Fuel Performance Comparison of Uranium Nitride and Uranium Carbide in VVER-1200 using OpenMC

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Supervisor: Dr. Majid Ali

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DEDICATION

To my parents, for their unending love and support.

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LIST OF SYMBOLS, ABBREVIATIONS AND ACRONYMS

PWR	Pressurized Water Reactor
VVER	Water-Water Energetic Reactor
ATF	Accident Tolerant Fuel
UN	Uranium Nitride
UC	Uranium Carbide
NPP	Nuclear Power Plant
LOCA	Loss of Coolant Accident
SBO	Station Black Out
HTGR	High-Temperature Gas-cooled Reactor
BDB	Beyond Design Basis
FCM	Fully Ceramic Microencapsulated
BOC	Beginning of Cycle
EOC	End of Cycle
MOC	Middle of Cycle
TRISO	Tri-Structural Isotropic
FA	Fuel Assembly
RCCA	Rod Cluster Control Assembly
RCP	Reactor Cooling Pump
BWR	Boiling Water Reactor
HWR	Heavy Water Reactor

ABSTRACT

Nuclear power is a reliable and large-scale source of GHG-free electricity. This study asses the viability of ATF fuel of uranium nitrate (UN) and uranium carbide (UC) as fuel for the VVER-1200 reactor. A comprehensive literature review has been conducted on the current state of global nuclear power and fuels. An in-depth overview of the VVER-1200 and Accident Tolerant fuels is presented and a review of the development of ATFs identified UN and UC as viable fuels for the VVER reactor. The study utilizes OpenMC to model the VVER-1200 core and compares the behaviour of ATF with conventional fuel. Key findings include comparable k-eff values implying similar neutronic behaviour. UO_2 and UC showed similar fission rates across the core while UN showed higher neutron flux and fission rate in the outer part of the core. The base Z44B2 showed increased flux and fission rate with UN as the fuel. ATF behaviour showed to be comparable to the UO_2 and thus is a potential alternative to conventional fuels. ATFs provide an additional level of safety because of higher melting points and higher thermal conductivity. This study can be further improved to investigate the depletion of ATFs so that the behaviours of the core over large periods of time, fission products and operator safety can be assessed. Base case k-eff value of 1.24795 are comparable to k-eff values generated by UN and UC.

Keywords: Nuclear Power, VVER, Uranium Nitride (UN), Uranium Carbide (UC), OpenMC, Pressurized Water Reactor (PWR), Accident Tolerant Fuels (ATF)

INTRODUCTION

1.1 Nuclear Power

Nuclear power is proven to be a reliable, cost effective and large-scale, source of GHG-free electricity. Nuclear power is a technology that uses the energy released by nuclear fission or fusion to generate electricity. It is one of the low carbon energy sources that can help mitigate the effects of climate change and enhance energy security. However, it also faces challenges such as safety, waste management, proliferation risks, and public acceptance.

One of the most widely used nuclear power technology is the pressurized water reactor (PWR), which accounts for about 65% of the operating nuclear power reactors worldwide. A PWR uses water as both coolant and moderator and operates at high pressure to prevent boiling. The water transfers heat from the reactor core to a steam generator, where steam is produced to drive a turbine and a generator. A PWR has several variants, such as the western PWR (WPWR), the Russian VVER, the Chinese CPR-1000, and the advanced PWR (APWR). These variants differ in their design features, such as fuel assemblies, control rods, steam generators, and safety systems.

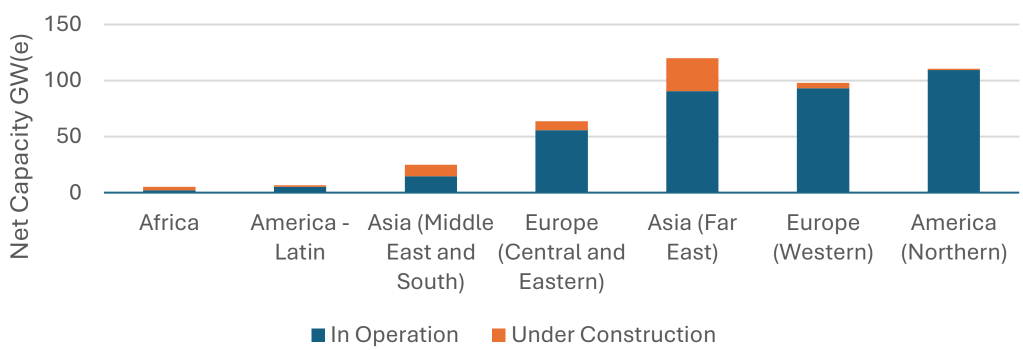

Figure 1.1: Regional distribution of nuclear power capacity [1]

By the end of 2019, there were 443 nuclear power reactors in operation around the world, with a combined capacity of 392.1 GW(e). During that year, 13 reactors were decommissioned, 6 were brought online, and 5 began construction. Asia was the main region for nuclear power development, both in the short and long term. It had 35 of the 54 reactors that were being built, and 61 of the 74 reactors that had started operating since 2005.

Power densities in light water reactors (LWR) can range between $50 - 70\ MW_{th}/m^3$ which is significantly greater than the average power density found in conventional power plant boilers burning fossil fuels [2]. Nuclear power plants (NPP) are increasing in competitiveness with fossil fuel power plants due to the increased service life, increased operability, implementation of load-follow conditions, and reduction in CAPEX & construction time.

The fuel for a light-water reactor is enriched uranium, which means it has a higher concentration of uranium-235, the fissile isotope of uranium. Uranium-235 can be split by neutrons and sustain a chain reaction. The fuel is formed into small ceramic pellets and arranged into long metal tubes called fuel rods. The fuel rods are grouped together into fuel assemblies, which are inserted into the reactor core.

The expected amount of uranium produced in the world in 2019 was about the same as in 2018, around 53 500 tonnes. Uranium exploration decreased considerably due to low prices, and new uranium projects were postponed. Many mines and processing plants that were operating before were put into a state of preservation and upkeep. The capacities for converting, enriching and making fuel from uranium were sufficient to satisfy the current and anticipated future needs.[1]

The high-power density that enables nuclear power to be economically viable also makes reactors susceptible to severe accidents. During a loss of coolant accident (LOCA), reactor fuel is subjected to an extremely high-temperature environment which leads to numerous unwanted behaviour including pellet-cladding interaction, cladding oxidation/hydriding, pellet dispersal and cladding embrittlement and fragmentation.[4] In light water reactors (LWR), a reactor scram greatly decreases power generation by suppressing the chain reaction, but a significant amount of heat is still generated through the decay of radioactive products present in the core. Power generation reduces to 7% immediately after the scram, 1% after four hours, and 0.2% after 10 days[4]. Power levels in LWRs are upwards of 3000 MWth, thus a reactor is producing a large amount of power, nearly 30 MW four hours after shutdown. Therefore, decay heat removal and tolerance to high temperatures are necessary to prevent core damage and degradation.

1.2 Reactor Technology

Nuclear fission is a process that generates heat and electricity by splitting atoms in nuclear reactors. There are different kinds of reactors that use different fuels, coolants, moderators, and designs. Some of the main reactor technologies are:

Light-water reactors (LWRs) are the most widely used reactors today. They use water for both cooling and moderating, and enriched uranium for fuel. There are two kinds of LWRs: pressurized water reactors (PWRs) and boiling water reactors (BWRs). PWRs have water under high pressure in the primary loop that carries heat to a secondary loop, where water turns into steam and spins a turbine. BWRs have water under low pressure in the primary loop that boils inside the reactor core and spins a turbine.

Heavy-water reactors (HWRs) are reactors that use heavy water for cooling and moderating, and natural or enriched uranium for fuel. The most common kind of HWRs is the CANDU reactor, which has horizontal pressure tubes with fuel bundles and heavy water. The heavy water in the primary loop carries heat to a secondary loop, where light water turns into steam and spins a turbine.

Gas-cooled reactors (GCRs) use CO_2 for cooling and graphite for moderating, and natural or enriched uranium for fuel. There are two kinds of GCRs: Magnox reactors and advanced gas-cooled reactors (AGRs). Magnox reactors have natural uranium metal fuel in magnesium alloy casing, and carbon dioxide for cooling. AGRs have enriched uranium oxide fuel in stainless steel casing, and carbon dioxide for cooling.

Liquid metal-cooled reactors (LMRs) use liquid metals for cooling, and do not need moderators because they use fast neutrons for fission. The most common kind of LMRs is the sodium-cooled fast reactor (SFR), which has liquid sodium for cooling and metal or oxide fuel. The sodium in the primary loop carries heat to a secondary loop, where another liquid metal or water turns into steam and spins a turbine. [1]

There are also other reactor technologies that are being developed or researched, such as small modular reactors (SMRs), high-temperature gas-cooled reactors (HTGRs), molten salt reactors (MSRs), supercritical water reactors (SCWRs), and fusion reactors. These technologies aim to improve the performance, safety, economics, and sustainability of nuclear power.

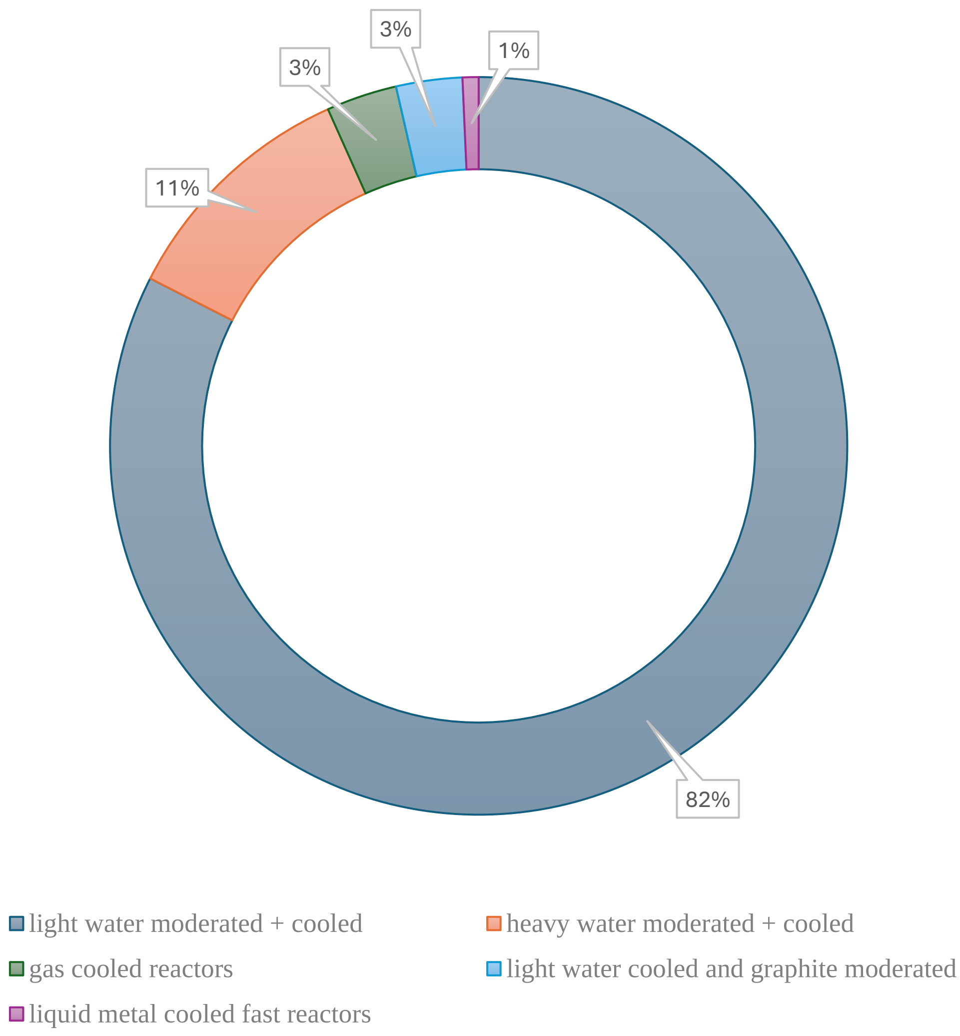

Figure 1.2: Global distribution of reactor types in operation (2019) [1]

1.3 Nuclear Fuels

Nuclear reactor fuels are substances that split atoms to produce heat and electricity in a nuclear reactor. There are different kinds of fuels that have different characteristics, such as their ingredients, form, size, and enrichment level. Some of the main factors that influence the selection and performance of nuclear reactor fuels are discussed.

Fuel cycle is the steps of fuel production, use, and disposal. Different fuels have different fuel cycles, depending on the kind of reactor, the availability of resources, the economics, and the environmental impacts. Fuels can be reused or reprocessed to get more energy or reduce waste, while others are stored away as spent fuel.

The amount of energy obtained from a unit mass of fuel is called burnup. Higher burnup means more effective use of fuel and less waste production, but also more difficulties in terms of fuel quality, safety, and handling. The burnup of a fuel depends on the kind of reactor, the power level, the operating time, and the fuel design.

Cladding covers and protects the fuel from the coolant and the environment. The cladding must resist high temperatures, pressures, irradiation, corrosion, and mechanical stresses. The cladding affects the heat transfer, neutronic properties, and chemical compatibility of the fuel.

The moderator's function is to reduce the energy level of the neutrons produced by fission, making them more likely to cause more fissions. The moderator can be part of the fuel or separate from it. The moderator affects the reactivity, efficiency, and safety of the reactor.[5]

Uranium oxide is the most popular kind of fuel for light water reactors (LWRs), which are the most common reactors today. Uranium oxide is a ceramic material that has a high melting point, a high density, and a good thermal stability. It is enriched to raise the concentration of uranium-235, the fissile isotope of uranium. Uranium oxide is shaped into small pellets and placed into long metal tubes called fuel rods. The fuel rods are grouped into fuel assemblies, which are put into the reactor core. Mixed oxide (MOX) is a fuel that has a mixture of uranium oxide and plutonium oxide. Plutonium is a product of uranium fission that can also be used as a fissile material. MOX can be used to reuse plutonium from spent fuel or weapons-grade material, or to raise the burnup of uranium fuel. MOX is also shaped into pellets and rods like uranium oxide, but it has different neutronic and thermal properties. MOX is mainly used in some LWRs and fast reactors. [6]

Metal fuels have metallic alloys of uranium or plutonium with other elements such as zirconium or molybdenum. Metal fuels have a high thermal conductivity, a high fissile density, and a good compatibility with liquid metal coolants. Metal fuels are usually used in fast reactors or research reactors, where they can achieve high burnup and breeding ratios. Metal fuels are shaped into cylindrical pins or plates that are clad with stainless steel or other metals.

Carbide fuel has compounds of uranium or plutonium with carbon. Carbide fuels have a high melting point, a high density, and a good resistance to irradiation damage. Carbide fuels are suitable for high temperature gas-cooled reactors (HTGRs) or fast reactors, where they can offer high performance and safety margins. Carbide fuels are shaped into spherical particles or cylindrical pellets that are clad with silicon carbide or other materials.[5]

1.4 Reactor Simulator

OpenMC is used as the computational code used for the neutronic calculation. OpenMC is a Monte Carlo neutron and photon transportation code developed by the open-source community. It is primarily function is in reactor physics research methods and can perform calculations such as fixed source, K values, and subcritical multiplication. OpenMC can compute continuous energy and multigroup transportation. It uses a native HDF5 format for particle interaction data that is generated from ACE files produced by NJOY. OpenMC can analyse and tally a wide range of physical quantities, making it suitable for depletion calculations, multigroup cross-section generation, Multiphysics coupling, and visualization of geometry and tally results. [7]

1.5 Problem Statement

Nuclear power has proven to be a reliable source of GHG free energy. As the contribution of nuclear power increases in the global energy mix, the need for safe reactors and reactor fuels is increasing. Accident tolerant fuels provide an extra layer of safety due to their thermal and neutronic properties. This paper explores multiple accident tolerant fuels, and a simulation is conducted to assess the viability of UN and UC as a fuel replacement for the VVER. The fuels are measured against conventional UO_2 fuel by modelling the reactor using the OpenMC neutron and photon transport code.

1.6 Summary

This section introduces nuclear power and its prevalence in the global energy mix. The distribution of various types of reactors is discussed and fuels that are commonly used in the industry are described. The section also describes OpenMC as a neutron simulator and its application to assessing various fuels. Finally, the problem statement is presented that this paper looks to explore

LITERATURE REVIEW

2.1 The VVER-1200 Reactor

The VVER is a pressurized light-water reactor with horizontal steam generators and hexagonal fuel assemblies. The VVER has a high level of inherent safety and a total of 49 power plants are under operation with approximately 1400 reactor-years of total operating time. The first VVER reactor was commissioned at NV NPP in 1964 and the VVER design has gone through improvements in safety, power operation characteristics, and economic efficiency. The VVER-1200 is a generation 3+ reactor designed and developed in Russia by OKB Gidropress. It is an evolution of the VVER-1000 reactor, with increased power output, improved safety features, and enhanced operational performance. The VVER-1200 has four primary coolant loops, each with a horizontal steam generator and a reactor coolant pump. The reactor core consists of 163 fuel assemblies, each with 312 fuel rods. The fuel is enriched uranium dioxide with an average enrichment of 4.95%. The reactor has 121 control rods for reactivity control and shutdown The VVER-1200 has greater thermal efficiency and is designed to operate at higher temperatures and pressure than previous VVER models, which allows it to generate more electricity from the same amount of fuel. This increased efficiency also results in lower fuel costs and reduced environmental impact. The VVER-1200 has several advanced safety features. These include an active and passive cooling system, which can rapidly cool the reactor in the event of an accident, and a containment building that is designed to withstand extreme external forces, such as earthquakes or airplane crashes. The VVER-1200 reactor is engineered to endure extreme events, including a complete power outage, a significant coolant leakage, or a core meltdown. A double-layered containment structure, featuring a steel liner encased in a concrete shell, safeguards the reactor. The reactor vessel itself resides within a protective shell capable of withstanding extreme temperatures and pressures. Additionally, a core catcher device is incorporated into the reactor core to trap and cool molten corium in the event of a meltdown. The VVER-1200 reactor is among the most sophisticated pressurized water reactor (PWR) designs. It is endorsed by the European Utility Requirements (EUR) and adheres to the safety standards set by the International Atomic Energy Agency (IAEA). [8]

The VVER-1200 reactor has passive safety systems that function autonomously, without the need for external power and human involvement. The Passive Heat Removal System (PHRS) effectively dissipates residual heat from the reactor core into the atmosphere through heat exchangers and air-cooling towers. The Passive Core Flooding System (PCFS) deals with a loss-of-coolant accident (LOCA), this system automatically injects borated water into the reactor core to maintain cooling. In addition, the Passive Containment Cooling System (PCCS) actively reduces the pressure and temperature within the containment building by spraying water onto the inner surface. The Hydrogen Recombiner System (HRS prevents the buildup of hazardous hydrogen gas within the containment by employing catalytic oxidation.[9]

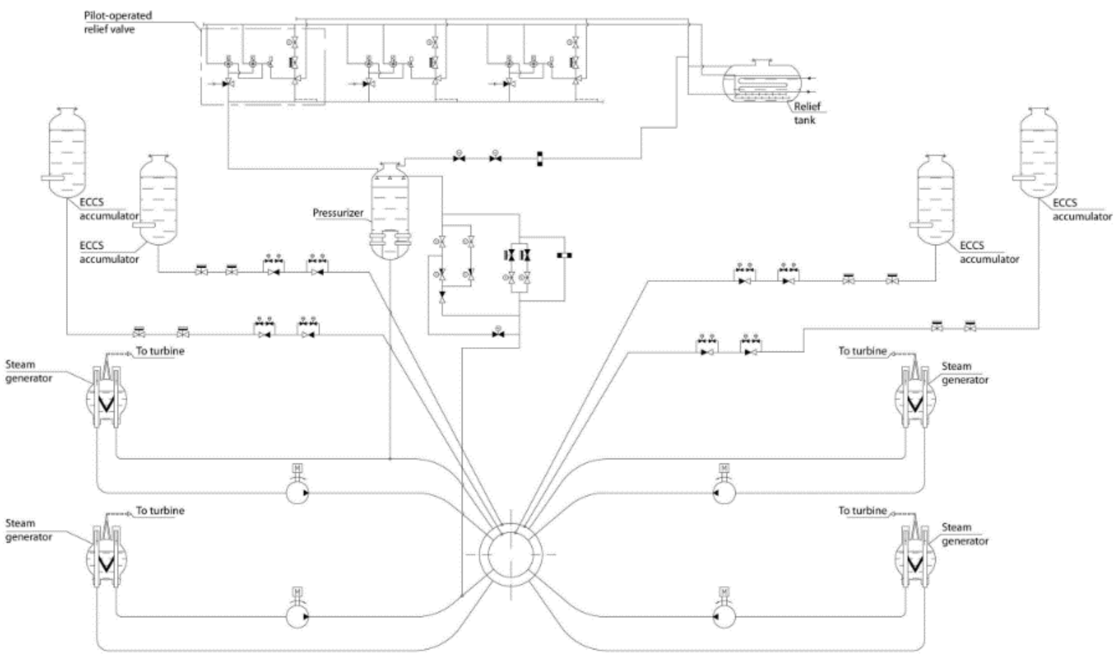

Figure 2.1: Schematic flow diagram of the primary circuit [9]

In terms of construction, the VVER-1200 is designed to be modular and easy to assemble. This reduces construction time and costs and makes it easier to transport and install the reactor components.[9] The VVER-1200 is currently in operation or under construction in several countries, including Russia, Belarus, Turkey, and Bangladesh. In Russia, the VVER-1200 is being used in the NoVo Voronezh II and Leningrad II nuclear power plants, and more reactors are planned for construction in the coming years. The total number of VVER-1200 reactors globally is 26, of which 3 are in operation, 9 are under construction, and 14 are planned. [10]

2.2 Accident Tolerant Fuel

Conventional UO_2 fuel shows weak resistance to a high-temperature environment. This leads to severe damage to the fuel, evidenced during the station blackout (SBO) at the Fukushima Daiichi nuclear power plant (NPP)[11]. The accident at Fukushima accelerated R&D of accident-tolerant fuels (ATF). The ATF program's primary motivation is to improve fuel safety and reliability of LWRs, and high-temperature gas-cooled reactors (HTGR) during beyond-design basis (BDB) accidents. Research is being conducted to develop innovative fuel compounds with enhanced thermophysical properties, lower operating temperatures, reduced hydrogen generation rates, enhanced retention of fission products, and increased capability to resist damage and degradation during a severe accident. [3] ATF can be classified into two categories: near-term and long-term. Near-term ATFs are based on modifications of the existing uranium dioxide (UO_2) fuel and zirconium alloy cladding while long term ATFs are based on new fuel and cladding materials. [6]

Advanced ceramic fuels have the advantage of having high heat conductivities and melting points. Uranium nitride (UN) and uranium carbide (UC) have better thermal conductivity and higher melting points than uranium dioxide [12]. UN is most used in NASA reactor designs NASA and interest in UC has been revived to be utilized in Fully Ceramic Microencapsulated (FCM) fuels such as TRISO particles. Yahya et al. demonstrated the viability of UN for the SMART reactor and Chaudri et al. proposed a fuel pellet design composed of UN and UC for the Super Critical Water Reactor (SCWR) [12][13].

Table 2.1: Thermal conductivity vs Temperature [13]

Property	UO_2	UN	UC
Density (kg/m^3)	10,600	14,000	13,000
Melting Temperature (°C)	2850	2850	2350
Thermal Conductivity (W/mK)	8.67	13.0	25.3

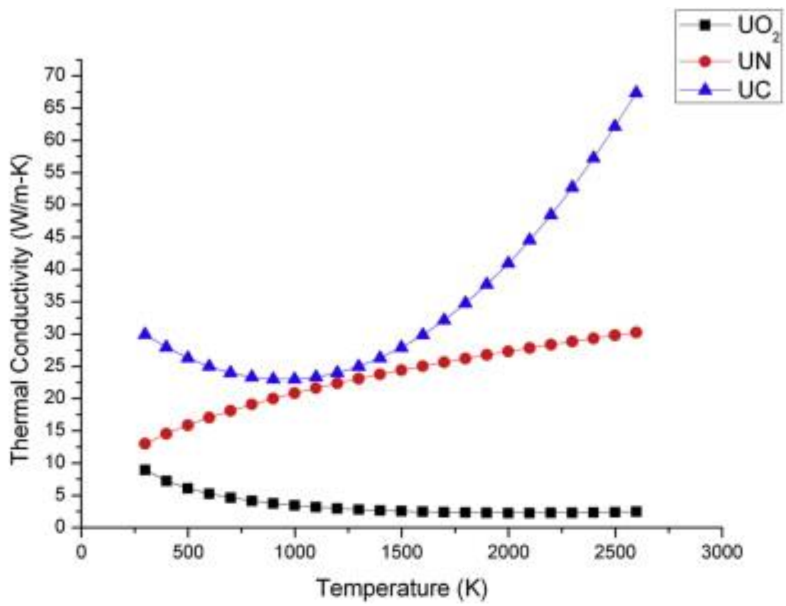

Figure 2.2 Thermal conductivity for UO_2, UN, and UC [13]

UN (Uranium Nitride) and UC (Uranium Carbide) are advanced nuclear fuel options that have shown promise in improving the safety and efficiency of nuclear reactors. Both UN and UC have higher thermal conductivity, higher melting points, and higher fuel densities compared to traditional UO_2 (Uranium Dioxide), making them more resistant to thermal stress and better suited for higher-temperature reactor designs. UN and UC also have a higher resistance to corrosion and irradiation damage, reducing the risk of fuel failure and nuclear accidents. [14] Studies have shown that UN and UC have excellent irradiation resistance and maintain their structural integrity even under extreme conditions.

Table 2.2: Properties of UO2, UN, and UC. [15][16]

Parameter	**UO_2**	**UN**	**UC**
Theoretical density (g/m^3)	10.96	14.32	10.5
Uranium density (g-U/cm3)	9.6	13.5	12.7
Specific heat capacity (J/kg K)	270	205	240
Melting point (C)	2800	2847	2525
Thermal conductivity (W/m K)	7.9 (200 C) / 3.35 (1000 C)	4 (200 C) / 20 (1000 C)	20.4 (570 C)
Thermal expansion - Linear (10^{-6} K^{-1})	10.1	9.4	10.9
Swelling rate (compared to UO_2)	1	0.8	
Release of fission gas	1	0.45	

2.3 Simulation technique

Neutron behaviour in a nuclear reactor can be modelled and analysed by using Monte Carlo simulations. This method is based on probability and tracks each neutron's movement and interactions in the reactor core. It considers different processes that affect neutrons, such as scattering, absorption, and fission. The method creates many random neutron histories and uses statistics to analyze the data. It can be used to study reactor parameters such as neutron flux, power distribution, criticality, and reactivity coefficients. The Monte Carlo method has many benefits for reactor simulations. It can model complex shapes and materials such as different fuel assemblies and control rod arrangements. Many types of neutron interactions, such as elastic and inelastic scattering, neutron capture, fission, and delayed neutron emission can be simulated accurately. In addition, can simulate different kinds of reactors, such as pressurized water reactors (PWRs), boiling water reactors (BWRs), and research reactors while measuring how uncertainties in input parameters affect reactor performance. However, the Monte Carlo method also has some drawbacks including high computational demand and statistical uncertainty. OpenMC is Monte Carlo simulations and utilizes python coding to generate and simulate an environment. In the current model the VVER-1200 reactor is designed and UO_2 is placed in the conventional loading pattern shown in table 3. The fuel is then replaced with UN and UC in the same loading pattern and enrichment levels to compare the behaviour and performance of ATF fuels in the VVER-1200 reactor.

2.4 Research Gap

Advanced Technology Fuels (ATF) are still undergoing development and rigorous testing by vendors and research organizations. Before ATF can be widely implemented in commercial reactors, several challenges need to be addressed. ATF must meet stringent safety and performance criteria established by regulatory authorities. Existing regulations are based on traditional UO_2/Zr fuel technology and may not be directly applicable or adequate for ATF. New or revised licensing and regulatory framework is essential for evaluating and approving ATF. In addition, ATF must undergo experimental and computational studies to demonstrate their safety and performance under both normal and accident conditions. Current fuel qualification and validation methods may not be entirely suitable or sufficient for ATF. Hence, new or improved fuel qualification and validation methods are required to verify and validate ATF. ATF may also necessitate new fuel fabrication and handling processes. Existing fuel fabrication and handling facilities may not be compatible or capable of handling ATF.

METHODOLOGY

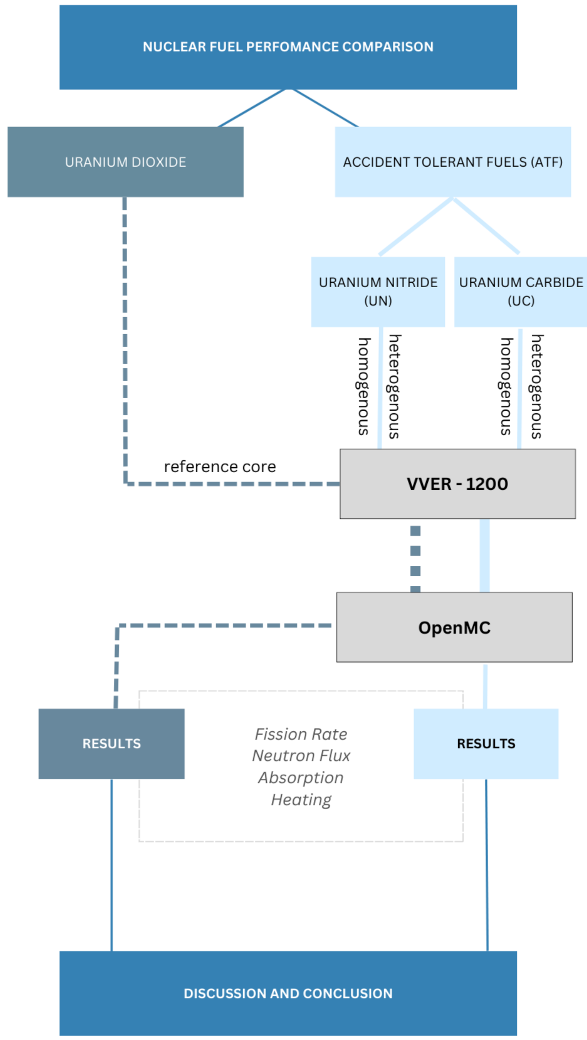

Figure 3.1: Methodology workflow

The objective of the simulation is to ascertain the viability of UN and UC as fuel for the VVER-1200 reactor. OpenMC is used to model the VVER core with a typical core configuration described in Table 3.2. UN and UC are replaced as fuel materials in homogeneous configurations. Comparison is made for the fission rate, neutron flux, absorption and heating against the behaviour of UO_2 in the reactor.

3.1 VVER-1200 Description

The Russian abbreviation VVER stands for 'water-water energetic reactor,' meaning light water is used for the coolant and moderator. The VVER-1200 is the successor to the VVER-1000 and has a similar design and core configuration. The VVER-1200 consists of four horizontal steam generators and reactor cooling pumps (RCP) and a single pressuriser kept at 16.2 MPa to prevent boiling within the core. The reactor is a vertical pressure vessel that houses the core, control rods, instrumentation sensors, core baffle, core barrel, and protective tube unit. The reactor is fixed in a concrete cavity with biological & thermal shielding, and cooling mechanism. The reactor fastening inside the concrete cavity prevents displacement from seismic impacts and pipeline breaks. The primary features of the VVER-1200 are given in Table 3.1.

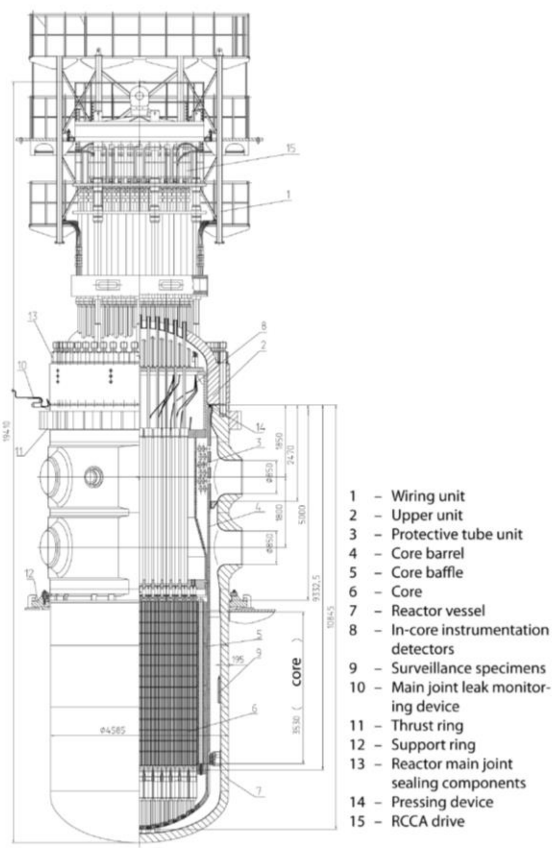

Figure 3.2: VVER-1200 Reactor Diagram [9]

Table 3.1: Primary features of VVER-1200 [9]

Parameter	
Reactor Type	Pressurized Light Water Reactor
Plant full thermal power	3200 MWth
Electric power gross	1170 MWe
Electric power net	1082 MWe
Power plant efficiency	33.9%
Plant design life	60 years
Power plant availability target	>90%
Number of FA	163
Rod cluster control assemblies (RCCA)	121
Primary pressure	16.2 MPa
Nominal steam generator pressure	6.9 MPs
Coolant	Light Water
Inlet coolant temperature	298.2 C
Outlet coolant temperature	329.5 C

Coolant volumetric flow rate	86000 m^3/hr
Coolant mass flow rate	23888 Kg/s
Core equivalent diameter	3.16 m
Core active length	3.75 m
Core power density	108.5 MW/m^3
Average linear heart rate	16.78 KW/m
Length of fuel cycle	12 months
Assembly pitch	23.51 cm
Rod pitch	1.275 cm
Control rod absorber material	B_4C + $Dy_2O_3TiO_2$
Fuel material	UO_2 and UO_2 + Gd_2O_3
Cladding material	Alloy E-110
Reactor coolant pumps	4
Soluble neutron absorber	H_3BO_3
Burnup of fuel	60 MWd/Kg
Neutron spectrum	Thermal Neutrons

3.2 Reactor Core Description

The VVER-1200 has 163 fuel assemblies (FA) arranged in an 8-ring hexagonal array. Each assembly is a hexagonal bundle of 331 rods out of which 312 are fuel rods and 19 are guide channels.

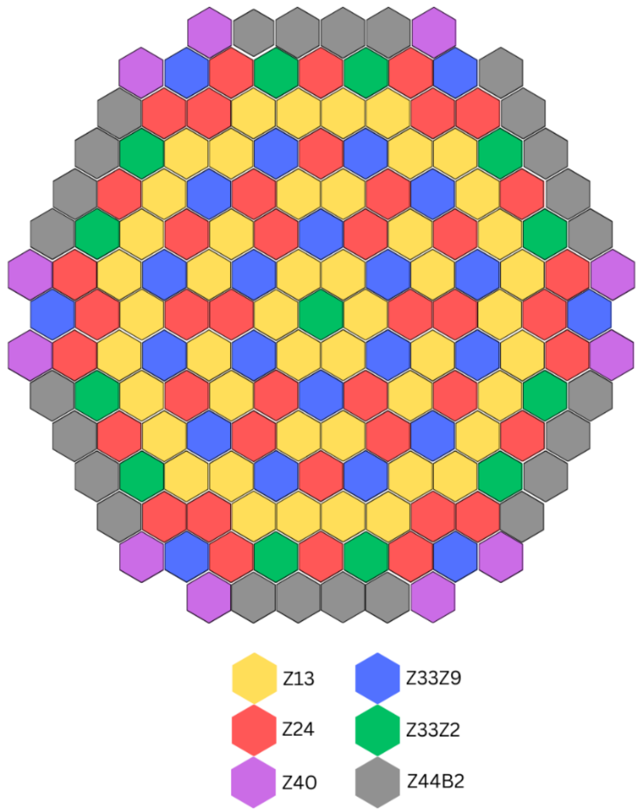

Figure 3.3: VVER-1200 reference core

The fuel assemblies are 4570 mm high, while the core height during a hot state is 3750 mm. The cladding is a zirconium alloy tube with sintered UO_2 pellets, and 121 Rod Cluster Control Assemblies (RCCA) are placed inside the core [9]. The RCCAs provide quick chain reaction suppression. aid in maintaining or transitioning power to a desired level, axial power levelling, and xenon suppression. There are six types of fuel assemblies with varying enrichment and weight percentage of the burnable absorber Gd_2O_3. Assemblies Z13, Z24, and Z40 consist of 312 fuel pins with 1.3%, 2.4%, and 40% enrichment, respectively. Z33Z9 has 9 pins with a mixture of burnable absorber Gd203. Fuel

Assemblies Z44B2 and Z33Z2 have 12 fuel pins with a mixture of the burnable absorber. The effective time of FA between refuelling for a 12-month fuel cycle is 8400 effective hours. The average burnup of fuel is up to 60 MWd/kg and 42 fresh FAs are placed into the core for a regular fuel cycle. A description of each assembly is summarized in Table 3.2.

Table 3.2: VVER 1200 fuel assembly configuration [8]

Fuel Assembly	Fuel Assembly Type	No of FAs in core	No of UO_2 pins / Ave enrichment (%)	No of Gd Pins /UO_2 enrichment%	Gd_20_3 concentration (%)
Z13	A	48	312/1.3	-	-
Z24	A	42	312/2.4	-	-
Z40	A	12	312/4.0	-	-
Z33Z9	C	24	303/3.3	9/2.4	8
Z44B2	B	24	300/4.4	12/3.6	5
Z33Z2	B	13	300/3.3	12/2.4	8

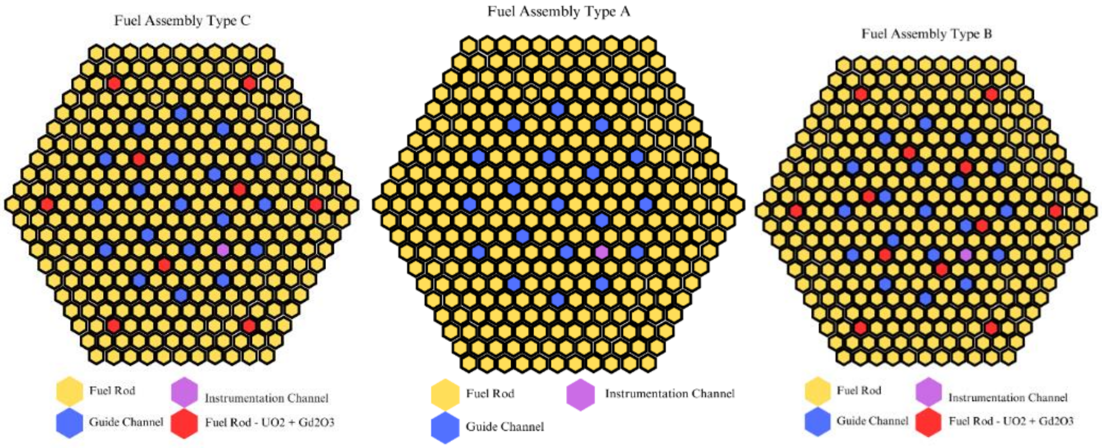

Figure 3.4: VVER Fuel assembly configurations

3.3 OpenMC Code

OpenMC is a neutron and photon transport simulation code that uses the python coding language. To operate, OpenMC requires four files in XML format. The materials.xml contains information on the elements, isotopes, and mixtures to simulate. Geometry.xml describes the spatial location of the materials defined earlier. Planes and prism are used to construct the required geometry and then divided into cells and universes for computation. Settings.xml list the location and number of neutrons to be simulated. Tallies defines the parameter to be studied by applying various filters for computation.

3.3.1 Materials

To define materials, the elements isotope and density must be defined. In addition, mixtures can be made by defining the elements and ratio of the simulated molecule. A sample code to add a material called au13, a UO_2 molecule with 2.3% enrichment can be seen below:

au13=openmc.Material(name='au13')

au13.add_element('U', 1.0, enrichment=1.3)

au13.add_element('O', 2.0)

au13.set_density('g/cc', 10.4)

The table below describes the materials needed to simulate a VVER-1200 core:

Table 3.3: List of VVER-1200 core materials

Material	Description
Au13	Uranium dioxide fuel with 1.3% enrichment
Au24	Uranium dioxide fuel with 2.4% enrichment
Au33	Uranium dioxide fuel with 3.3% enrichment
Au36	Uranium dioxide fuel with 3.6% enrichment
Au40	Uranium dioxide fuel with 4.0% enrichment
Au44	Uranium dioxide fuel with 4.4% enrichment
Gd2O3	Burnable absorber
water	Moderator H_2O
zirconium	Cladding material
niobium	Cladding material
helium	Gas gap
Reflector material	Neutron reflector
Alloy	Zirconium and niobium mixture

Fuel mix 1 Uranium dioxide and burnable absorber mixture (8%)

Fuel mix 2 Uranium dioxide and burnable absorber mixture (5%)

3.3.2 Geometry

After defining materials, the core geometry of the VVER reactor. The geometry of the Pin, fuel assembly and core lattice are defined by generating surfaces and assigning regions bound by surfaces. The materials then can be placed in a volume defined by the regions. Multiple regions can then be placed in a lattice to hexagonal lattice. An example of the geometry of a fuel rod is shown below.

```
fuel_or2 = openmc.ZCylinder(surface_id=510, r=0.38)

clad_ir2 = openmc.ZCylinder(surface_id=511, r=0.3865)

clad_or2 = openmc.ZCylinder(surface_id=512, r=0.455)

fuel_region2 = -fuel_or2 & -assembly_z1 & +assembly_z0

gap_region2  = +fuel_or2 & -clad_ir2 & -assembly_z1 & +assembly_z0

clad_region2 = +clad_ir2 & -clad_or2 & -assembly_z1 & +assembly_z0

moderator_region2 = +clad_or2 & -assembly_z1 & +assembly_z0

fuel_cell2  = openmc.Cell(cell_id=1520, fill=au13,   region=fuel_region2)

gap_cell2   = openmc.Cell(cell_id=1521, fill=helium, region=gap_region2)

clad_cell2  = openmc.Cell(cell_id=1522, fill=alloy,  region=clad_region2)

water_cell2 = openmc.Cell(cell_id=1523, fill=water,  region=moderator_region2)

au13_u = openmc.Universe(cells=[fuel_cell2, gap_cell2, clad_cell2, water_cell2])
```

The values of the fuel rod, fuel pitch, lattice pitch and core diameters are mentioned in Table 3.1.

3.3.3 Tallies

The tallies section requires coding of a mesh to define points to take various measurements. The measured value is known as the score. In this study the following scores are simulated for the VVER-1200 reactor.

Table 3.4: Scores and tallies generated by OpenMC

Score	Description
Fission	Fissions per unit volume per unit time
Neutron flux	Neutrons passing through a unit area per unit time
Absorption	Absorption per unit volume per unit time
Heating	Energy deposited per unit volume per unit time

3.3.4 Settings

The settings section defines the number of batches to compute in the Monte Carlo Simulation, the bounding area of the simulated neutrons and the neutron density in the core. The settings code can be seen below:

```
settings_file.batches = batches

settings_file.inactive = inactive

settings_file.particles = particles

bounds = [-187.5, -187.5, -108.3, 187.5, 187, 91.7]

uniform_dist = openmc.stats.Box(bounds[:3], bounds[3:], only_fissionable=True)

settings_file.source = openmc.source.Source(space=uniform_dist)
```

3.3.5 Geometry Visualization

OpenMC used the Python API to generate 2-D slice plots of the geometry. However, for 3D visualization, OpenMC can generate voxel plots. Voxel plot data is written to an HDF5 file that can subsequently be converted to a standard mesh format (VTK). VTK files then can be opened via ParaView. Figure 3.5 shows a 3-D voxel plot of the VVER geometry generated by ParaView.

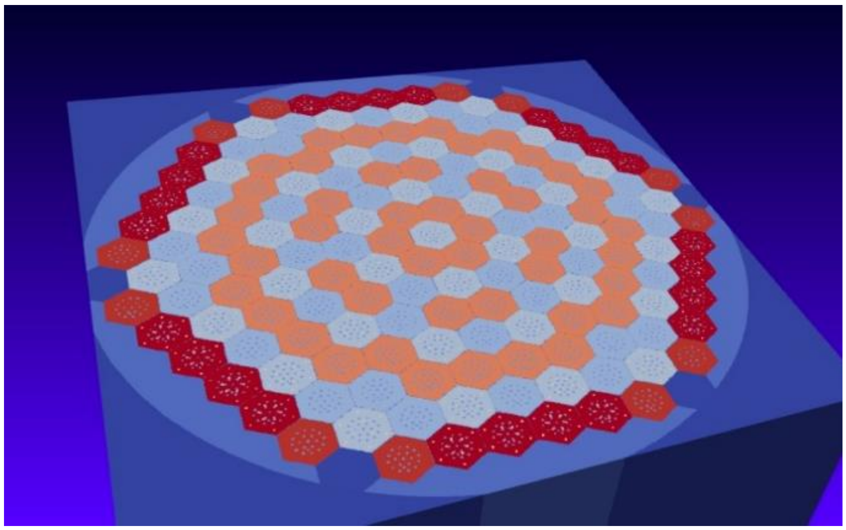

Figure 3.5: 3-D visualization of the VVER reactor generated by ParaView

3.4 Summary

This section sets out the methodology used in the simulation. The first section describes in detail the configuration of the VVER-1200 reactor and its operating parameters. The VVER-12200 core is looked in further detail to identify the fuels materials, core geometry and distribution. The section describes in detail the python code used including materials, geometry, tallies and settings.

RESULTS AND DISCUSSION

OpenMC generates tally data in an HDF5 and text file. The HDF5 can then be converted to a VTK to be visualized with ParaView. To create a baseline, OpenMC is run with the conventional loading of the VVER-1200. Data for fission, flux, absorption, and heating is generated by applying a mesh bounding the core geometry. The mesh bounding is visualized in Figure 4.1.

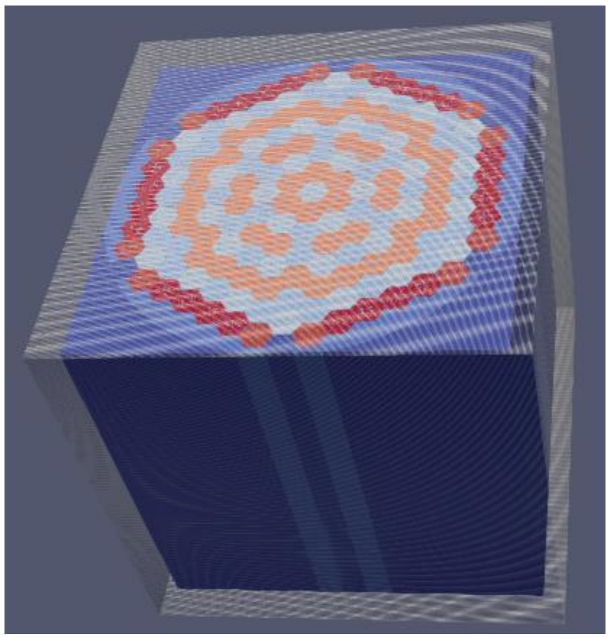

Figure 4.1: VVER-1200 geometry with Mesh Bounding

4.1 K-Effective

K-effective (k-eff) is a fundamental parameter that characterizes the neutron multiplication in a nuclear reactor. It is calculated by dividing the number of neutrons produced in one generation to the number of neutrons lost in the same generation due to absorption or leakage. The value of k-eff describes whether a reactor is critical subcritical (k-eff < 1), (k-eff = 1), or supercritical (k-eff > 1).

The k-eff value is crucial for assessing the stability and safety of a nuclear reactor. A subcritical reactor will eventually shut down, while a supercritical reactor may lead to an uncontrollable chain reaction, potentially resulting in a nuclear meltdown. Therefore, accurately determining the k-eff is vital for reactor design, operation, and safety analysis. OpenMC calculates K-eff via collision, track-length, and absorption to provide a combined value. K-eff is calculated for the base case (UO_2) and case 1 (UN) and case 2 (UC) and is shown in Table 4.1.

Table 4.1: Comparison of k-eff.

Reactor Configuration	k-eff (Collision)	k-eff (Track-Length)	k-eff (Absorption)	Combined k-eff
Base Case (UO_2)	1.24798 +/- 0.00012	1.24791 +/- 0.00014	1.24792 +/- 0.0010	1.24795
Case 1 (UN)	1.13788 +/- 0.00035	1.13791 +/- 0.00037	1.13799 +/- 0.00036	1.13791
Case 2 (UC)	1.25316 +/- 0.00013	1.25311 +/- 0.00015	1.25301 +/- 0.00011	1.25305

4.2 Fission Rate

UO_2 serves as a baseline to compare the simulation results with ATF fuels. OpenMC can score fission rate, neutron flux, absorption, and heating. The results are visualized through surface heat maps generated by ParaView. OpenMC measures fission rates in units of fissions per unit volume per unit time. The typical unit used is fissions/cm^3/s (or fissions per cubic centimetre per second). This quantity represents the number of fission events occurring within a given volume per unit time.

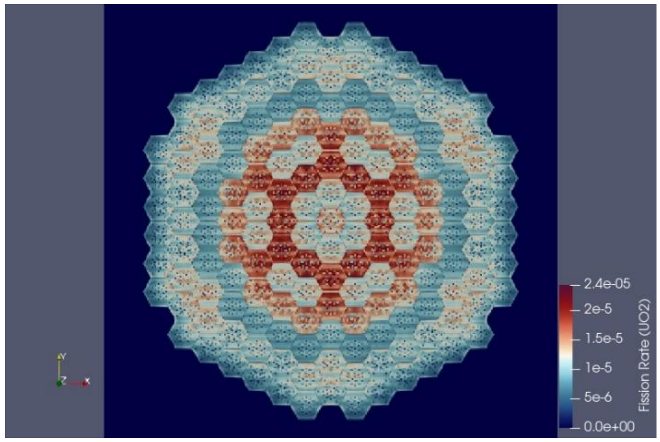

Figure 4.2: Fission rate UO_2

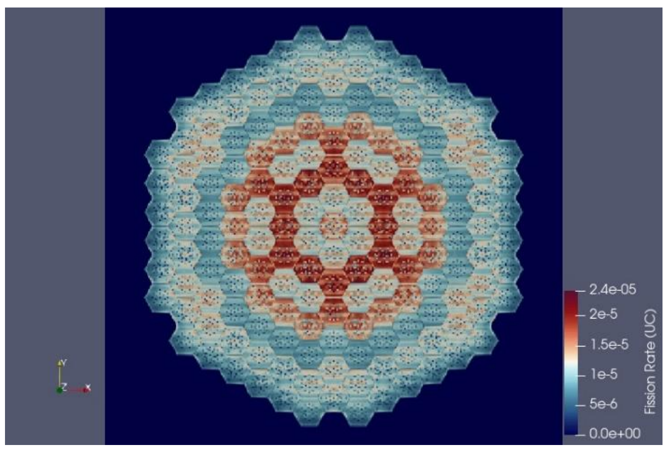

Figure 4.3: Fission rate UC

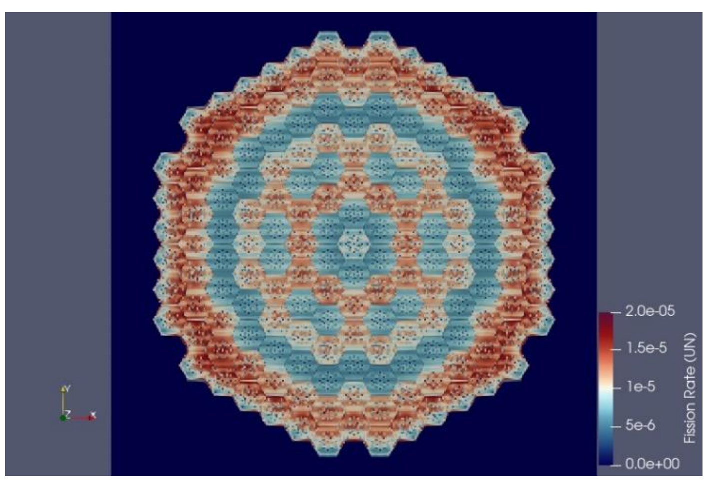

Figure 4.4: Fission rate UN

Figure 4.2 shows a heat map of fission seen in the VVER-1200 with conventional UO_2 loading. The maximum fission occurs close to the centre of the core. The maximum fission rate of 2.4 x 10^{-5} is observed in the 3rd ring of the core which consists of assemblies Z24 and Z33Z9. Figure 4.3 shows the fission rate heat map for UC which shows a very similar distribution and behaviour as $U0_2$. However, the fission distribution is considerably different when UO_2 is replaced with UN. As seen in figure 4.4, there are more areas with higher fission rate values but with a marginally smaller value of 2.5 x 10^{-5}. There is still significant fission in assemblies Z24 and Z33Z9, but maximum fission is now occurring in the outer part of the core in assemblies Z40 and Z44B2. This can be attributed to the higher enrichment present in the assemblies.

4.3 Neutron Flux

The neutron flux is defined as the number of neutrons passing through a unit area per unit time. OpenMC measures neutron flux in units of neutrons per square centimetre per second (neutrons/cm²/s). This quantity describes the density of neutrons in a particular region and is an important parameter in nuclear engineering calculations.

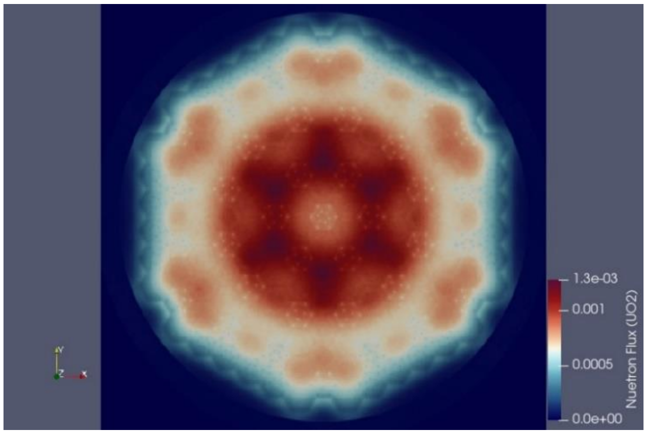

Figure 4.5: Neutron flux UO_2

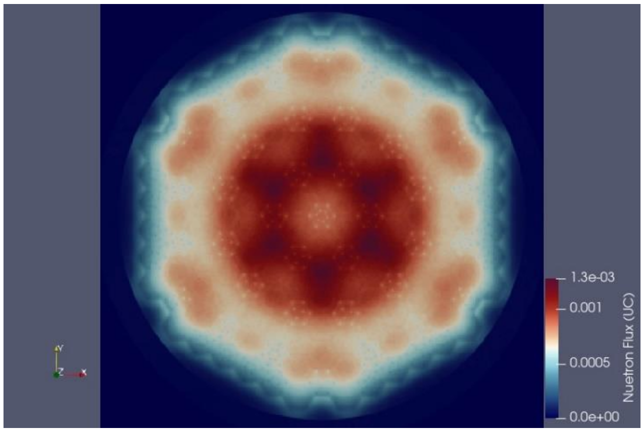

Figure 4.6: Neutron flux UC

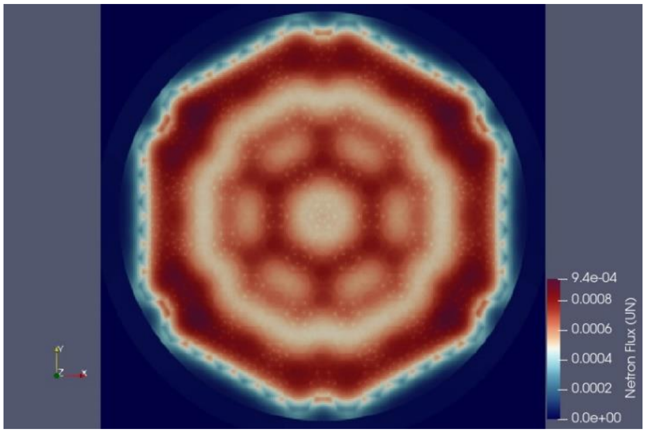

Figure 4.7: Neutron flux UN

The neutron flux created by conventional UO_2 loading is shown in figure 4.5. A clear correlation of flux and fission can be seen as fission events are the primary contributor to the neutron flux in any given space. In this case the Z24 assemble has the largest flux at 1.3×10^{-3} neutrons/cm²/s. Similarly due to the increased fission in case 2 (UN) a larger flux can be seen. Along with Z24, assemblies Z40 and Z44B2 contribute more to generate the higher flux. The peak flux measured in this case is 9.4×10^{-4} located on the outer ring of the core. Case 3 (UC) neutron flux is similar to the base case (UO_2) fission results.

4.4 Absorption

Absorption rates are measured in units of absorption per unit volume per unit time. The typical unit used is absorptions/cm³/s. This quantity represents the number of neutrons being absorbed within a given volume per unit time.

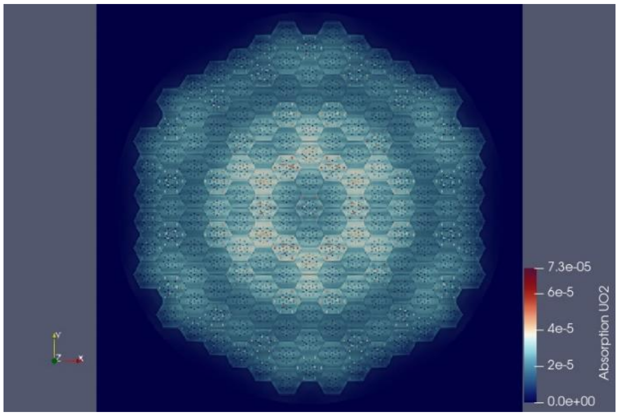

Figure 4.8: Absorption UO_2

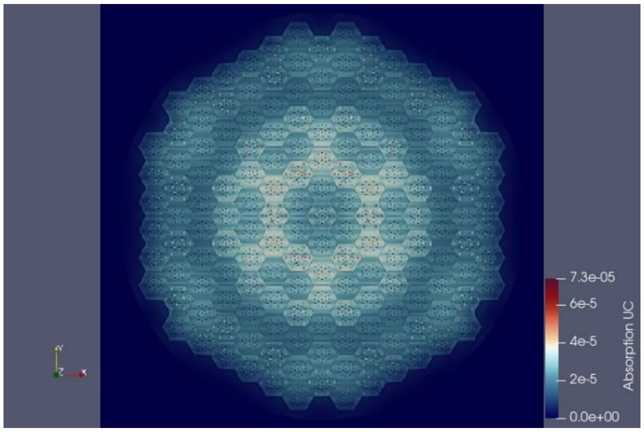

Figure 4.9: Absorption UC

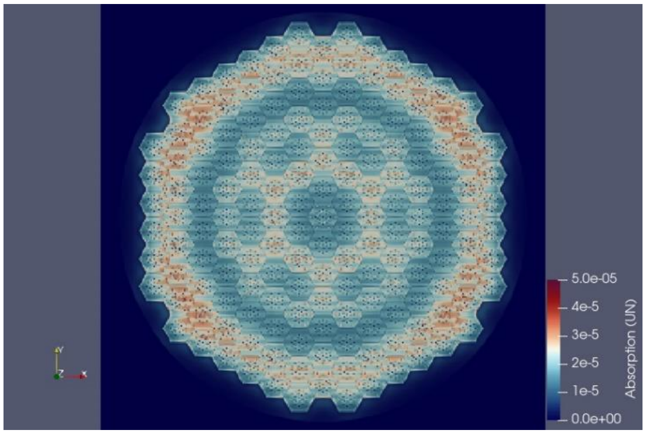

Figure 4.10: Absorption UN

Figure 4.8 shows the absorption map generated by UO_2 with a maximum value of 7.3 x 10^{-5}. Absorption contributed negatively to the k-eff of the reactor system. Figure 4.10 shows increase absorption in the outer ring however with a lower value of 5 x 10^{-5}. As in the previous cases, UC shows a similar absorption pattern as UO_2.

4.5 Heating

OpenMC measures heating rates in units of energy deposited per unit volume per unit time. The typical unit used is watts per cubic centimetre (W/cm^3) or joules per second per cubic centimetre ($J/s/cm^3$). This quantity represents the amount of energy being deposited within a given volume per unit time, which contributes to the overall heating of the material.

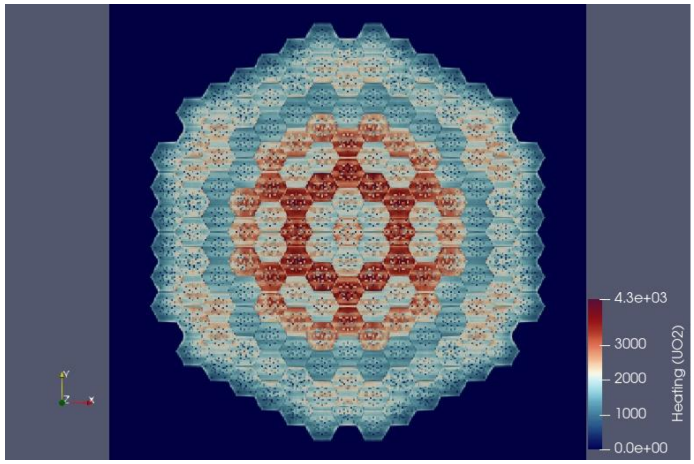

Figure 4.11: Heating UO_2

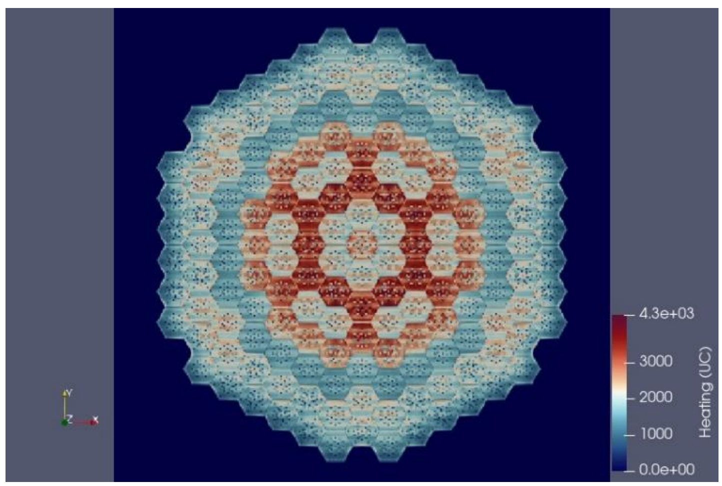

Figure 4.12: Heating UC

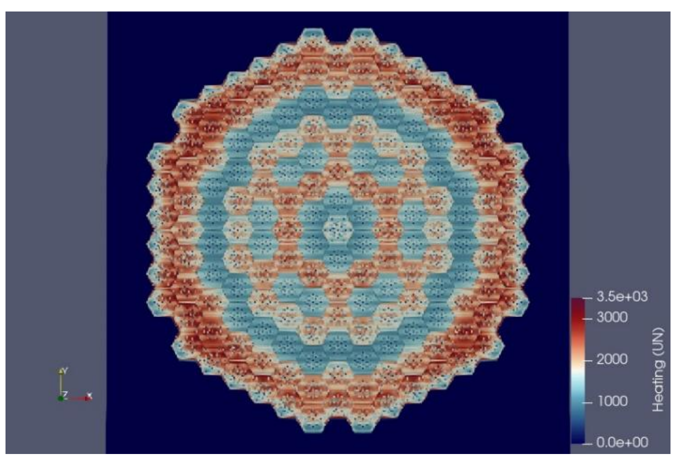

Figure 4.13: Heating UN

Heating is directly proportional to the amount of fission. In all cases the heating map matches very closely to the fission maps. In the base case heating is concentrated in the middle of the core with a maximum value of 4.3 x 10^3. Figure 4.13 shows the heat map generated by case 2 (UN). Although more areas show high heating, the maximum value is slightly lower at 3.5 x 10^3. Case 3 (UC) shows a similar heating pattern to the base case of UO_2.

4.6 Summary

The section shows the results of the OpenMC Monte Carlo simulation. ParaView is used to visualize the output. The output of the base case of UO_2 for fission, neutron flux, absorption and heating are generated. Then UC and UN are replaced in the core with the same enrichment levels. The images generated are then compared to see the viability of UN and UC as an ATF for VVER-1200.

CONCLUSION

The study showed the viability of ATF fuel UN and UC for the current generation VVER-1200 reactor. ATF will allow the VVER to be operated with an additional layer of safety. When compared to UO_2, UC provides high thermal conductivity at high temperatures as shown in figure 2.2. The VVER core was modelled in OpenMC, and a baseline is generated by simulating the conventional loading. UO_2 is then replaced with UN and then UC with the same enrichment distribution. OpenMC tallies are generated by providing a mesh filter and a score. The mesh filter is visualized in figure 4.1 and the scores recorded are k-eff, fission rate, neutron flux, absorption and heating. OpenMC calculates k-eff using track length, collision and absorption to estimate a combined k-eff. The k-eff generated by each case is shown in Table 4.1. The k-eff generated by the base case is 1.24795 and the k-eff of the core generated by UN and UC is comparable to that figure which implies similar neutronic behaviour in the cores. The highest fission rate in the base case is seen closer to the centre of the core in Z24 and Z33Z9. UC shows a very similar pattern of fission rate and thus a similar power output can be implied. UN however shows higher fission rates on the outer part of the core and a different fission rate pattern. The increased high fission zones will result in a higher energy output. The neutron flux generated by UC is also very similar to UO_2. Areas of high neutron flux also correspond to areas where a high fission rate is observed. UN showed an increased neutron flux in the outer ring of the core in assemblies Z40 and Z44B2, possibly due to increased enrichment. The heating and absorption patterns in UO_2 and UC also closely resemble each other while UN shows higher heating in the outer ring of the core. In conclusion, ATFs provide a higher level of safety when faced with LOCA conditions. If ATFs can be shown to be viable alternatives in current technologies to conventional UO_2 fuel, the reliability and safety of VVERs currently in use can be increased. UC showed to perform very similar to UO_2 while UN showed increased fission and flux. This study can be further improved to investigate the depletion of ATFs so that the behaviours of the core over large periods of time, fission products and operator safety can be assessed.

5.1 Future Work

This work is a small and first step in introducing the use of ATF in conventional reactors present in the world. ATFs provide higher operating safety, but many steps must be taken before they are implemented. Detailed simulations are required to accurately assess the behaviour of fuel and the reactor over long periods of time.

In terms of this work, OpenMC can also simulate behaviour over time to simulate core degradation and overall radioactivity. Depletion parameters can be added to this code to generate outputs for the entire core life cycle. After ATFs are considered a theoretically viable option for VVER-1200 fuel, the next hurdle is fabrication and sourcing. The production process and manufacturing lifecycle of various ATFs can be studied including UN and UC to ascertain an economic viability.

5.2 Summary

The study explored the viability of ATF fuel for the current generation VVER-1200 reactor. The detailed review of literature identifies UN and UC as potential ATFs. ATFs allow reactors to be operated with an additional layer of safety. A baseline is studied with conventional UO_2 fuel using the OpenMC simulation. After generating a baseline, UN and UC are simulated with the same enrichment levels as the base case. The k-eff generated by the base case is 1.24795 and UN/UC show similar neutronic behaviour. In the base case, fission is concentrated in the centre of the core and UC shows a comparable fission distribution. UN shows a different pattern with fission rates higher that UC in the outer part of the core. UN also shows a higher neutron flux in the outer part of the core. Assemblies Z40 and Z44B2 had the maximum fission rates. ATF were shown to be viable and potential alternative to conventional fuel allowing for better safety due to higher melting points. Behaviour of the core over larger periods of time and ATF reactivity can be assessed as a next step to this initial study.

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