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

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Abstract: Nuclear power is a reliable and large-scale source of GHG-free electricity. This study asses the viability of ATF fuel of uranium nitride (UN) and uranium carbide (UC) as fuel for the VVER-1200 reactor. A comprehensive overview of the VVER-1200 and Accident Tolerant fuels is conducted. 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 U_{O2} 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)

1. Introduction

Nuclear power is proven to be a reliable, cost effective and large-scale, source of GHG-free electricity. Power densities in light water reactors (LWR) can range between $50 - 70\ \mathrm{MW_{th}/m^3}$ which is significantly greater than the average power density found in conventional power plant boilers burning fossil fuels [1]. 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 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. 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. 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.[2] 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 [3].

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[5]. 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.

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)[6]. 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[4].

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 [7]. 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) [7][8].

Table 1 Thermal conductivity vs Temperature [8]

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

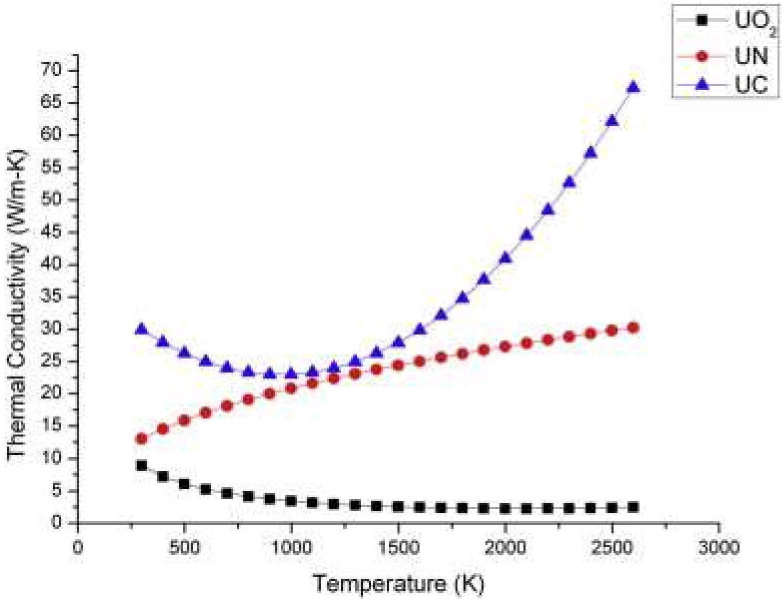

Figure 1 Thermal conductivity for UO_2, UN, and UC [8]

In this paper, the viability of UN and UC as a fuel replacement for the VVER is measured against conventional UO_2 fuel by modelling the reactor using the OpenMC neutron and photon transport code.

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2. Methodology

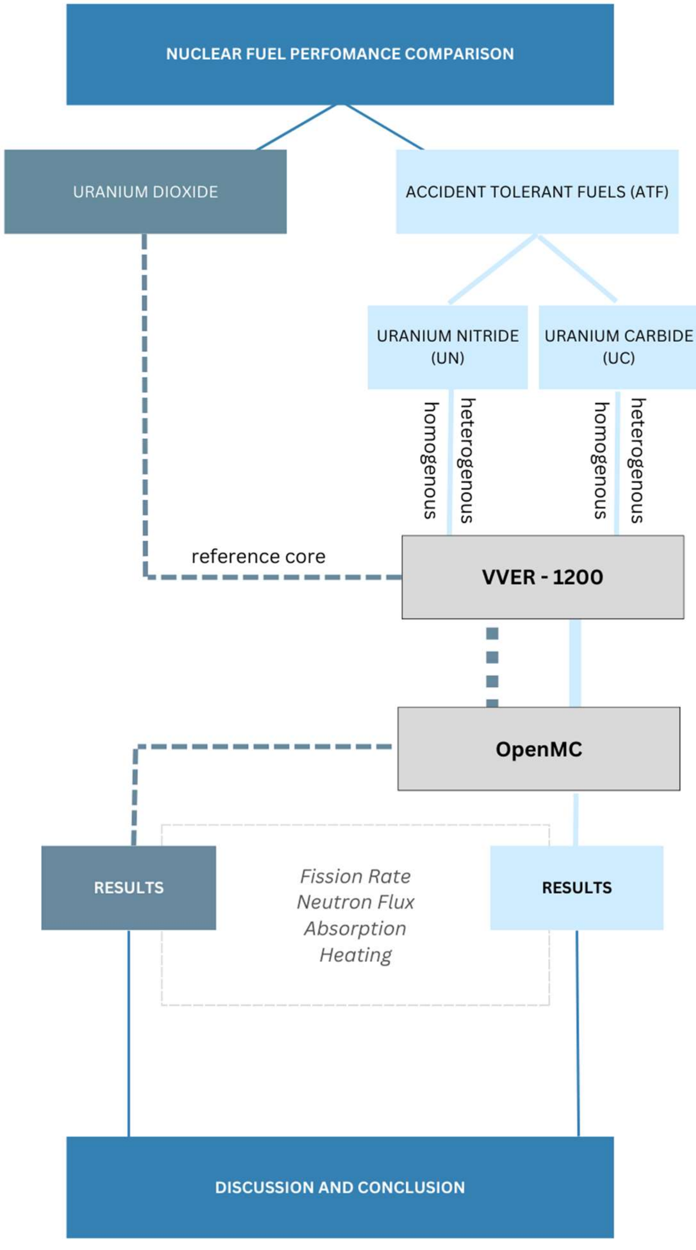


Figure 2 Methodology Flow Chart

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 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.

2.1 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 pressurizer 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.

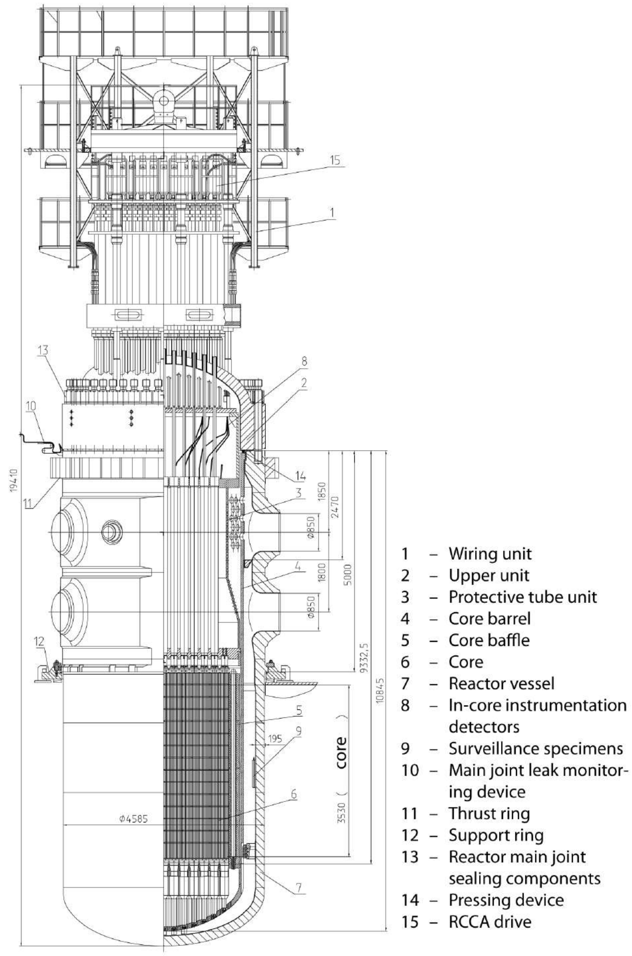


Figure 3 VVER-1200 Reactor Diagram [2]

The primary features of the VVER-1200 are given in Table 2.

Table 2 Primary features of VVER-1200 [2]

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

2.2 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.

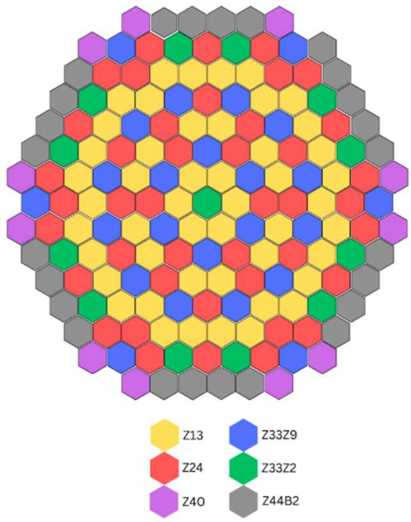
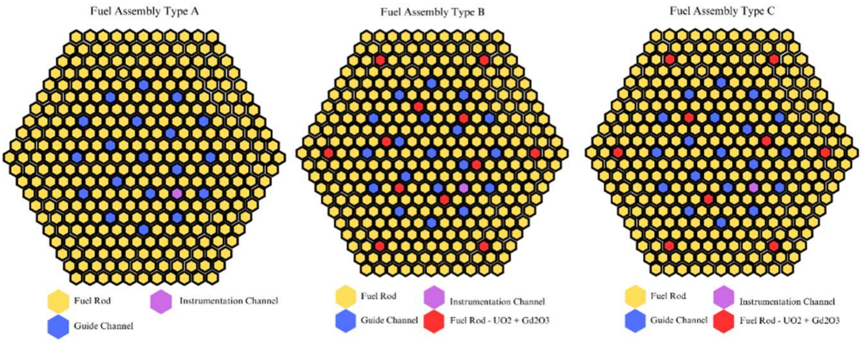


Figure 4 VVER-1200 Reference Core

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 [2]. 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.

Table 3 VVER 1200 fuel assembly configuration [9]

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



2.3 OpenMC Code

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. [10]

2.3.1 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 5 shows a 3-D voxel plot of the VVER geometry generated by ParaView.

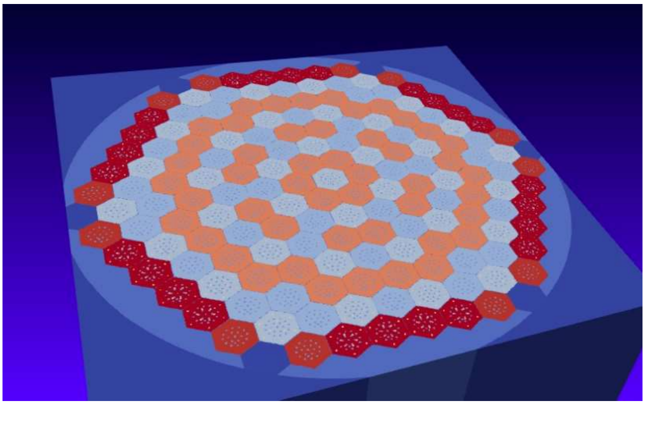


Figure 5 3-D visualization of the VVER reactor.

2.4 Fuel Comparison

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. [11] Studies have shown that UN and UC have excellent irradiation resistance and maintain their structural integrity even under extreme conditions.

Table 4 Properties of UO2, UN, and UC. [12][13]

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 UO2)	1	0.8	
Release of fission gas	1	0.45	

OpenMC is used to simulate the behaviour of UN and UC as fuel for the VVER reactor. UO_2 is replaced with UN and UC with the same enrichment levels and a homogenous distribution in the reactor.

3. 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 core as described in Table 3. Data for fission, flux, absorption, and heating is generated by applying a mesh bounding the core geometry. The mesh bounding is visualized in Figure 6.

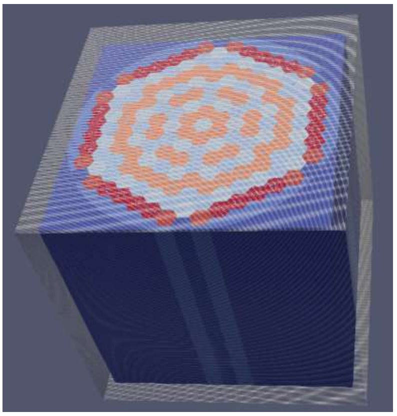


Figure 6 Geometry with Mesh Bounding

3.1 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 5.

Table 5 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

3.2 Fission Rate

UO2 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/cm³/s (or fissions per cubic centimetre per second). This quantity represents the number of fission events occurring within a given volume per unit time.

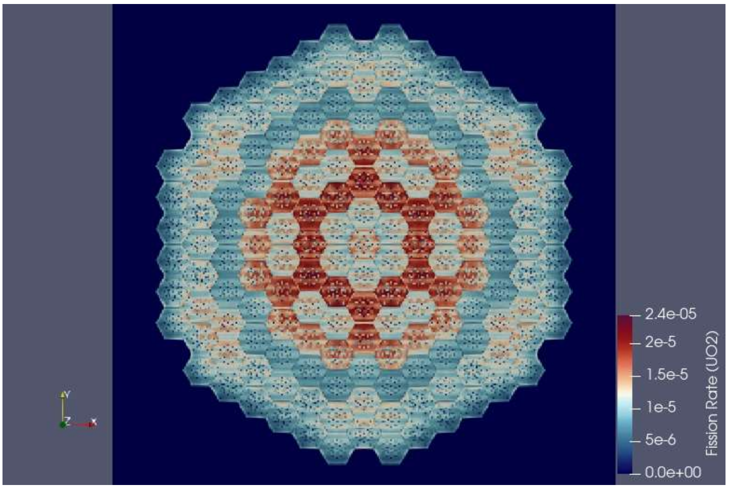


Figure 7 Fission Rate UO_2

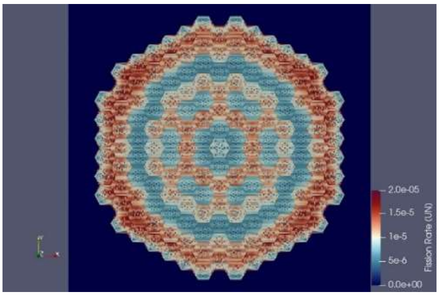


Figure 8 Fission rate UN

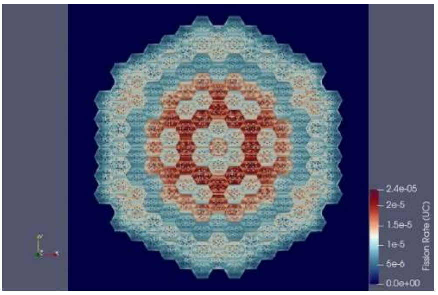


Figure 9 Fission Rate UC

Figure 7 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 9 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 8, 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.

3.3 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.

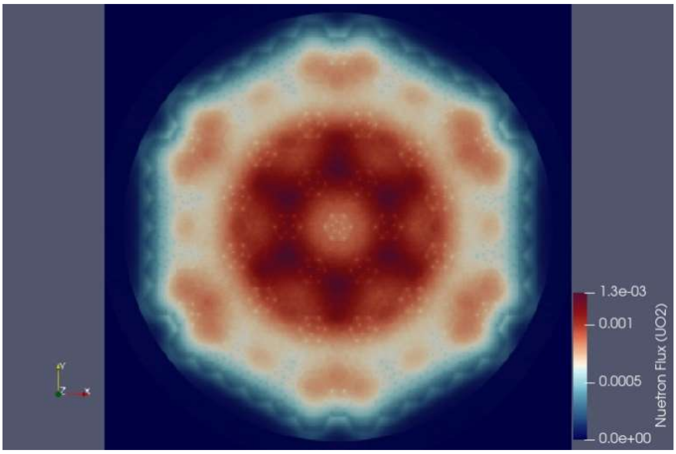


Figure 10 Neutron Flux UO2

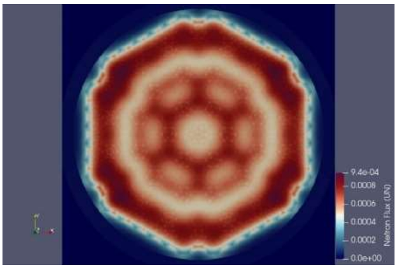


Figure 11 Neutron Flux UN

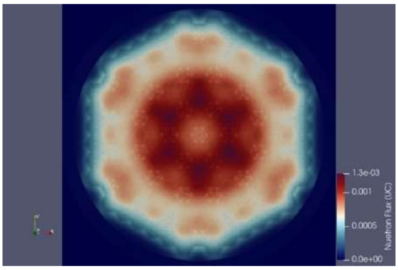


Figure 12 Neutron Flux UC

The neutron flux created by conventional UO2 loading is shown in figure 10. 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 x 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 x 10-4 located on the outer ring of the core. Case 3 (UC) neutron flux is similar to the base case (UO2) fission results.

3.4 Absorption

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

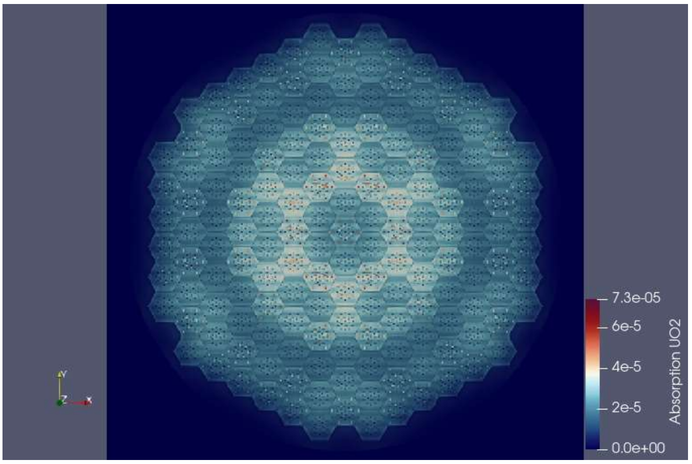


Figure 13 Absorption UO_2

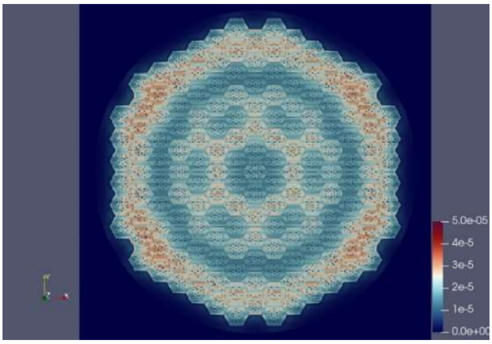


Figure 14 Absorption UN

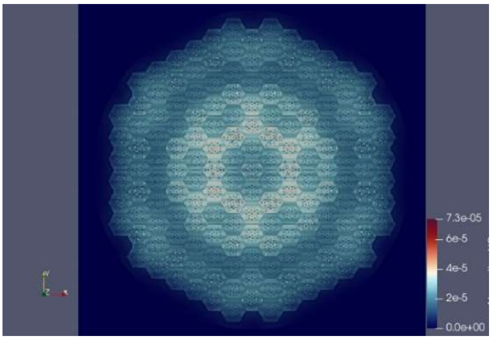


Figure 15 Absorption UC

Figure 13 shows the absorption heat 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 14 shows increase abruption 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.

3.5 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.

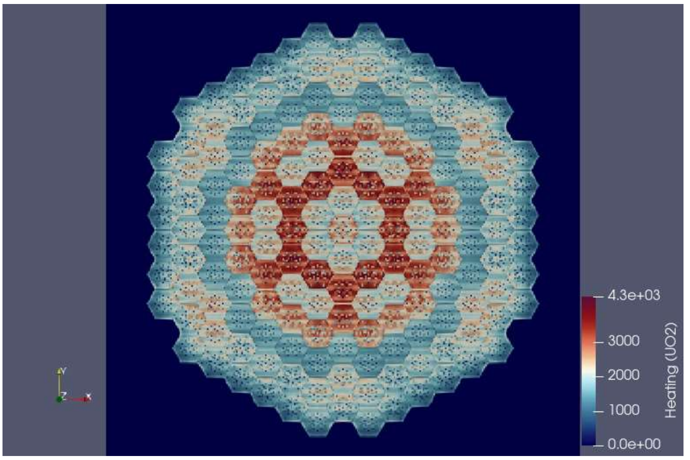


Figure 16 Heating UO_2

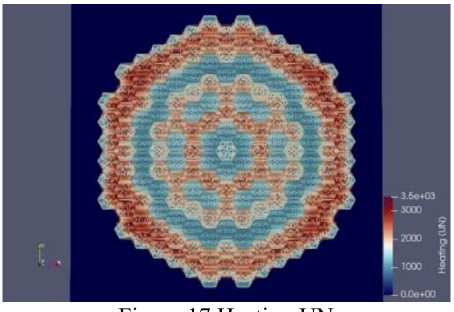


Figure 17 Heating UN

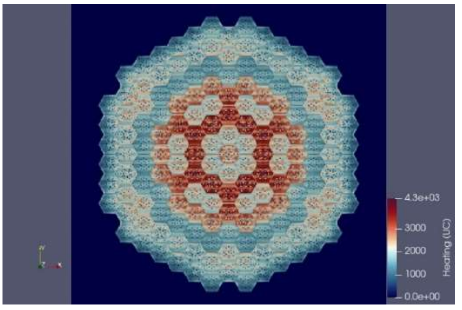


Figure 18 Heating UC

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 17 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. 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. 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.

The k-eff generated by the base case is 1.24795 and UN/UC show similar neutronic behaviour. The fission rate 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.

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