Neutronic Analysis of the Westinghouse Demonstration Lead Fast Reactor

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Abstract – *The DLFR reactor is a pre-conceptual design for a lead-cooled fast reactor developed by the Westinghouse Electric Company. The reactor is a demonstration version of the project and it is intended to prove the feasibility and cost-effectiveness of the technology, prior to commercial deployment. For the purpose of this paper, a DLFR reactor core model was created in OpenMC software, through which the effects of two fuel types – uranium dioxide and uranium nitride – on the neutronic parameters were studied. Moreover, the paper presents a number of advantages of fast reactors over the more commonly used thermal reactors. A series of simulations were carried out using the Monte Carlo method for two fuel configurations of the DLFR reactor core. The output data analyzed included the effective neutron multiplication factor, neutron flux as a function of neutron energy, conversion ratio, and isotope mass change as a function of time and burnup. Based on the obtained results, it can be concluded that uranium nitride is a promising alternative fuel relative to uranium dioxide, feasible for use in new types of nuclear reactors. In addition, it has been shown that minor actinide production is significantly lower in fast reactors compared to thermal reactors. This indicates that the greater use of fast-spectrum reactors can contribute significantly to reducing the long-lived nuclear waste disposal problem.*

Keywords: LFR, Monte Carlo, OpenMC, neutronic analysis, uranium nitride

I. Introduction

Significant progress has been made in recent years in the development of advanced nuclear reactors, known as generation IV reactors. Compared to older units, they are expected to be characterized by a significant reduction in long-lived waste production via more efficient fuel consumption (increased burnup) and closed fuel cycles, improved safety through advanced safety systems, and reduced investment risk. In 2000, at the initiative of the US Department of Energy, the Generation IV International Forum (GIF) was established and selected six reactor concepts with the highest potential for deployment [1]. This group includes Gas-Cooled Fast Reactor (GFR), Molten Salt Reactor (MSR), Very High-Temperature Reactor (VHTR), Supercritical-Water-Cooled Reactor (SCWR), Sodium-Cooled Fast Reactor (SFR), Lead-Cooled Fast Reactor (LFR). In this paper, the concept of an LFR reactor will be discussed.

II. Lead-Cooled Fast Reactors

II.A. Technology Overview

LFR reactors can cover a wide range of power outputs – from small modular reactors with electrical outputs of 50-150 MW, to large power plants of up to 1200 MW. Due to the high medium temperature reaching 550°C (later up to 800°C) high efficiencies of up to 45% can be achieved. Because of the high temperature of lead, generated energy can also be used to supply district heating. In LFR reactors, the pressure in the primary cycle is at the atmospheric pressure, resulting in an increased safety and lower construction costs due to the absence of high-pressure maintenance systems. Unlike SFRs, which require three circuits due to the chemical reactivity of sodium with water and oxygen, LFRs require only two circuits, further reducing plant construction costs.

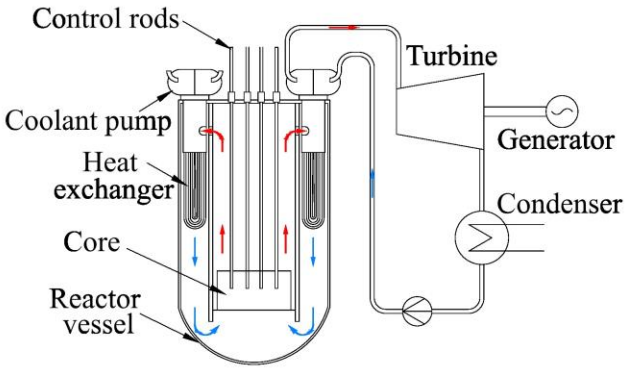

Fig. 1. Simplified LFR power plant diagram.

LFRs fall into the category of liquid metal-cooled reactors. Using a medium with better physical properties than the water used in light water reactors (LWRs), the secondary cycle of the power plant can be either a supercritical Rankine cycle or a supercritical Brayton cycle. In this technology, similar to SFRs, the entire primary circuit of the LFR reactor is contained within a large vessel filled with the working medium, as shown in Figure 1.

II.B. Fast Neutron Spectrum

Most of the world's power reactors utilize the thermal neutron spectrum. The uranium used in LWRs consists of a 3-5% isotope content of ^{235}U, with the remainder being ^{238}U. As a fertile isotope, its thermal neutron-induced fission cross section is virtually zero. The high neutron capture cross section in the thermal neutron energy region results in the transmutation of a certain amount of ^{238}U to ^{239}Pu. The ^{239}Pu is a fissile isotope, therefore in the thermal neutron region it has a high fission cross section and an almost equally high neutron capture cross section. Upon thermal neutron absorption, only 64% of the ^{239}Pu undergoes fission reactions and the remaining 36% undergoes an (n, γ) reaction. This results in the formation of the ^{240}Pu isotope, which can then transmute to ^{241}Pu and ^{242}Pu [2]. These isotopes, and all the transuranics that follow, are characterized by a high neutron capture cross section and a low thermal neutron fission cross section (with the exception of ^{241}Pu, which has an odd number of neutrons). A simplified diagram of transmutation process leading to the production of minor actinides in LWRs is shown in Figure 2.

Transuranic isotopes formed as a result of transmutation pose a long-term spent fuel storage problem, as they have half-lives of thousands and millions of years. Table I gives a summary of the half-lives of selected transuranic isotopes formed in the core of a nuclear reactor.

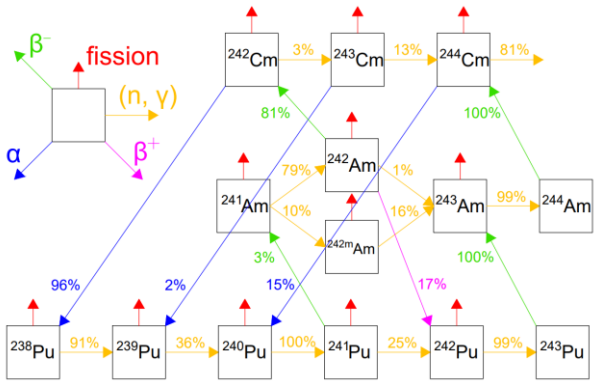

Fig. 2. Transuranic isotope depletion chain in LWRs with specific reaction probabilities [2].

Table I Half-life comparison of selected long-lived actinides.

Isotope	$t_{1/2}$ [years]
Neptunium-237	$2.144 \cdot 10^6$
Plutonium-240	6561
Plutonium-242	$375 \cdot 10^3$
Americium-241	432.2
Americium-243	7370
Curium-245	8500

In fast reactors, the high-energy neutrons produced in fission reactions are not moderated. By using materials with a low scattering cross section, the fast neutrons maintain their high energy (or are only slightly slowed down). For fertile isotopes, a sharp increase in the probability of fission is observed in the fast spectrum in parallel with a decrease in the neutron capture cross section (as for fissile isotopes). For neutron energies above 1.5 MeV, the probability of ^{238}U fission is even greater than the probability of a neutron capture reaction. In nuclear reactors using the fast neutron spectrum, any actinide isotope can be fissioned, but the probability of this reaction occurring for isotopes with an odd number of neutrons is many hundreds of times lower than in thermal reactors. By utilizing fast neutrons, it may be possible to reduce significantly the quantity of transuranic isotopes produced in the reactor, the accumulation of which reduces the reactivity of the core, and to solve the problem of the long-lived radioactive waste disposal [3].

Another advantage of fast reactors over thermal reactors is that when a nucleus is fissioned by a fast neutron, more neutrons are produced on average than when it is fissioned by a thermal neutron. The resulting excess neutrons can initiate more fission reactions. The excess neutrons in the core also make it possible to breed the nuclear fuel more efficiently, thereby extending the duration of the fuel cycle. A fast reactor designed for this purpose can produce more fissile material than it consumes, therefore reactors of this type are called breeder reactors.

II.C. Lead Coolant Properties

Today, sodium and lead are the most commonly proposed materials for fast reactor coolants. The coolant used in fast reactors must have a high neutron scattering cross section, a low neutron capture cross section, and a high mass number in order to dissipate the energy of the neutrons hitting the nucleus more efficiently. Lead fulfills all these criteria, making it a superb coolant from a neutronic point of view. Lead also has excellent physical properties for heat transfer. The thermal conductivity of lead is 35.9 W/(m·K) (at 20℃), compared to 0.598 W/(m·K) for water, making it more efficient at removing heat from the core and achieving core exit temperatures of up to 800°C. Lead has a very high boiling point of 2021ºC, which allows atmospheric pressure to be maintained in the primary circuit of the reactor [4].

The disadvantage of lead, however, is its high melting point of 327.5ºC, which can cause some operational problems with the risk of the medium solidifying. The density of lead is up to 10 times that of water and is 11.34 g/cm^3 at 20ºC, which increases the weight of the system and requires additional structural reinforcement. Moreover, lead isotopes can also transmute to produce the isotope ^{210}Po, a very strong alpha emitter, which must also be considered in the reactor design.

III. Uranium Nitride Fuel

In commercial nuclear reactors currently in operation, the vast majority use fuel that is made from uranium dioxide (UO_2). An alternative fuel to UO_2 can be uranium nitride (UN), which has on average 30% higher uranium density than uranium oxide, making it possible to reduce fuel volume. At a temperature of 1000°C, the densities of UO_2 and UN are 10.63 g/cm^3 and 13.99 g/cm^3, respectively [5, 6]. Higher fuel density also results in a potentially higher fuel burnup, a longer fuel cycle duration, and an increased conversion ratio. In addition, the thermal conductivity of uranium nitride is much higher than that of uranium dioxide. At 20ºC the thermal conductivity of UO_2 is 7.67 W/(m·K) and for UN fuel it is 14.06 W/(m·K) [6, 7]. The main disadvantage of UN fuel is its high production cost associated with the need to enrich the natural nitrogen (consisting of approximately 99.6% ^{14}N and 0.4% ^{15}N) in the ^{15}N isotope to nearly 99.9%. The ^{14}N isotope has a higher neutron capture cross section than the ^{15}N isotope, resulting in a lower neutron flux in the core.

IV. Simulation

IV.A. OpenMC Monte Carlo Code

The core of the DLFR lead-cooled fast reactor was created in OpenMC, a free, open-source software developed in 2011 by the University of Massachusetts Institute of Technology and Argonne National Laboratory [8]. The principle of its operation relies on the stochastic Monte Carlo method application. Monte Carlo simulations are a type of numerical method that estimates the occurrence probability of some event based on random variables. In nuclear core applications, the stochastic method eliminates the need to solve time-consuming neutron transport equations (the Boltzmann equation), which are impossible to solve for very complex systems. Each nuclear reaction has a certain probability of occurrence, dependent on its probability distribution. Based on that, it is possible to trace the history of a neutron from its origin to its absorption or escape from the system and obtain the rate of each nuclear reaction.

IV.B. Westinghouse DLFR Core Model

The core of the Demonstration Lead-Cooled Fast Reactor (DLFR) conceptual nuclear reactor of Westinghouse Electric Company's design was modeled using the OpenMC software. The reactor core input data was taken from a document that is part of the "Advanced Demonstration and Test Reactor Options (ADTRO)" study prepared for the U.S. Department of Energy [9].

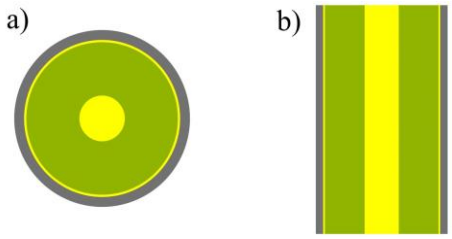

Fig. 3. Cross-section in the xy plane (a) and xz plane (b) of the DLFR reactor fuel rod (green - fuel pellet, yellow - helium, gray - steel cladding).

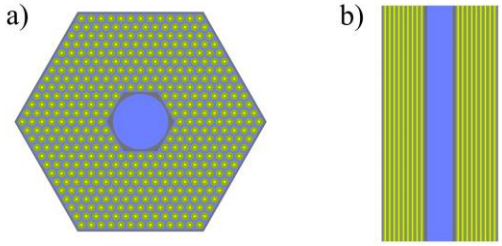

Fig. 4. Cross-section in the xy plane (a) and xz plane (b) of the DLFR reactor fuel assembly (green - fuel pellet, yellow - helium, gray - steel cladding, blue - lead).

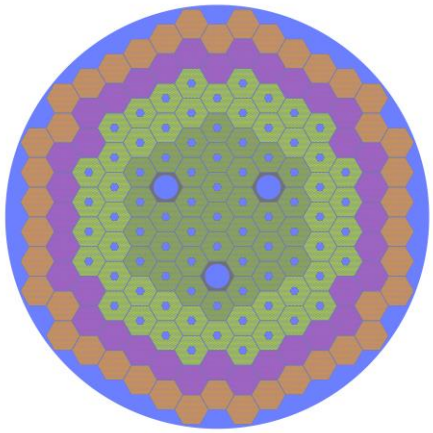

Fig. 5. Cross-section of the DLFR reactor core (dark green - fuel with 17.5% enrichment, light green - fuel with 19.9% enrichment, yellow - helium, gray - steel, blue - lead, pink - Zircaloy-4, orange - boron steel).

The DLFR reactor features a hexagonal core consisting of 82 fuel assemblies and 3 safety assemblies surrounded by 78 shielding assemblies. The fuel assemblies are divided into inner assemblies with enrichment of 17.5% and outer assemblies with 19.9% enrichment. The fuel area is surrounded by 36 shielding assemblies acting as neutron reflectors and 42 shielding assemblies serving as neutron absorbers. The height of the active part of the core is 70 cm, while the core diameter (including shield assemblies) is equal to 430 cm. The total mass of the fuel inside the reactor for UO_2 and UN is equal to 19755 kg and 25999 kg, respectively. Figures 3 through 5 show the modeled fuel rod, fuel assembly, and the DLFR reactor core.

IV.C. Simulation Settings

The calculations were carried out using two nuclear libraries: ENDF/B-VII.1 and JEFF-3.3 [10, 11]. Simulation parameters for fresh fuel (at time t = 0 s) were set for 10000 neutrons per cycle, with the number of active and inactive cycles equal to 500 and 50, respectively. Depletion calculations were performed using 10000 neutrons per cycle, with the number of active and inactive cycles equal to 120 and 15, respectively. For both types of fuel, the thermal power of the reactor was set to 500 MW. All simulations were conducted with control/safety rods placed outside the active core area.

V. Simulation Results

V.A. Effective Neutron Multiplication Factor

Table II Comparison of k_{eff} results for UO_2 and UN fuels.

Fuel type	Nuclear library	
	ENDF/B-VII.1	JEFF-3.3
Uranium dioxide (UO_2)	1.13462 ± 0.00034	1.13475 ± 0.00033
Uranium nitride (UN)	1.18500 ± 0.00036	1.18522 ± 0.00035

Table II summarizes the obtained k_{eff} results at the initial stage for UO_2 and UN and the two nuclear libraries. The differences in k_{eff} values between the core with UO_2 fuel and UN fuel are 5038 pcm for calculations using the ENDF/B-VII.1 library and 5047 pcm for simulations using the JEFF-3.3 library, in favor of uranium nitride fuel. Figure 6 shows the change in k_{eff} as a function of burnup for both fuels. For the core depletion simulation made with uranium dioxide fuel, the reactor becomes subcritical ($k_{eff} < 1$) at a fuel burnup of 91.49 MWd/kg (3366.16 days) and 87.57 MWd/kg (3221.72 days) for the ENDF/B-VII.1

and JEFF-3.3 libraries, respectively. With uranium nitride fuel, the reactor becomes subcritical at a fuel burnup of 132.7 MWd/kg (6842.44 days) and 125.71 MWd/kg (6779.41 days), depending on the library used. The application of uranium nitride fuel makes it possible to increase the fuel burnup level by 41.21 MWd/kg (ENDF/B-VII.1) and 38.14 MWd/kg (JEFF-3.3) relative to uranium dioxide fuel, thus making it possible to extend the total time period of a fuel element in the core by 3476.28 days and 3557.69 days, respectively.

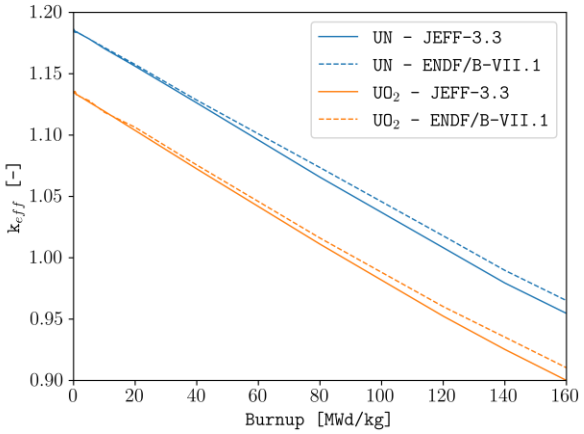

Fig. 6. Change in k_{eff} as a function of fuel burnup for UO_2 and UN fuel.

V.B. Neutron Flux

Figure 7 depicts neutron flux per unit lethargy as a function of neutron energy for both fuel types. The neutron flux obtained for uranium dioxide fuel is on average higher than for uranium nitride fuel. The peak neutron flux for fuel with UO_2 and UN is $3.63 \cdot 10^{13}$ n/(cm^2 · s) and $3.16 \cdot 10^{13}$ n/(cm^2 · s), respectively. The neutron flux values obtained can be influenced by such factors as the rate of fission reactions and absorption in the fuel, the energy of fission neutrons, and the number of neutrons released in the fission event.

Capture and fission cross section plots of selected transuranic isotopes and neutron flux in the core of a UN-fueled DLFR reactor are presented in Figure 8. In order to efficiently fission minor actinides, it is necessary to achieve the lowest possible ratio of the neutron capture cross section to the fission cross section. By shifting towards higher neutron energies, the ratios become progressively lower. In order to fission these isotopes more efficiently, the neutron flux inside the core should also be shifted towards the fast neutron energies.

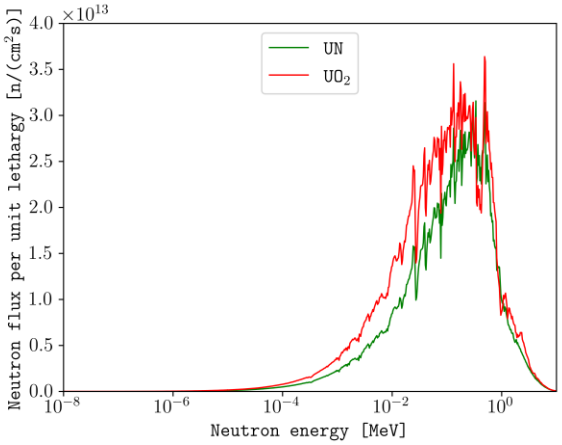

Fig. 7. Neutron flux per unit lethargy relative to the neutron energy in the core with UO_2 and UN fuel.

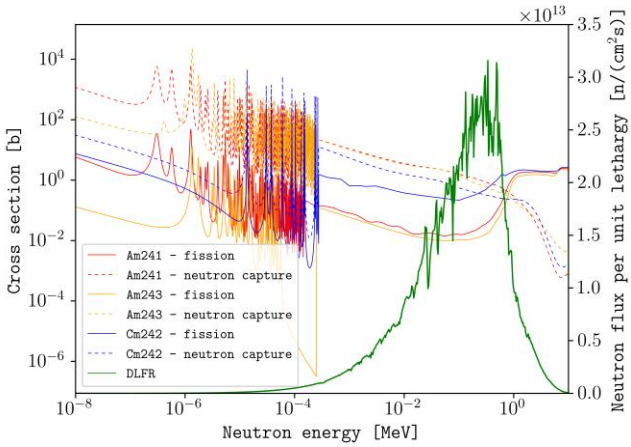

Fig. 8. Neutron flux in the UN-fueled DLFR core, neutron capture cross sections and fission cross sections for selected transuranic isotopes.

V.C. Conversion ratio

Conversion Ratio (CR) values were compared for both types of fuels. CR is a quantity, which can be defined as a ratio of the fertile nuclide capture rate to the fissile nuclide absorption rate. The conversion ratios were calculated as the quotient of the (n, γ) reaction rate in the fertile ^{238}U material, and the sum of the absorption reaction rates in the fissile materials – ^{235}U, ^{239}Pu, and ^{241}Pu. Figure 9 presents a comparison

of calculated conversion ratios for uranium dioxide and uranium nitride fuel as a function of burnup (for the JEFF-3.3 library). The values of the fuel conversion ratio for UO_2 and UN over the entire fuel burnup range are 0.453-0.720 and 0.456-0.700, respectively. At the early stages of fuel burnup, the conversion ratio values for both types of fuel are very close to each other, but with an increasing residence time of fuel elements in the reactor core, the CR for UO_2 fuel increases relative to the value for UN.

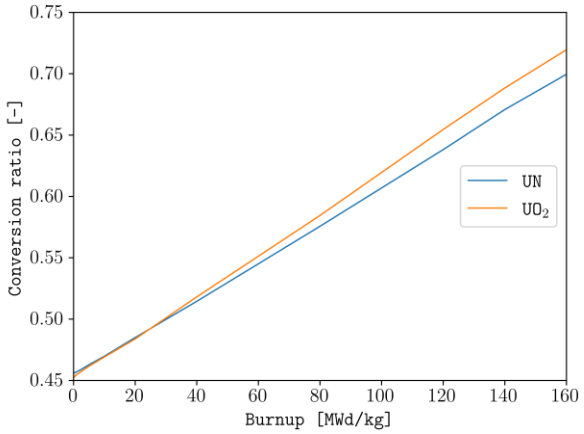

Fig. 9. Conversion ratios for the core with UO_2 and UN fuel as a function of burnup.

In fast spectrum reactors, due to the higher number of neutrons produced in the fission reaction and the higher probability for the reaction to occur, fuel CRs are usually higher than in PWRs and BWRs, in which they are around 0.6 [12]. In the analyzed DLFR reactor core, the average value is 0.586 for UO_2 fuel and 0.578 for UN fuel. Its relatively low values, especially at the beginning of the fuel campaign, are due to the high level of fuel enrichment, up to 19.9%. To improve the CR value, one possible option is to use fuel containing in its initial state a few percent of ^{239}Pu, which has a higher number of neutrons produced in the fission reaction than ^{235}U. The second option, used in breeder reactors, is placing assemblies containing depleted uranium in the peripheral part of the core, which is known as a blanket.

V.D. Actinides Mass Change

The final data obtained are the mass changes of selected isotopes as a function of fuel burnup and time, carried out for simulations using UN fuel and the JEFF-3.3 library. In the modeled DLFR reactor core, fresh fuel consists of 17.5% to 19.9% of the ^{235}U isotope (depending on the location of the fuel assembly in the core), with the remainder being the ^{238}U. The initial mass of fuel in the core is 25999 kg, comprising 21133 kg of ^{238}U isotope and 4866 kg of ^{235}U isotope. As illustrated in Figure 10, as fuel burnup progresses, the masses of these isotopes decrease due to their fission or transmutation. At a fuel burnup level of 132.7 MWd/kg, when the reactor core becomes subcritical (end of fuel cycle), ^{238}U and ^{235}U isotopes account for about 70.2% and 6.8% of the total fuel mass, respectively.

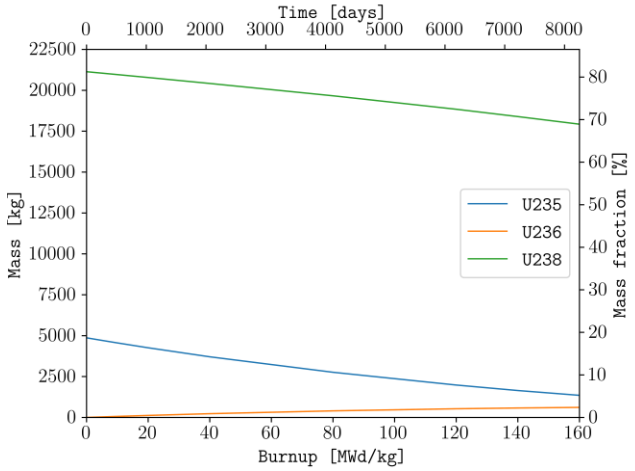

Fig. 10. Mass of uranium isotopes as a function of fuel burnup and time.

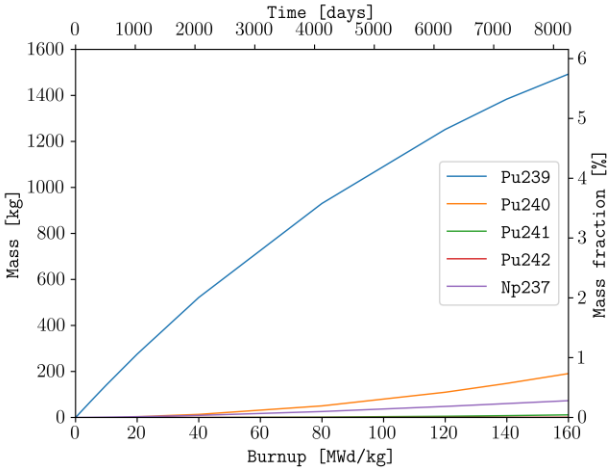

Fig. 11. Mass of plutonium isotopes and Np-237 as a function of fuel burnup and time.

As a result of a successive radiative capture of neutrons by actinide nuclei, plutonium isotopes are formed in significant quantities, as shown in Figure 11. The most abundant of the recorded plutonium isotopes is the fissile ^{239}Pu isotope, which has a mass of 1336 kg at a burnup of 132.7 MWd/kg, accounting for 5.1% of the total fuel mass. In thermal reactors, the resulting fissile ^{239}Pu isotopes and, in much smaller quantities, ^{241}Pu, contribute to a relatively large percentage of the total thermal energy production in the core. Due to the low level of fuel enrichment in LWRs (3-5%), more than 40% of the fission energy produced comes from the fission of ^{239}Pu and ^{241}Pu isotopes [13]. Considering the high level of fuel enrichment in the DLFR reactor (reaching 17.5% and 19.9%), the contribution of plutonium isotope fissions to total energy production is relatively much smaller than in thermal reactors. Of all the minor actinides, ^{237}Np isotope is by far the most produced. It is mainly formed by neutron capture by the ^{236}U nucleus and the subsequent beta-minus reaction.

Figure 12 illustrates the increasing amount of the most significant minor actinides (aside from ^{237}Np) as a function of fuel burnup and time. The largest amount of the resulting material is the ^{241}Am isotope, whose total mass in the fuel at a burnup of 132.7 MWd/kg is about 1.31 kg. Given the very low mass of the other minor actinides (including actinium, thorium, protactinium, berkelium, californium, einsteinium, and fermium), they were not included in the analysis. The total mass of the minor actinides formed in the DLFR core is about 61.63 kg, of which as much as 60.24 kg is the ^{237}Np isotope. With the high burnup of fuel in the DLFR reactor core, at the end of the fuel campaign, the mass of decay products is 3880 kg, which accounts for up to about 14.9% of the total fuel mass.

In reactors utilizing the fast neutron spectrum, including LFR-type reactors, it is feasible for a relatively small amount of minor actinides to be formed. In LWRs, the average content of minor actinides is 0.1-0.2%, which mainly consists of neptunium, americium, and curium isotopes [14]. Table III provides a comparison of the average mass contribution of minor actinides in the fuel of LWRs and their mass contribution in the modeled core for three levels of fuel burnup. In the DLFR reactor core with uranium nitride fuel, at a burnup of 20 MWd/kg and 60 MWd/kg, the content of minor actinides in the total fuel mass is 0.0125% and 0.067%, respectively. These values are several times lower than for LWRs. It is only at the end of the DLFR reactor's fuel cycle (burnup rate of 132.7 MWd/kg) that the production of minor actinides is at a similar level to that of LWRs, at 0.237%. This occurs with as much as three times longer residence time of the fuel element in the DLFR reactor core than in LWRs, equal to 18.75 years.

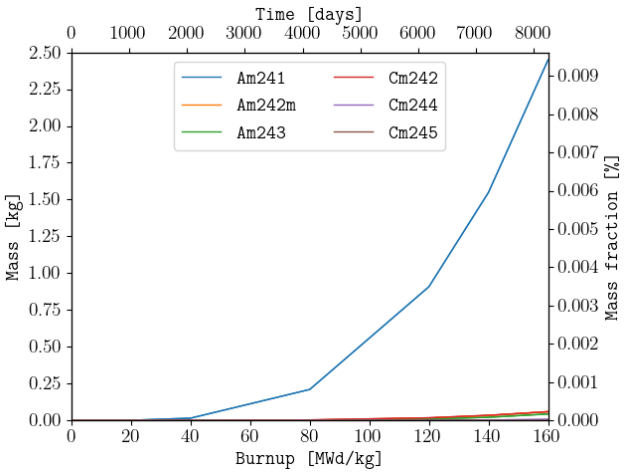

Fig. 12. Mass of americium and curium isotopes as a function of fuel burnup and time.

Table III Average mass contribution of minor actinides in fuel in LWRs and the DLFR reactor for different levels of fuel burnup.

Parameter	LWRs		DLFR		
Burnup [MWd/kg]	20	60	20	60	132.7
Fuel element time inside the core [years]	2	5	2.83	8.48	18.75
Minor actinides percentage fraction in spent fuel [%]	0.1	0.2	0.0125	0.067	0.237

VI. Conclusions

This paper presents the effect of two nuclear fuel types on the most basic neutronic parameters in the LFR reactor. Moreover, a comparison of reactors using the fast and thermal neutron spectrum in terms of long-lived nuclear waste production is presented by performing Monte Carlo simulations using the OpenMC code.

The initial state k_{eff} values obtained in the simulation are higher for uranium nitride fuel, at 1.18500 and 1.18522 (depending on the library used), compared to the values of 1.13462 and 1.13475 for uranium dioxide fuel. The higher k_{eff} value significantly affects the potential operating time of the reactor. The core becomes subcritical after 3366.16 days (91.49 MWd/kg) and 6842.44 days (132.7 MWd/kg) for UO_2 and UN fuel, respectively. This means that the use of uranium nitride fuel makes it possible to extend the residence time of the fuel element in the core by up to 3476.28 days and to increase the fuel burnup rate by 41.21 MWd/kg relative to uranium dioxide fuel.

The use of UN fuel results in an average lower neutron flux than that of UO_2 fuel, but it is shifted towards higher neutron energies, allowing a more efficient utilization of transuranic isotopes. The most probable reason for the higher neutron energy in the core with UN fuel is a lower amount of neutron scattering reactions occurring in the fuel itself, due to the presence of only one nitrogen atom in the UN compound compared to two oxygen atoms in the UO_2 compound.

The conversion ratio for uranium dioxide fuel was found to be slightly higher than that for uranium nitride fuel, especially during the final burnup period of the fuel. The values of the conversion ratio in the analyzed core over the entire burnup period are 0.586 for UO_2 fuel and 0.578 for UN fuel. Fast reactors usually tend to have higher fuel efficiency compared to LWRs, which have conversion ratios averaging 0.6. The low fuel efficiency of the DLFR reactor is mainly due to high fuel enrichment of up to 19.9%.

Changes in the mass of isotopes as a function of time and burnup for a UN-fueled core are also presented. One of the most important advantages of fast reactors over thermal reactors is the lower production of minor actinides, which is why the amount produced in the DLFR core was compared with that in thermal reactors. A burnup simulation conducted showed that the mass share of minor actinides for the modeled core is significantly lower than in PWR reactors. At a burnup of 60 MWd/kg, the mass contribution of minor actinides in the DLFR reactor core is 0.0668%, compared to about 0.2% in PWR reactors. This demonstrates that the use of fast reactors can make a significant contribution to solving the problem of long-lived radioactive waste storage.

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