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ARTICLE

Molybdenum with MOX Nuclear Fuel to be Used for the Second Load of Generation IV ALLEGRO Nuclear Reactor Using the Monte Carlo Method

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Abstract: A new nuclear fuel consisting of 80% MOX and 20% molybdenum is proposed to be used in Gen IV reactors (ALLEGRO Reactor). The average temperature drop on the fuel (ATDF) decreased by about 153 °C with respect to the non-mixed MOX with a consequent decrease of the average temperature on the fuel-rod axis (ATFA) by 166.4 °C. This temperature reduction can be utilized to increase the coolant outlet temperature (T_{out}), thereby enhancing the efficiency of the thermodynamic cycle of the coolant (ETCC). The MALBRN computational system was used to address the neutronic problem using the Monte Carlo method (MCM) and the thermal-hydraulic problem using correlations available in the literature. A comparison of the new fuel with standard nuclear fuels, such as carbides (CFs) and nitrides (NFs), was conducted based on thermal properties. The new fuel exhibits an ATDF comparable to those of CFs and NFs. Moreover, the new fuel enables coolant outlet temperatures to reach high values (up to 1140.4 °C), facilitating advanced applications for generation IV reactors. As a result, a very high ETCC (up to 64.90%) can be achieved. However, this improvement comes at the cost of a higher plutonium content in the final fuel (26.84% compared to 20.35%).

Keywords: ALLEGRO and Gen IV reactors, Carbide and Nitride fuels, MOX fuel, Molybdenium, MALBRN computation system, Monte Carlo method.

PACS: 25.85.−w Fission reactions.

1. Introduction

The world trend towards the use of renewable energy remains modest, with renewable energy sources still unable to meet the growing demand for energy consumption worldwide. For example, in Europe, renewable energy accounts for only 22% of total energy consumption [1], while global energy demand is expected to increase by up to 47% by 2050 [2]. This highlights the continued necessity of nuclear energy to play a critical role in global energy consumption scenarios.

ALLEGRO is a research reactor designed to demonstrate Gen IV technology which means that this reactor should operate using a fuel that can stand a high-power density and high temperatures. The fuel temperature is intended to be over 2000 °C, while the fuel power density should be at least 100 MW/m^3 in the reactor core [3].

Gen IV reactors, often regarded as the reactors of the 21st century, are currently under development, with ALLEGRO serving as a representative example [4].

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Gen IV reactors will have many new and advanced characteristics, such as sustainability, good protection of public health and the environment, and financial risks comparable to those of conventional energy projects. They will be also safe and reliable.

Although this paper focuses on how to increase the thermal conductivity of MOX fuel to compete with the CFs and NFs, an equally important objective is to benefit from the new higher conductivity to reduce the maximum temperature drop on the fuel (MTDF) and increase the outlet temperature of the coolant (T_{out}) to increase the efficiency of the thermodynamic cycle of the coolant (ETCC), which should not be less than 47% [4]. For comparison, current efficiencies are 34–36% for most existing nuclear plants, 39% for some advanced designs, 40% for modern coal-fired plants, and approximately 60% for combined cycle gas turbine (CCGT) plants [5]. Achieving higher T_{out} would enable more advanced applications for Gen IV reactors, such as hydrogen production, district heating, and industrial transformation processes.

MOX fuel is widely regarded as a strong candidate for nuclear reactors due to its high melting point, exceeding 2000 °C (3025 K) [6], and its extensive international operational experience with reliable performance under irradiation. However, its primary drawback, which may be a major one, is its thermal conductivity [6] (see Fig. 1).

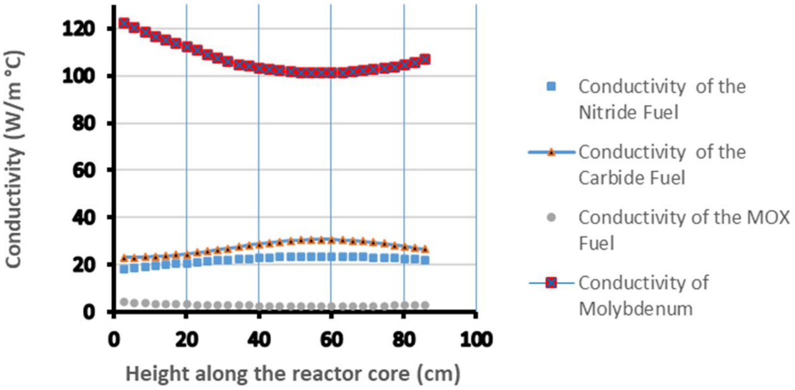


FIG. 1. Comparison of the conductivities of MOX, CFs, NFs, and molybdenum.

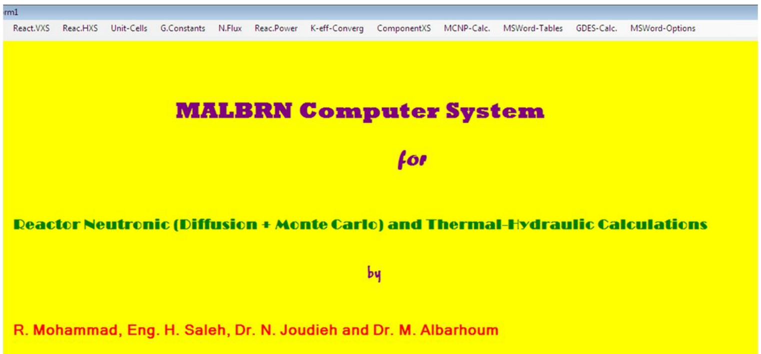
Other candidate fuels are carbides (U-Pu) C and nitrides (U-Pu)N, which have good thermal conductivity but poor international operating experience [7]. Although the Moly fuel is actually receiving high attention as a fuel for research reactors, it does not seem to be suggestible as a fuel for Gen IV reactors, uranium being enriched while in the MOX fuel uranium is only natural.

The best solution for Gen IV nuclear reactors is to enhance the thermal conductivity of MOX fuel. This paper explores the feasibility of achieving this by incorporating molybdenum into MOX fuel. Molybdenum is a metal with a high melting point (2623 °C [6]), excellent performance under irradiation, and proven application in nuclear reactors as a component of stainless steel, widely used in cladding and containment materials.

European countries participating in the ALLEGRO project have outlined a multi-stage process for qualifying ALLEGRO as a Gen IV reactor. The final stage involves operating the reactor with a MOX core, featuring coolant inlet and outlet temperatures of approximately 400 °C and 850 °C, respectively. Using this as a benchmark, this study focuses on how MOX fuel can compete with carbide (CFs) and nitride (NFs) nuclear fuels in this reactor while addressing the challenges associated with CFs and NFs in nuclear applications [6].

2. Codes and Programs Used to Solve the ALLEGRO Problem

The MALBRN System is a software package consisting of many programs that work in harmony to achieve semi-automatic work, with user input playing a pivotal role in guiding the calculations. The system features user-friendly dropdown menus (as shown in Fig. 2), allowing users to design reactor components, whether physical or modeled. Reactor components are modeled when the reactor neutronics are calculated with a diffusion code (DC) (like the code GDES which is included in the system, where GDES is a DC locally developed in 2020 during a Ph.D. thesis [8]). Calculation with a DC requires the homogenization of the reactor component with the WIMS code [9], a cell code used for the calculation of the macroscopic XS of the reactor components. If the reactor contains materials not included in the WIMS cross-section library, the system employs the Monte Carlo method (MCM) available within the MALBRN System to perform the calculations [10]. The user writes a general free-format input file to solve both the neutronic and thermal-hydraulic problems of the reactor.



MALBRN Computer System

for

Reactor Neutronic (Diffusion + Monte Carlo) and Thermal-Hydraulic Calculations

by

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FIG. 2. User interface of the MALBRN computer system.

The input file component data include dimensions, material densities, and material thermo-physical properties as functions of temperature (most of them are embedded in the MALBRN system as databases) The pre-processing programs available in the MALBRN system get out the required data for each type of calculation, whether neutronic or thermal-hydraulic. Reactor components are described in the input file only as they are physically. The interface programs transform this description to be suitable for WIMS-modeled components or MCM without modeling.

When the neutronic calculations are performed by the MALBRN system other post-processing programs act to use the neutronic results to calculate the thermal-hydraulic parameters, such as the temperature distribution along the core of the coolant, the temperature drop on the fuel (TDF), the temperature drop on the clad (TDC), the temperature drop between the clad and the coolant (TDCC), and the coolant flow-rate required to achieve a fixed temperature whether it is the T_{out} or the temperature on the fuel-rod axis (TFA).

Additional calculations such as the reactivity of the reactor for a certain k_{eff} (effective multiplication factor) are available as well. Results (whether neutronic, thermal-hydraulic, or a combination of both) are presented in MS Word tables, while all graphical outputs, such as drawings, are displayed directly on the PC screen.

The MALBRN System also supports bilingual operation, offering language options in Arabic and English. Furthermore, the system provides detailed information about component dimensions and reactor statistics, enabling users to better understand how the system interprets their reactor structure.

2.1 Reactor Modeling with MALBRN

Once the MCM is run by the MALBRN computational system, the neutronic fluxes, the thermal power distribution along the core, and the initial excess reactivity (IER) in the reactor are all calculated. Based on the thermal power generated along the reactor core, all the thermal-hydraulic parameters are then calculated, including the temperature drop on the fuel (TDF), on the clad (TDC), and between the clad and the coolant (TDCC) in addition to the coolant temperature distribution along the core of the reactor. The coolant flow rate is also calculated to achieve a certain T_{out} for the coolant.

The ALLEGRO reactor considered in this study differs from that proposed by some European members of the ALLEGRO Project (see Table 1). These differences arise from our decision to set the Initial Excess Reactivity (IER) close to 62 mk to extend the in-core fuel cycle duration. In contrast, the originally positioned control rods (CRs) and shut-down rods (SDRs) were configured to operate with an IER of approximately 20 mk. Consequently, we needed to shift and rearrange the positions of both the CRs and SDRs, as detailed in Table 2.

TABLE 1. Comparison of reactor parameters used in this paper with those proposed by the European countries participating in the ALLEGRO Project [11].

Item:	European Value	Local Value
Power of the reactor (MW)	75	75
Power density in the core (MW/m^3)	100	102.71
Power density in the fuel material (MW/m^3)	Not Available	254.1
Fissile core coolant fraction (%)	35.07	35.07
Fissile Core mass flow rate (kg/s)	53.5	53.5
Cladding Material/Total Cladding Surface area in the core(cm^2)	SS\2422486	SS\2422486
Helium Inlet/Outlet Temperature (°C)	260/530	260/530
Operating helium pressure (Mpa)	7	7
Fissile core height (cm)	86	86
Core Volume (m^3)	0.7302	0.7302
Fuel Volume in the core (m^3)	0.2952	0.2952
No of fuel rods in the core	13689	13689
No of Fuel Assemblies in the core	81	81
No of fuel rods/Fuel Assembly	169	169
No of Radial Reflector Assemblies	174	174
No of RS Assemblies in the core	98	98
Pressure Vessel Material	Stainless Steel (SS)	SS

TABLE 2. Distribution of the control devices in our ALLEGRO and the European ALLEGRO.

Row No. in the core	European ALLEGRO			Local ALLEGRO		
	CRs	SDRs	ITs	CRs	SDRs	ITs
5	1					1
6			1			1
7						
8		2		2		
9	1				1	
10			1	1		
11	1	1	2	1	1	2
12			1			1
13	1		1			
14	2				2	
15						
16			1			
17		1				1

3. Results

The most important parameters for the MOX fuel are reported in Table 3. The ALLEGRO reactor can operate with about 62 mk IER with 20.35% Pu in the MOX fuel. The inlet temperature of helium at the bottom of the core is 400 °C and the outlet temperature of the coolant is about 850 °C.

TABLE 3. The resulting neutronic and thermal-hydraulic parameters for ALLEGRO reactor using pure MOX fuel with SiC clad.

Item	Value
Type of fuel used in the Reactor / Pu% in the fuel	PuO2+UO2 / 20.35
Coolant Mass Flowrate (kg/s) / Coolant thermodynamic efficiency	32.1 / 0.529
K-effective of the Reactor / Reactivity in the Reactor (mk)	1.066474 / 62.327
Fuel density (g/cm^3) / Cladding Material	10.4 / SiC
Temperature at the Fuel Rod Axis (°C): Max / Average	1384.8 / 1076
Temperature at the Clad Internal Surface (°C): Max / Average	1089.2 / 887.7
Temperature of He (°C): Outlet / Inlet	849.7 / 400
Temp. Drop Fuel-Clad (°C) Max / Average	312.61 / 188.3

The same parameters for the MOX + 20% Mo, NFs, and CFs are shown in Tables 4, 5, and 6, respectively. All these results were obtained for a coolant T_{in}/T_{out} = 400/850 °C.

If the TFA is fixed at 1140 °C instead of fixing T_{out} at 850 °C, the results summarized in Table 7 are obtained. Moreover, with a SiC clad, the outlet temperature could potentially be raised to around 1500 °C, resulting in a new coolant cycle efficiency of 64.9%, as shown in Table 8.

TABLE 4. Neutronic and thermal-hydraulic parameters for the ALLEGRO reactor using MOX with 20% MO, with a coolant outlet temperature of approximately 850 °C.

Item	Value
Type of fuel used in the Reactor / Pu% in the fuel	Mo+U-Pu-O2 / 26.84
Coolant Mass Flowrate (kg/s) / Coolant thermodynamic efficiency	32.1 / 0.529
K-effective of the Reactor / Reactivity in the Reactor (mk)	1.066541 / 62.389
Fuel density (g/cm^3) / Cladding Material	10.36 / SiC
Temperature at the Fuel Rod Axis (°C): Max / Average	1121.1 / 909.6
Temperature of He (°C): Outlet / Inlet	849.7 / 400
Temp. Drop Fuel-Clad (°C) Max / Average	35.38 / 21.9
Percentage of Mo in the fuel(%)	20

TABLE 5. Neutronic and thermal-hydraulic parameters for the ALLEGRO reactor using NFs.

Item	Value
Type of fuel used in the Reactor / Pu% in the fuel	UN+PuN / 15.6
Coolant Mass Flowrate (kg/s) / Coolant thermodynamic efficiency	32.1 / 0.529
K-effective of the Reactor / Reactivity in the Reactor (mk)	1.066252 / 62.134
Fuel density (g/cm^3) / Cladding Material	14.3 / SiC
Temperature at the Fuel Rod Axis (°C): Max / Average	1119.3 / 910.3
Temperature at the Clad Internal Surface (°C): Max / Average	1089.2 / 887.7
Temperature of He (°C): Outlet / Inlet	849.7 / 400
Temp. Drop Fuel-Clad (°C) Max / Average	34.44 / 22.6

TABLE 6. Neutronic and the thermal-hydraulic parameters for the ALLEGRO reactor using CFs.

Item	Value
Type of fuel used in the Reactor / Pu% in the fuel	UC+PuC / 15.13
Coolant Mass Flowrate (kg/s) / Coolant thermodynamic efficiency	32.1 / 0.529
K-effective of the Reactor / Reactivity in the Reactor (mk)	1.067305 / 63.056
Fuel density (g/cm^3) / Cladding Material	13.6 / SiC
Temperature at the Fuel Rod Axis (°C): Max / Average	1112.3 / 905.8
Temperature at the Clad Internal Surface (°C): Max / Average	1089.2 / 887.7
Temperature of He (°C): Outlet / Inlet	849.7 / 400
Temp. Drop Fuel-Clad (°C) Max / Average	27.32 / 18.1

TABLE 7. Neutronic and thermal-hydraulic parameters for the case of MOX with 20% MO, with the fuel-axis temperature fixed at 1140 °C.

Item	Value
Type of fuel used in the Reactor / Pu% in the fuel	Mo+U-Pu-O2 / 26.84
Coolant Mass Flowrate (kg/s) / Coolant thermodynamic efficiency	31.1 / 0.537
K-effective of the Reactor / Reactivity in the Reactor (mk)	1.066541 / 62.389
Fuel density (g/cm^3) / Cladding Material	10.36 / SiC
Temperature at the Fuel Rod Axis (°C): Max / Average	1140.2 / 923.5
Temperature of He (°C): Outlet / Inlet	864.2 / 400
Temp. Drop Fuel-Clad (°C) Max / Average	35.53 / 22.1
Percentage of SiC in the fuel(%)	20

TABLE 8. Neutronic and thermal-hydraulic parameters for the case of MOX with 20% MO, with the fuel-axis temperature fixed at 1499 °C.

Item	Value
Type of fuel used in the Reactor / Pu% in the fuel	Mo +U-Pu-O2 / 26.84
Coolant Mass Flowrate (kg/s) / Coolant thermodynamic efficiency	19.5 / 0.649
K-effective of the Reactor / Reactivity in the Reactor (mk)	1.066541 / 62.389
Ful density (g/cm^3) / Cladding Material	10.36 / SiC
Temperature at the Fuel Rod Axis (°C): Max / Average	1499 / 1178.5
Temperature of He (°C): Outlet / Inlet	1140.4 / 400
Temp. Drop Fuel-Clad (°C) Max / Average	38.12 / 23.5
Percentage of SiC in the fuel(%)	20

4. Discussion

Going back to the base case for the MOX fuel, where the outlet temperature of the coolant is nearly 850 °C, we can see that the efficiency of the thermodynamic cycle of the coolant (ETCC) is about 52.9%, a good and high value for the ETCC. The required flow rate of the coolant for this case is 32.1 kg/s, and the maximum temperature drop on the fuel (MTDF) is about 312 °C.

These data are relative to the MOX fuel with a SiC clad. It is important to note that the temperature on the fuel-rod axis (TFA) is about 1385 °C, a high temperature compared with some European criteria for the fuel-rod axis temperature (1140 °C [12]).

When the inlet and outlet temperatures of the coolant are fixed, the maximum temperature on the fuel-rod axis (MTFA) is about 1119.3 °C for the case of the NFs and approximately 1112.3 °C for the case of the CFs (see Tables 5 and 6). As stated earlier, with a coolant flow rate of 32.1 kg/s, the average temperature drop on the fuel is approximately 188.3 °C for the MOX, compared to about 35.38 °C for the MOX mixed with 20% molybdenum (Table 4), yielding a gain of approximately 152.92 °C. This gain can be utilized to raise the helium output temperature (T_{out}). However, the tradeoff is an increase in the plutonium content of the fuel, which rises to 26.84% from 20.35%. Figure 3 compares the temperature drops on the fuel for the four cases discussed. While there is a significant difference in the temperature drop on the fuel between the case of MOX and the other three cases, the differences among CFs, NFs, and MOX mixed with 20% Mo are minimal.

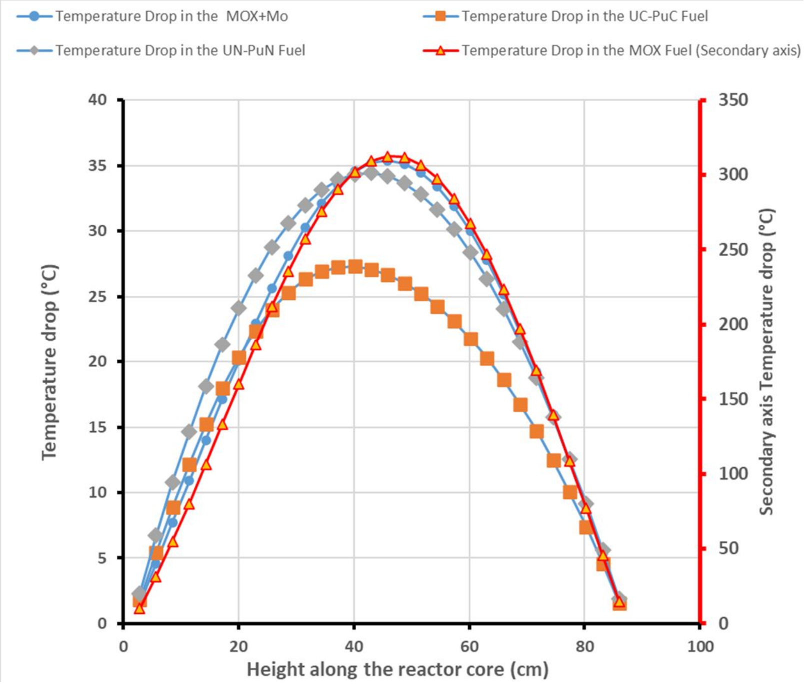

Fig. 3. Comparison of the temperature drops on the fuel for the four fuel types: MOX, MOX with 20% MO, CFs, and NFs in the ALLEGRO reactor.

As seen from Table 3, fixing the outlet temperature at 850 °C results in a fuel-axis maximum temperature less than the permitted 1140 °C criterion for the fuel center temperature. This suggests that fixing the fuel-axis temperature instead could yield a coolant cycle efficiency of 53.7%, compared to 52.9% as shown in Table 7, with minimal changes to both the MTDF and ATDF.

A further increase in the ETCC is achievable with SiC cladding by raising the TFA to approximately 1499 °C, which would result in a new ETCC of nearly 64.9%. At this point, the MTDF and ATDF remain at manageable values of 38.12 °C and 23.5 °C, respectively. With these conditions, the T_{out} could reach 1140.4 °C, enabling highly advanced applications of Gen IV reactors.

The molybdenum content in the fuel can also be further increased to achieve thermal conductivity surpassing that of both carbide and nitride fuels.

5. Conclusion

The MOX fuel mixed with 20% molybdenum is a good candidate for use in Gen IV nuclear reactors, competing with both carbide and nitride fuels. Furthermore, its performance can be enhanced by increasing the molybdenum content. Although this would result in a higher plutonium content in the final MOX (exceeding 26.84%), it would enable a significantly higher outlet temperature for the coolant, opening up opportunities for advanced applications of Gen IV reactors.

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