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Computational model for thermohydraulic analysis of an integral pressurized water reactor with mixed oxide fuel (Th, Pu)O_2

Mariana Cecilia Betancourt[1,2], Pedro E. Moraes Santos[2], Leorlen Y. Rojas Mazaira[2], Carlos R. García Hernandez[1], Dany S. Dominguez[3], Carlos A. Brayner[4] and Jesús A. Rosales García[1]

[1] *mariana.cbetancourt@gmail.com*

[1] *Instituto Superior de Tecnologías y Ciencias Aplicadas (InSTEC), Universidad de La Habana, Ave. Salvador Allende No. 1110, Quinta de los Molinos, La Habana, 10400, Cuba*

[2] *Departamento de Energia Nuclear – Universidade Federal de Pernambuco, Ave. Prof. Luiz Freire, 1000. Cid. Universitária, CEP 50740-540, Recife, PE, Brasil*

[3] *Universidade Estadual de Santa Cruz, Campus Soane Nazaré de Andrade, Rodovia Jorge Amado, Km 16, Bairro Salobrinho CEP 45662-900, Ilhéus, BA, Brasil*

[4] *Centro Regional de Ciências Nucleares do Nordeste – CRCN-NE, Avenida Professor Luiz Freire, 200, 50740-535, Recife, PE, Brazil*

ABSTRACT

The use of advanced generation III+ and IV nuclear reactors, and their applications, has become important, seen as a means capable of contributing to the global transition to more sustainable, affordable and reliable energy systems. This technology, which could be integrated into future carbon-free electric power generation systems with high proportions of different renewable energy sources, includes Small Modular Reactors (SMR). There are about 100 different proposed projects of Generation III+ and IV, of which about 50 are SMR concepts, in various stages of development and of different types of technologies. Other important

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issues for achieving the long-term sustainability of nuclear energy are the proper use of its fuel sources and the improvement of nuclear waste management. Therefore, fuels based on a mixture of oxides have been used successfully in several countries. In addition, the incorporation of thorium-based fuel is a current challenge for the new designs of advanced reactors. The present paper focuses on the analysis of a small modular integral pressurized water reactor (iPWR) with Thorium-Plutonium Oxide (Th-Pu MOX) mixtures. A thermohydraulic model is developed using the Ansys CFX program, which allows the calculation of the temperature distribution in the section where the highest power is produced within the SMR IPWR core (critical section). The temperature distributions in the fuel, clad and coolant were calculated with the objective of verifying that they were within the safety limits.

Keywords: SMR, MOX, CFD

1. INTRODUCTION

The use of nuclear energy has been one of the best alternatives to supply electricity on a large scale and reduce carbon dioxide emissions into the atmosphere. Its contribution to climate change mitigation has been important in preventing the annual emission of around 2 billion tons of carbon dioxide. Current reserves are large enough to guarantee nuclear fuel production for decades. On the other hand, some challenges emerged, such as the storage or disposal of long-lived radioactive waste and the nonproliferation of nuclear weapons.

The nuclear reactor type with the greatest global impact throughout history and with the most ambitious development plans is the Pressurized Water Reactor (PWR). The use of advanced generation III+ and IV nuclear reactors, and their applications, has become important, seen as a means capable of contributing to the global transition to more sustainable, accessible, and reliable energy systems. This technology, which could be integrated into future carbon-free electricity generation systems and with high proportions of different renewable energy sources, includes small modular reactors (SMR) [1].

According to the IAEA, Small Nuclear Reactors are those nuclear reactors with electrical power less than 300 MW(e). The term "modular" in the context of SMR refers to a single reactor or module that can be grouped with other modules to form a larger nuclear power plant. A module is defined as a reactor and a steam supply system. Each module is independent and can be turned off without affecting other modules [2].

From the earliest times of nuclear energy development, thorium has been considered a potential fuel that could complement or even replace natural uranium. In recent years, the proliferation resistance necessity, longer fuel cycles, increased burning, reduced plutonium stores, and in situ use of replicated fissile material have led to renewed interest in thorium-based fuel cycles. The thorium fuel cycle is an attractive way to produce long-term nuclear energy with low radioactive waste. In addition, the transition to thorium could be accomplished by incinerating weapons-grade plutonium (WPu) or civilian plutonium. ThO_2 has favorable thermophysical properties due to its higher thermal conductivity and lower coefficient of thermal expansion compared to UO_2. Therefore, fuels based on ThO_2 are expected to perform better than mixed oxides based on UO_2. Th-based fuel cycles have intrinsic resistance to proliferation due to the formation of 232U through reactions (n,2n) with 232Th, 233Pa and 233U, by the following likely reactions in Equations (1), (2) and (3). From the same consideration, 232U could be used as an attractive carrier for highly enriched uranium (HEU) and weapons-grade plutonium (WPu) to prevent their proliferation for non-peaceful purposes [3]–[5].

$$^{232}\mathrm{Th} \xrightarrow{(\mathrm{n},\gamma)} {}^{233}\mathrm{Th} \xrightarrow{(\beta-)} {}^{233}\mathrm{Pa} \xrightarrow{(\beta-)} {}^{233}\mathrm{U} \xrightarrow{(\mathrm{n},2\mathrm{n})} {}^{232}\mathrm{U} \quad (1)$$

$$^{232}\mathrm{Th} \xrightarrow{(\mathrm{n},\gamma)} {}^{233}\mathrm{Th} \xrightarrow{(\beta-)} {}^{233}\mathrm{Pa} \xrightarrow{(\mathrm{n},2\mathrm{n})} {}^{232}\mathrm{Pa} \xrightarrow{(\beta-)} {}^{232}\mathrm{U} \quad (2)$$

$$^{232}\mathrm{Th} \xrightarrow{(\mathrm{n},2\mathrm{n})} {}^{231}\mathrm{Th} \xrightarrow{(\beta-)} {}^{231}\mathrm{Pa} \xrightarrow{(\mathrm{n},\gamma)} {}^{232}\mathrm{Pa} \xrightarrow{(\beta-)} {}^{232}\mathrm{U} \quad (3)$$

This paper focuses on the analysis of a small modular reactor (SMR) and integral pressurized water reactor (iPWR) type using thorium-plutonium oxide (Th-Pu MOX) fuel mixtures. The main objective is to develop a computational model of the critical section of the core, where the greatest power is produced, that allows the calculation of the most important thermohydraulic parameters. Using the developed model, the temperature and power profiles released in the hottest channel, and the temperature and density profiles of the water in the cooling zone were calculated.

2. MATERIALS AND METHODS

2.1. Core size and configuration

The conceptual design of the reactor core analyzed was based on the characteristics of the iPWR-type SMR, which has a nominal power of 180 MW (e) per module [6]. The reactor core consists of 69 fuel assemblies standard Westinghouse Company, loaded into a 21.5 cm square lattice pitch, which has a mirror-symmetrical configuration octant. Each fuel assemblies contain 264 fuel rods, 24 guide tubes for control rods and an instrumentation tube in the center [2], [7]. In [6], a feasibility assessment of the use of MOX (Th,Pu)O_2 mixtures in the core of an iPWR was studied, considering the core partially loaded with MOX fuel, to ensure an extended cycle of 48 months. One-third of the core (24 fuel assemblies) has been loaded with MOX fuel, while the rest has UO_2 fuel (*Figure 1*). Plutonium, obtained from the first recycling of an irradiated fuel originally composed of slightly enriched UO_2, is recycled once into a mixture with Thorium, 13.14% PuO_2 and 86.86% ThO_2 (*Table I*). The plutonium vector characteristic of first recycling has a high proportion of fissile isotopes. In this case, the obtained new fissile isotope will be 233U. As no new plutonium is produced, the final plutonium vector will be poorly enriched in fissile fuel.

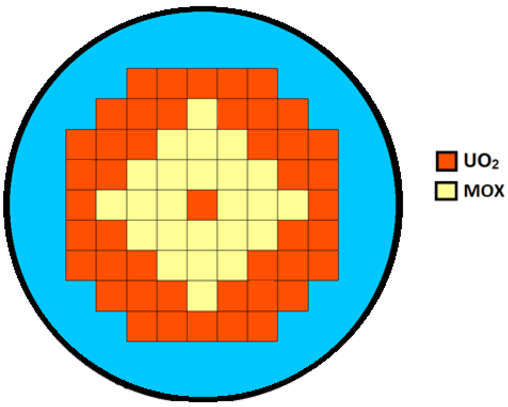
Table I. Composition of MOX fuel assemblies.

MOX (Th,Pu)O_2	
Pu 238	2.7 %
Pu 239	51.05 %
Pu 240	24.22 %
Pu 241	12.80 %
Pu 242	7.30 %
AM 241	1.92 %
Total de Pu	**13.14 %**
U235	**--**
U238	**--**
Total de U	--
Total de Th232	**86.86 %**

Another distinctive feature of the proposed iPWR core design is the non-use of soluble boron in the coolant for global reactivity control. The removal of soluble boron has advantages in terms of design simplification. Not using chemical shim produces a large negative value of the moderator temperature reactivity coefficient, mainly at the beginning of the cycle (BOC), which provides a robust inherent reactivity control mechanism, like a boiling water nuclear reactor [8]. However, controlling the large excess reactivity of the core using only burnable absorbers and control rods is another major challenge for core design. Several studies about mPower fuel cycle design and reactivity management strategies have been published [7]–[10]. The core was designed to achieve a fuel cycle length of 4-year in a one-batch core design. Refueling and shuffling of fuel assemblies are not allowed. This feature gives priority to proliferation resistance [8].

For the neutronic calculations in [6], the probabilistic methods implemented in the SERPENT code (version 2) were used. Simulations are not limited to two-dimensional set geometries and the code can also be used to model any full-core three-dimensional configuration. Serpent code allows you to calculate the axial power distributions in both the fuel assemblies and subchannels, which will be used in the thermohydraulic calculation to obtain the temperature profiles [11]. The core was considered clean of combustible absorbers and without inserted control rods, operating at hot coolant and fuel temperatures, and poisoned by Xe135. Core peak power factors were normalized to full power. Water was considered as the axial and lateral reflector material. For the subchannel axial power distribution calculations, one million stories and 1500 cycles were used; and each fuel element was divided into 100 axial zones of 0.024 m.

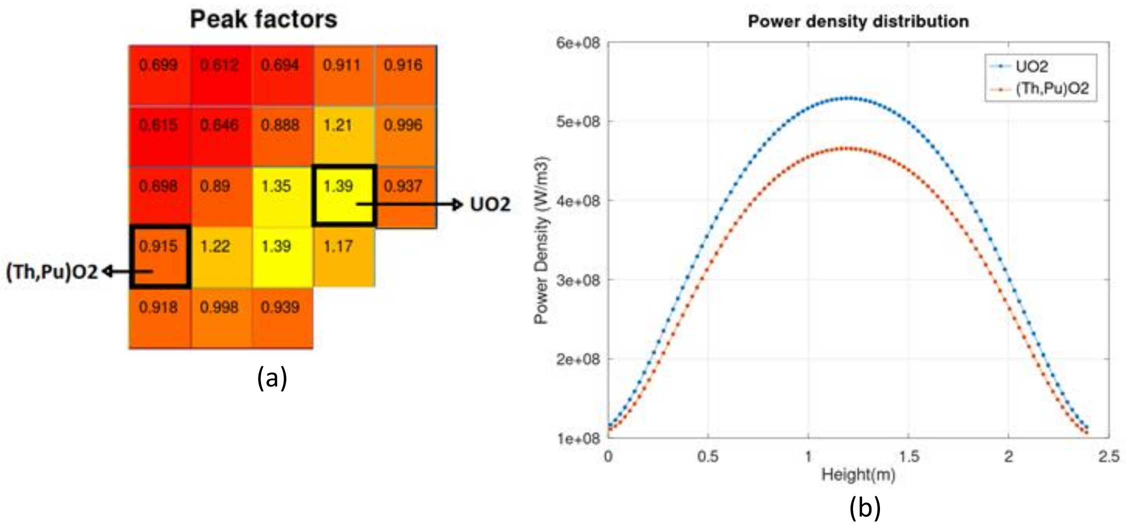
Figure 1. *MOX fuel distribution in the core.*



Source: Author

*Figure 2*a shows the radial distribution of the core peak power factors at quarter symmetry at the beginning of the cycle (BOC). The highest power fuel assembly in the core, with a peak factor of 1.39, corresponds to the position of a UO_2 fuel assembly. Among the assemblies loaded with MOX (Th, Pu)O_2 fuel, the one with the highest power has a peak factor of 0.915 [6]. Since both fuels have different behavior for their thermophysical properties, a thermohydraulic study of the subchannel that generates more power in the core was carried out (corresponds to fuel UO_2), and a study of the subchannel that generates more power for assemblies with fuel MOX (Th, Pu)O_2. *Figure 2*b shows axial power density distribution calculated by Serpent code for the subchannels to be analyzed.

Figure 2. *The radial distribution of the core peak power factors at quarter symmetry and axial power density distribution at the beginning of the cycle (BOC)*



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2.2. Description of the computational model for the thermohydraulic analysis

One of the thermohydraulic design limits of the fuel is that the temperature reached cannot exceed its melting point. The maximum temperature that is reached in the fuel depends on the thermal conductivity and the linear power density in the fuel rods. Reactor coolant pressure is maintained by an electrically heated pressurizer located above the steam generator, providing stable operation and pressure response during all operating conditions. Reactor bulk coolant temperature must be kept below the saturation point so that there is no boiling in the core; this results in a subcooling of approximately 32 K at the core outlet. The core power density of the B&W mPower reactor is approximately 65 kW/liter, significantly lower than the power density of a large PWR [8]. *Table II* shows the main thermohydraulic parameters used in the model to carry out the thermohydraulic study of the hottest section of the core. The thermohydraulic calculations were performed with Ansys CFX.

Table II. Thermohydraulic parameters.

Parameter	Value
Thermal Power	530 MW
Pressure	14.8 MPa
Inlet temperature	290 ºC
Outlet temperature	318.8 ºC
Core mass flow	3345 kg/s

The use of CFD techniques has been a reliable alternative to predict thermohydraulic behavior in nuclear reactors. A distinctive feature of CFD simulations is the approach it takes to the description of physical processes, as it uses a spatial distribution of them, allowing the capture of local phenomena, which are of vital importance for the design and safety of nuclear reactors. The thermohydraulic calculations for this work were performed with the Ansys CFX program. Ansys CFX is a general-purpose CFD code that is part of Ansys' suite of applications focused on analyzing engineering simulation problems. The program is composed of four modules that, from the input of a geometry and a mesh, allow a CFD simulation to be carried out: the pre-processing and post-processing modules (Ansys CFX-Pre and Ansys CFD-Post, respectively) [12]. For the construction of the geometry and mesh, two other applications integrated with Ansys CFX 2020.R1 are used, Ansys Designer Modeler and Ansys Meshing.

To verify that the fuel meets the thermal limits, it is necessary to analyze the fuel assembly with the greatest power. Taking advantage of symmetry conditions to simplify calculations and optimize available computational resources, the hottest subchannel of the highest power fuel assemblies was simulated. The dimensions of the subchannel designed by Westinghouse were taken from [13], considering an active length of 240 cm.

The mesh type and the number of elements used to discretize the space depends on the geometry and the required precision of the solution. In the present study, a structured mesh was used to adapt to the channel geometry. The geometry was decomposed into several parts to obtain a more structured mesh and optimize the computational resources used. In the vicinity of the walls, mesh refinement is performed to ensure that the velocity and temperature gradients are correctly resolved. To verify the independence of the solution with the mesh, a study with several configurations was carried out. With a mesh of 3 876 000 elements and 4 202 801 nodes, a mesh-independent solution is reached. *Figure 3* and *4* shows the cross-section of the subchannel. The mesh is generated by the multizone method, which is based on the interlacing of independent zones, providing an automatic decomposition of the geometry into scan regions and free regions.

Figure 3. *Superior view of the fuel subchannel geometry and mesh used in the domain discretization.*

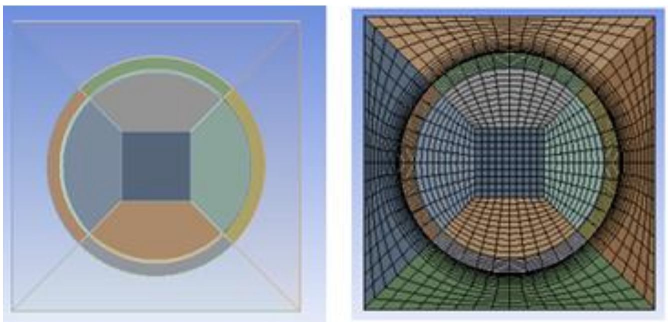

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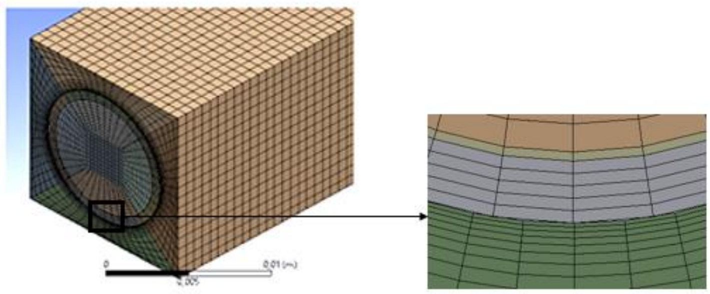
Figure 4. *Fuel subchannel mesh used.*



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To verify the quality of the mesh, an evaluation is performed using the quality indicators Skewness, Aspect Ratio and Orthogonal Quality. The Skewness parameter, which determines how close a face or cell is to the ideal, that is, equilateral or equiangular, with 0 being ideal (optimal) and 1 being completely degenerate (worst), for the present work, a maximum value of 0.5. The Aspect Ratio parameter is the ratio of the longest edge length to the shortest edge length. Must be equal to 1 for an ideal mesh; in the study, 28.66 was obtained for the maximum. Another parameter evaluated was the Orthogonal Quality, which involves the angle between the vector joining two mesh nodes (or control volume) and the normal vector for each surface of integration point (n) associated with that edge. For this parameter, 1 is considered an optimal value and 0 a bad value, resulting in a value of 0.632 for the minimum. The mesh obtained for the modeling performed meets the requirements of the quality indicators, guaranteeing the reliability of the results.

The material properties of water taken according to the International Association for the Properties of Water, from the library of materials provided by CFX, IAPWS-IF97, which is a formulation of water and properties of steam prepared for industrial uses, where the formulations must be designed for fast and complex calculations. This state equation is valid between 1 and 1000 bar and between 0°C and 800°C. The advantage of using IAPWS-IF97 is that the dependence of material properties on both pressure and temperature can be taken into account simultaneously [14].

The three-dimensional flow field under single-phase flow conditions in the subchannel has been evaluated using the standard k-epsilon turbulent model. Since the 1970s, the most widely used turbulence models for high Reynolds number flow are the models of two equations of the k-ε type. These models close the RANS (Reynolds Averaged Navier-Stokes) system of equations that governs the mean flow by approximating the effect of turbulence using a turbulent viscosity, which varies with position and with time as a function of the kinetic energy and its dissipation rate ε [15].

2.3. Thermophysical properties of (Th, Pu)O_2

The specific heat (Cp_{ThO_2}) of $(Th_{1-y}Pu_y)O_2$ mixed solid solutions was calculated from the literature values of specific heats of ThO_2 (Cp_{ThO_2}) and PuO_2 (Cp_{PuO_2}). The following equations were used to calculate the Cp_{ThO_2} [16].

$$Cp_{(\mathrm{Th}_{1-y}\mathrm{Pu}_y)\mathrm{O}_2} = (1-y)Cp_{ThO_2} + yCp_{PuO_2} \tag{4}$$

$$Cp_{ThO_2} = 55.9620 + 51.2579 * 10^{-3}T - 36.8022 * 10^{-6}T^2 + 9.22452 * 10^{-9} * T^3 - 5.7403 * 10^5 T^{-2} \tag{5}$$

$$Cp_{PuO_2} = \frac{347{,}4 * 571^2 e^{\left(571/T\right)}}{T^2\left[e^{\left(571/T\right)} - 1\right]^2} + 3.95 * 10^{-4} T + \frac{3.860 * 10^7 * 1.967 * 10^5}{RT^2} e^{\left(-1.965 * 10^5/RT\right)} \qquad (6)$$

Where T is the temperature and $R = \sqrt{0.965}$.

Thermal conductivity assessment for $(Th,Pu)O_2$ mixed solid solutions were provided by the Division of Radiometallurgy, Bhabha Atomic Research Center, Mumbai, India. The best-fit equation for thermal conductivity of $(Th_{1-y}Pu_y)O_2$ of 95% theoretical density as a function of composition (y) and temperature (T) was derived (Equation 7), which is valid from 873 to 1873K [16].

$$\lambda_{95}(W/mK) = \frac{1}{-0.08388 + 1.7378y + (2.62524 \cdot 10^{-4} + 1.7405 \cdot 10^{-7} y)T} \qquad (7)$$

3. RESULTS AND DISCUSSION

With the axial distributions of the power density calculated by the SERPENT code, the thermohydraulic study of the subchannels was carried out. The present study was made at the beginning of the cycle (BOC), that is, with fresh fuel. As a first result, it was possible to obtain the distribution of the coolant temperature at the outlet. It is observed that the highest temperature is obtained in the area close to the cladding, where heat transfer from the cladding to the water occurs. The water temperature has a variation in this section of 587.07-594.84 K for the MOX fuel subchannel, and a variation in this section of 590.978-598.56 K for the UO_2 subchannel.

In *Figure 5* the axial water temperature in the wall and the axial temperature at the center of the fuel for both subchannels are shown. The maximum water temperature reached is 610.326 K for MOX (Th, Pu)O_2 and 613.3 K for UO_2, lower than the saturation temperature (614.23 K) for the refrigerant pressure. The maximum fuel temperature reached is 1622.24 K for the MOX (Th, Pu)O_2 fuel, well below the melting point (3651 K), and 1544.54 K for the UO_2 fuel, below the melting point (3120 K).

Figure 5. *Axial water temperature in the casing wall and the axial temperature at the center of the fuel for both subchannels.*

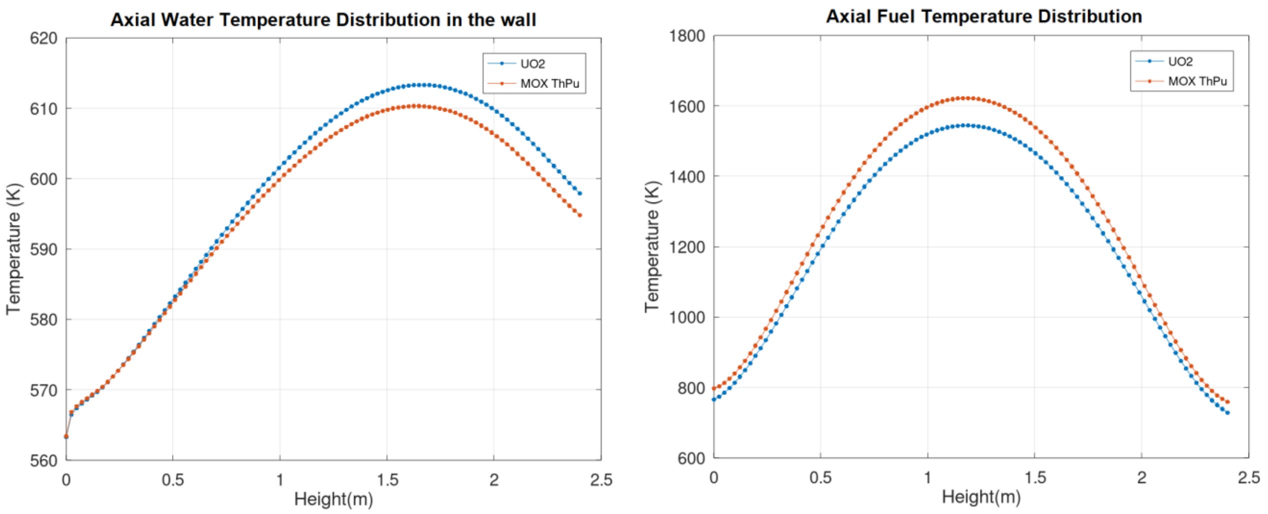
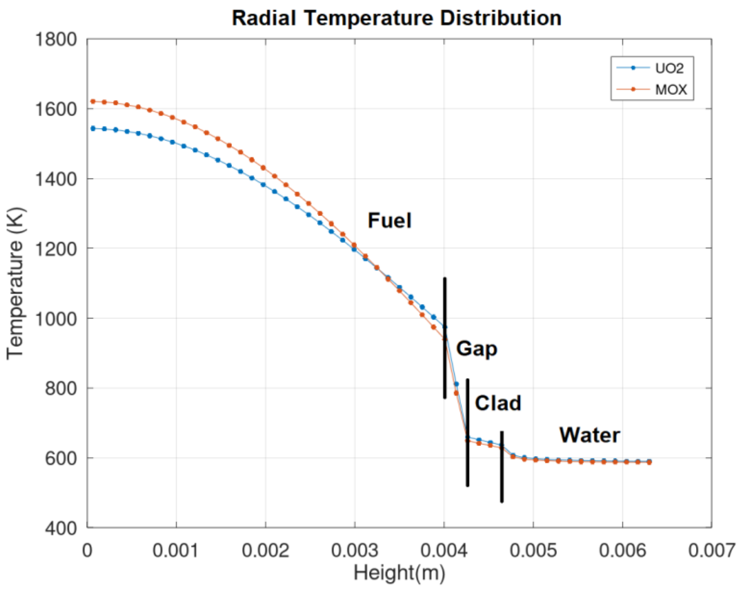


Figure 6 shows the temperature radial distribution. There is a sharp drop in temperature as the radius of the fuel element increases, especially in the gap area (helium). The maximum temperature found in the cladding was 655.83 K for MOX (Th, Pu)O_2 and 667,024 K for UO_2, well below 1477.59 K, reported as a limit value for the accident regime.

Figure 6. *Radial temperature distribution.*



4. CONCLUSION

A three-dimensional model was developed and implemented using the Computational Fluid Dynamics code to evaluate the thermohydraulic behavior of a critical SMR reactor fuel assembly using a mixture of uranium and thorium oxides (Th, Pu)O_2. The axial power distribution was obtained in the critical subchannel of the reactor core, and in the highest power subchannel using MOX fuel, for neutronic calculation was used the Serpent code. The temperature profiles in the subchannels were calculated. It was observed that the MOX fuel reaches a maximum temperature of 1622.24 K being below the melting point (3651 K), while the UO_2 fuel has a maximum temperature of 1544.54 K for the UO_2 fuel, below the melting point (3120 K). The maximum temperature reached by the cladding was also evaluated and a value of approximately 655.83 K and 667,024 K was obtained for MOX (Th, Pu)O_2 and UO_2, respectively, showing a good result against the value of 1477.59 K, reported as a threshold value for accident regime.

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