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Analysis of Optimum Accident Tolerant Fuel and Cladding Behavior in Advanced Pressurized Water Reactor

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ABSTRACT

In PWR reactors, a higher temperature than the normal operation rate causes an increase in the oxidation rate between the fuel and the clad (UO_2 / Zircaloy), and this results in the release of large quantities of hydrogen, which leads to an increase in pressure and temperature inside the reactor core and also on the walls of the pressure vessel, and perhaps partial or total damage to the reactor core. This research examines the development of new types of fuel such as Uranium Nitride (UN), Uranium Silicate (U_3 Si_2). Also, two types of clads such as Silicon Carbide and (Fe-Cr-Al) alloy are tested. The neutronic and thermal properties of these new types have been studied, as they are characterized by the low probability of fuel interaction with cladding, as well as the presence of good neutronic and thermal properties in terms of thermal conductivity and heat capacity, which lead to an improvement in the safety margin during operation and also in the event of nuclear accidents.

INTRODUCTION

In light of the event that occurred at the Fukushima Daiichi nuclear power plant in March 2011, there has been an increased research efforts into accident tolerant fuel (ATF) and cladding materials [1]. Accident Tolerant materials are defined as those that provide significantly increased response time in the event of an accident while providing improved performance than the standard UO_2/Zircaloy fuel rods during accident and normal operation [2]. One of the most significant issues in the Fukushima Daiichi accident was the oxidation of Zircaloy that lead to a large inventory of Hydrogen within the core.

The Iron Chromium-Aluminum (Fe-Cr-Al) was proposed to be used as a cladding material due to its low oxidation rate. Oxidation rate for FeCrAl are approximately much lower than the oxidation rate of Zircaloy, The Ferritic alloy (Fe-Cr-Al) has low oxidation behavior with water and steam in the range of normal reactor operations and in the case of severe accident conditions. Also it has better thermodynamic, metallurgical and mechanical properties[3,4]. Silicon Carbide (SiC) which is also used in gas cooled fast reactors has antioxidant capability in steam environment. Uranium Nitride (UN) fuel has higher thermal conductivity and higher content of fissile isotopes than UO_2 which implies economic and long fuel cycle. U_3Si_2 has a number of advantageous thermophysical properties, including; high density

(11.3 gU/cm^3), high thermal conductivity at room temperature (15 W/mK). These properties also support its use as an accident tolerant fuel. Because of its high thermal conductivity, U_3Si_2 operates at a much lower temperature and experiences lower thermal gradients than UO_2. As a result, it is subject to lower thermal stresses, which should mitigate pellet cracking, [5,6, 7, 9].

The motivation for transitioning away from zirconium-based fuel cladding in light water reactors to significantly more oxidation-resistant materials thereby enhances safety margins during severe accidents. In this study, the neutronic and thermal properties of Fe-Cr-Al

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and Silicon Carbide alloys are analyzed and compared with Zircaloy. Also, two types of fuel namely, Uranium nitride (UN) and Uranium silicide (U_3Si_2) are investigated and compared with the traditional UO_2 fuel.

Gamble K. A. [1] Studied U_3Si_2 fuel and FeCrAl clad under normal and accident conditions both thermophysical and oxidation behavior are analysed. Brown N. R. [2] Studied the Neutronic analysis of UN (Uranium Nitride) under different porosity and additives to UN such as ZrO_2 , U_3Si_2 , U_3Si_5 , UB_4 . Rahman M. H. [5] Studied microstructure aspects of SiC particles in Aluminum matrix. Metzeger K. E. [8] model the behavior of U_3Si_2 with the available thermophysical data to predict the cladding temperature and swelling using BISON code. Terrani K. A. [10] studied oxidation behavior, microstructure under burnup for coated Zirconium, Ferritic Alumina forming alloy cladding and Silicon Carbide. Qiu B.[11] reviewed on thermohydraulic and mechanical physical properties of SiC , FeCrAl , and Ti_3SiC_2 as Accident Tolerant Fuel cladding. In the present Study three types of fuel UO_2, UN and U_3Si_2 in addition to three types of cladding Zr- alloy, SiC and FeCrAl are investigated as an Accident Tolerant fuel (ATF) and cladding from neutronic and thermalhydraulic point of view. K_{eff} , cycle length and discharge burnup are used as neutronic indicator while thermal conductivity (k) and thermal capacity (Cp) is used as thermal indicator.

MATHEMATICAL AND COMPUTATIONAL MODEL

In the following section, both neutronic and thermodynamic models are established to study the neutronic and thermal properties of different clad and fuel types. The behavior of thermal conductivity and heat capacity with temperature are considered as an indicator of the thermal properties of the clad and fuel materials.

Neutronic Model

MCNPX code, [12], has been used to design a computer model for an assembly of advanced PWR reactor. The assembly is 17 x17 fuel rods. It contains 264 fuel rods and 24 positions for burnable poison or control rod and one central position for instrumentation [13]. The horizontal and vertical layout of the model is illustrated in Figure 1. The outer dimension is 21.4 x21.4 cm. The fuel rod pitch is 1.264 cm. fuel rod radius is 0.4096 cm, outer clad radius is 0.475 cm and a thin layer of Helium between fuel and clad with thickness of 0.0083 cm. Figure 2 illustrates the model of the fuel, clad and coolant. Three types of clads are tested, Zircaloy-4 (Zr), silicon Carbide (SiC) and Ferritic steel alloy (Fe-Cr-Al) with density 6.6 g/cm^3, 3.21 g/cm^3, and 7.15 g/cm^3, respectively. The ratio between isotopes in Ferretic steel is 74:21:5, respectively, [9].

Three types of fuel are also considered in the analysis namely, UO_2, UN, and U_3Si_2 with fixed enrichment 4.95 %. The assembly is burned in a typical operating conditions in pressure and temperature for PWR reactor. High fuel burnup with sixteen time steps up to the multiplication factor approach one is allowed for each case. The power assigned to the assembly during burnup is 20 MW. Reflective boundary conditions are considered for all peripheral boundaries and 50 cm of water is considered on the top and bottom of the assembly. ENDF-VI is the neutron cross section library for the materials in the model. Table 1 illustrates the density of clad and fuel used in the paper and Table 2 illustrates Chemical composition of Zr-4.

Table (1): Clad and Fuel density

Clad and Fuel type	Zr-4	SiC	FeCrAl	UO_2	U_3Si_2	UN
Density (g/cm^3)	6.6	3.21	7.15	10.2	11.56	13.5

Table (2): Chemical Composition of Zr-4

Isotope	Zr	Sn	Fe	Cr	O
Weight fraction %	98.43	1.2	0.18	0.07	0.12

Several neutronic parameters such as cycle length, discharge burnup and breeding capability are compared for all of the three fuel types. Also thermal properties parameters such as heat capacity (Cp) and thermal conductivity (k) are examined. For cladding material, three cases for Zr, SiC and Fe-Cr-Al, assuming UO_2 fuel in all cases, are compared to analyze the accident tolerant cladding materials.

Thermodynamic Model

Thermal conductivity (k) and heat capacity (Cp) are the key parameters for thermal properties. A higher thermal conductivity results in a lower fuel rod temperature and smaller temperature gradient. The following formula are used to study the behavior of both k and Cp over the entire range of normal and accident conditions in the PWR reactor.

U_3 Si_2 Fuel

Thermal conductivity and heat capacity of U_3Si_2 fuel are computed using temperature dependent empirical relations which are given in reference [8].

$$k\left(\frac{w}{k.m}\right) = 7.98 + 0.0051 \times (T - 273.15) \quad \textbf{(1)}$$

Where, T is temperature in K. This expression is valid for temperatures from room temperature to 1473.15 K. A relationship for the specific heat Cp (J/kg.K) of U_3Si_2 was derived in [8] as,

$$Cp(\text{J/kg.K}) = 199.0 + 0.104 \times (T - 273.15) \quad \textbf{(2)}$$

Where, T is temperature in ^{o}K.

UN Fuel

First, the thermal conductivity for 100% dense UN fuel is calculated from [15], using the following equation:

$$k\left(\frac{w}{k.m}\right) = 1.37T^{0.41} \quad \textbf{(3)}$$

For Heat Capacity, Cp, the correlation used in the current analysis is given by [15] as,

$$Cp = 0.2029\left(\frac{\theta}{T}\right)^2 . \frac{exp\left(\frac{\theta}{T}\right)}{\left(exp\left(\frac{\theta}{T}\right)-1\right)^2} + 3.766x10^{-5}\,T + \frac{1.048x10^{9}}{T^2} . exp\left(-\frac{18081}{T}\right) \quad \textbf{(4)}$$

Where, Cp (KJ/mole.k) and $\theta = 365.7 \quad K$

FeCrAl Alloy

The thermal conductivity of FeCrAl Alloy is given by [11], where T is temperature in (K)

$$k\left(\frac{w}{k.m}\right) = 3.72 + 0.042T - 7.2x10^{-6}\,T^2 + 1.56573x10^{-9}\,T^3 \quad \textbf{(5)}$$

The heat capacity, Cp (J/kg.k), is also given by:

$$Cp(\text{J/kg.k}), = -211.55 + 3.7854T - 6.227x10^{-3}\,T^2 + 3.63774x10^{-6}\,T^3, if\ T \le 854\,K \quad \textbf{(6)}$$

$$Cp = 2113.39 - 2.543T + 1.12x10^{-3}T^2,\ if\ 854\,K < T \le 991\,K \quad \textbf{(7)}$$

$$Cp = 208.78 + T - 6.86x10^{-4}\,T^2 + 1.7173x10^{-7}T^3,\ if\ 991\,K < T \le 1776\,K \quad \textbf{(8)}$$

SiC Alloy

The thermal conductivity is given by:

$$k = 1.2 + 0.002\,T + 0.62x10^{-4}T^2\ (\text{W/m. C}) \quad \textbf{(9)}$$

And, the heat capacity (J/Kg.K) is given by :

$$Cp(\text{J/Kg. K}) = 0.925.65 + 0.3772\,T - 7.9259x10^{-5}\,T^2 - \frac{3.1946x10^{7}}{T^2} \quad \textbf{(10)}$$

The thermal conductivities and heat capacities for the traditional UO_2 and Zircaloy are extracted from reference [14, 15], respectively.

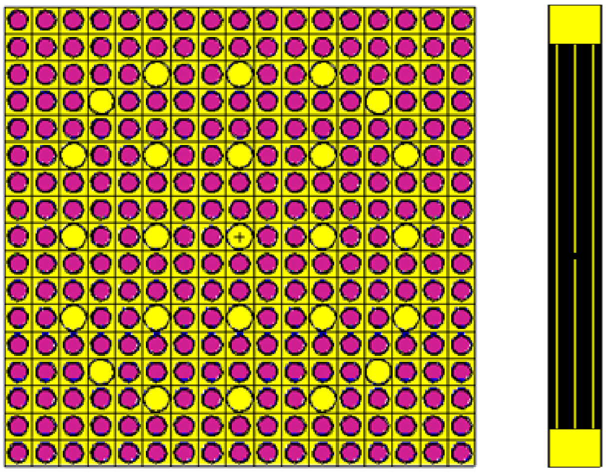

Fig. (1): Horizontal and vertical Layout of MCNPX model

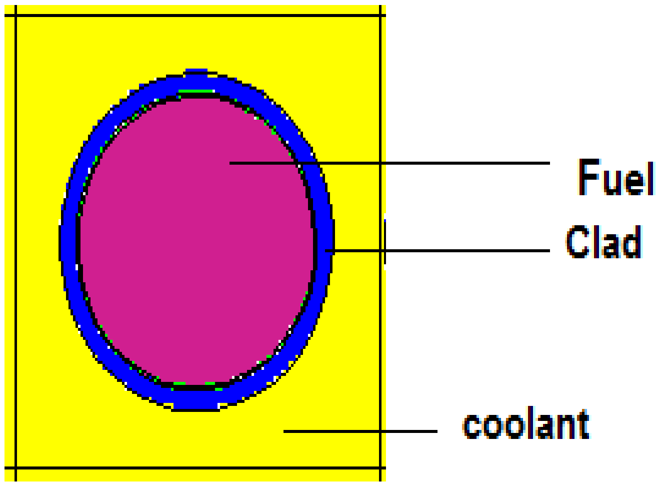

Fig. (2): MCNPX computer model for the Fuel rod

RESULTS AND DISCUSSIONS

Figure 3 illustrates the multiplication factor for an assembly with 3 different cladding materials and UO_2 fuel. The results show that K_{inf} is higher in the case of SiC clad over the entire operation time up to 1000 days. Table 3 shows the value of K_{inf} at initial time (t=0.0). The ferretic steel alloy (FeCrAl) shows significant reduction in the value of K_{inf} because absorption cross section for iron and Chromium are 2.53 and 3.1 barns respectively, [16], in comparisons with those of silicon and Zirconium of 2.33 and 0.18 barns, respectively.

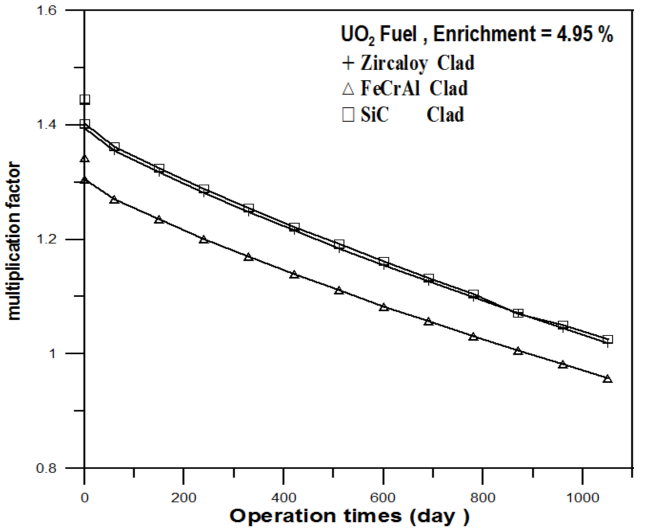

Fig. (3): Variation of K_{inf} versus operation time (day) for different cladding Materials

Table (3): Multiplication factor for composition of UO_2 Fuel and 3 different types of Cladding

Clad	Zircaloy-4	SiC	FeCrAl
K_{inf}	1.43621±0.00063	1.4450±0.00076	1.34309±0.00054

Figure 4 illustrates the multiplication factor for the assembly for 3 different fuel types UO_2, UN and U_3Si_2 with Zircaloy clad. UN is higher in K∞ because it has the higher density of 13.5 g/cm^3 as compared to U_3Si_2 and UO_2 which is 11.3 and 10.4 g/cm^3, respectively. Higher density implies higher ^{235}U fissile isotope content and also higher fuel cycle. Uranium fraction in U_3Si_2, UN and UO_2 are 0.962, 0.944 and 0.88, respectively. For this reason, UN and U_3Si_2 have comparable cycle length to each other.

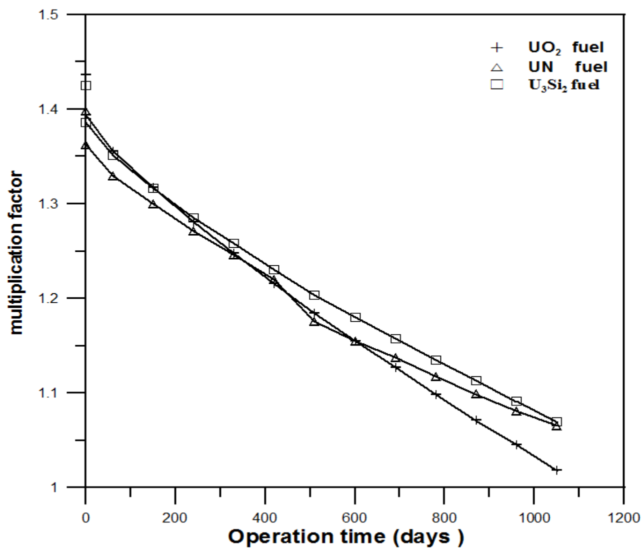

Fig. (4): Variation of K_{inf} versus operation time (day) for different fuel types

Figure 5 illustrates ^{235}U and Pu – fissile isotope in atom/barn.cm versus operation times (days) for UO_2 fuel. An operation time of 1050 days is fixed between all 3 fuel types. For example ^{235}U at initial time and 1050 day is 1.16x10^{-3} and 2.9 x10^{-4} atom/barn.cm. The burnup for ^{235}U during this period is 75 % and the concentration of Pu - fissile approaches to 1.88x10^{-4} atom/barn.cm (Pu-fissile isotopes is the summation of both 239Pu and 241Pu).

Figure 6 illustrates ^{235}U and Pu –fissile isotope in atom/barn.cm versus operation times (days) for UN fuel. At 1050 days of cycle length, ^{235}U concentration at initial time and 1050 day is 1.617x10^{-3} and 6.78 x10^{-4} atom/barn.cm. The burnup for ^{235}U during this period is 58 % and the concentration of Pu- fissile approaches to 2.77x10^{-4} atom/barn.cm.

Figure 7 illustrates ^{235}U and Pu –fissile isotope in atom/barn.cm versus operation times (days) for U_3Si_2 fuel. At 1050 days of cycle length, ^{235}U concentration at initial time and 1050 day is 1.435x10^{-3} and 2.434 x10^{-4} atom/barn.cm. The burnup for ^{235}U during this period is 64 % and the concentration of Pu- fissile approaches to 2.65x10^{-4} atom/barn.cm.

Figures 4, 5 and 6 compare between burnup of ^{235}U and breeding of Pu-fissile isotopes for all three fuel type UO_2, UN and U_3Si_2. The results indicate that UO_2 is the higher fuel burnup 75 % while UN fuel is the higher initial ^{235}U concentration. UN fuel is the higher fuel breeding with Pu-fissile concentration of 2.77 x10^{-4} atom/barn.cm.

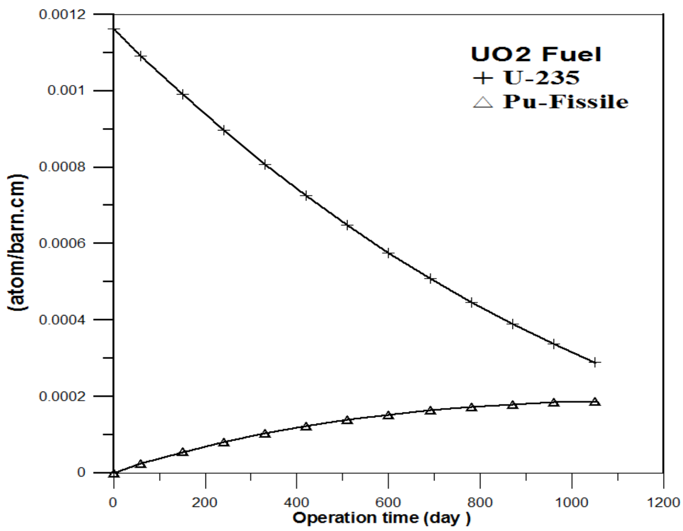

Fig. (5): U-235 and fissile plutonium (atom/barn.cm) versus operation time (days) for UO_2 Fuel

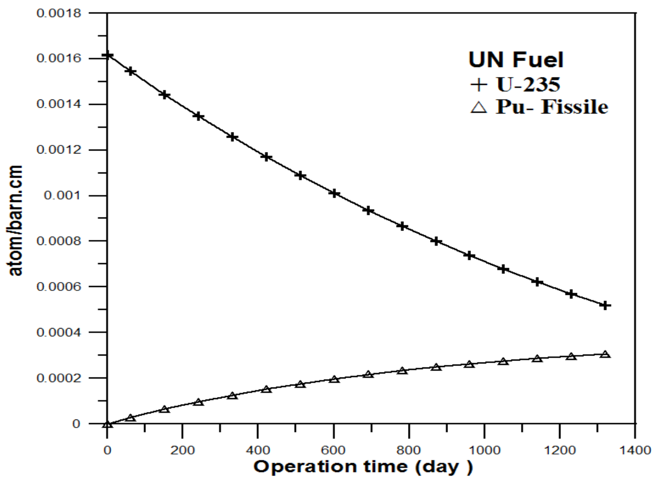

Fig. (6): U-235 and fissile Plutonium (atom/barn.cm) versus operation time (days) for UN Fuel

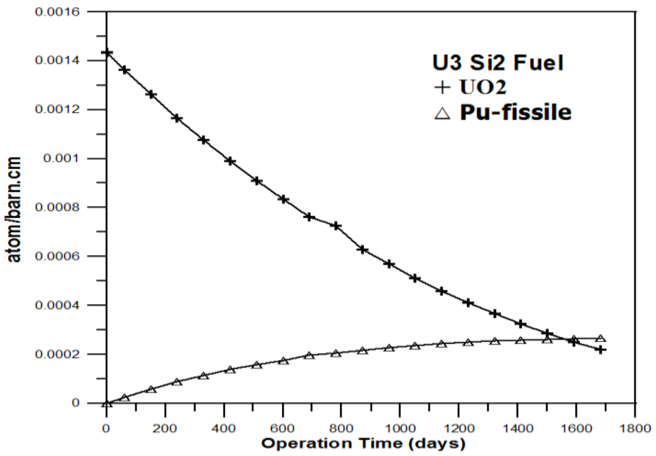

Fig. (7): U-235 and fissile Plutonium (atom/barn.cm) versus operation time (days) for U_3Si_2 Fuel

Figure 8 illustrates the fuel burnup (GWd/T) versus operation time (days) for the three fuel types; i.e., UO_2, UN and U_3Si_2 fuel. The results indicate that UO_2 have highest burnup (GWd/T) and UN is the lowest between the three types.

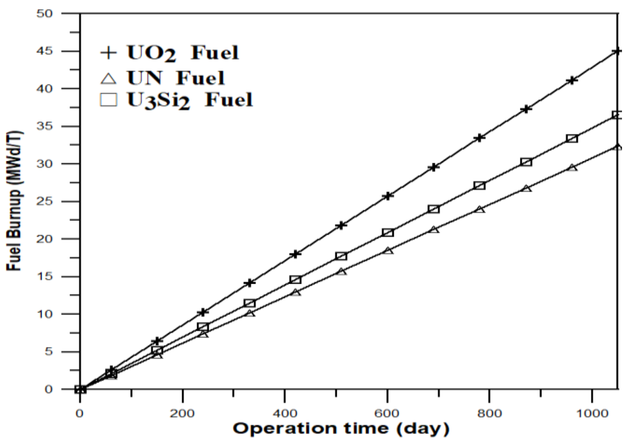

Fig. (8): Fuel burnup (GWd/T)versus operation time (day)

Figure 9 illustrates Thermal Conductivity (W/m. K) versus fuel temperature (K) for typical fuel materials namely UO_2, U_3Si_2 and UN. The results indicate that UO_2 thermal conductivity decreases with increasing temperature, while it increases for both U_3Si_2 and UN. Increasing thermal conductivity with temperature rise during accident conditions reduces the fuel centerline temperature and improves the safety margin of the fuel. UN has the superiority for thermal conductivity.

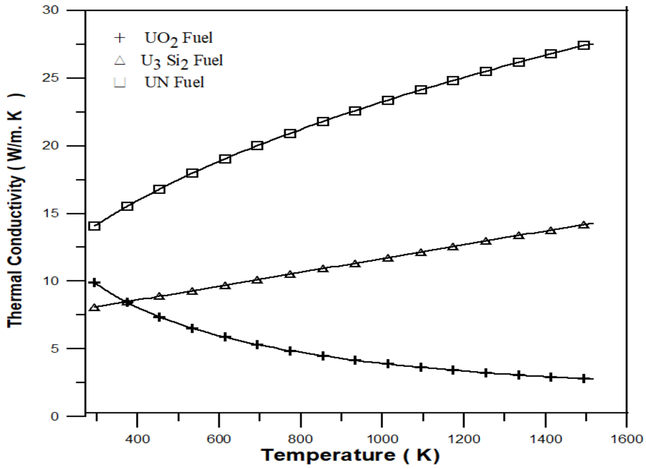

Fig. (9): Thermal Conductivity (W/m. K) versus fuel temperature (K) for different fuels

Figure 10 illustrates thermal conductivity (W/m. K) versus fuel temperature (K) for clad materials namely Zircalloy-4, FeCrAl Alloy and SiC. During normal operating conditions of the reactor (600 K), Zircalloy and FrCrAl alloy have higher thermal conductivities than that of SiC. But, at higher temperatures, thermal conductivity of SiC increases dramatically with temperature to values much higher than thermal conductivities of the other two cladding types.

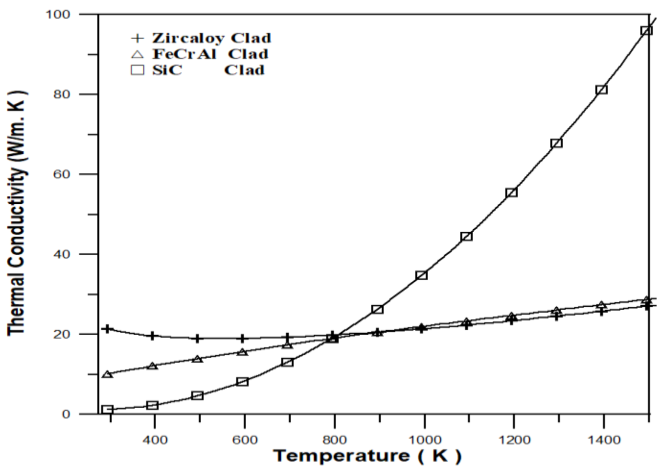

Fig. (10): Thermal Conductivity (W/m. K) versus fuel temperature (K) for different clad materials

Figure 11 illustrates heat capacity (J/Kg. K) for Zircalloy-4, FeCrAl Alloy and SiC cladding materials versus temperature (K). Zircalloy-4 has discontinuity at temperature 1100 K due to phase transition from α phase to β phase [15]. SiC heat capacity is an increasing function of temperature and has the highest values between the three cladding types.

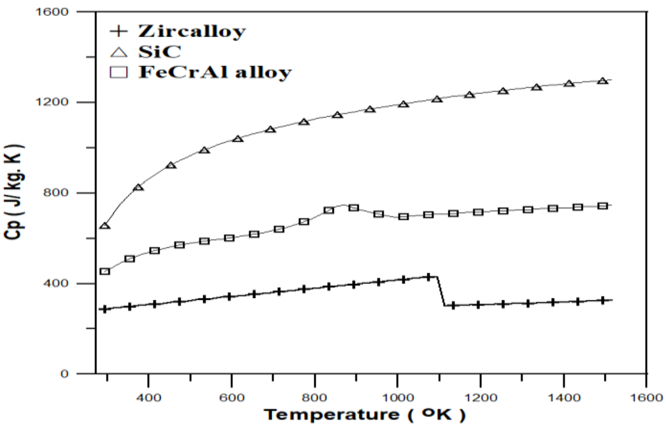

Fig. (11): Heat Capacity (J/Kg.K) for clad materials versus temperature (K)

Figure 12 illustrates heat capacity (J/Kg. K) for fuel materials namely UO_2, U_3Si_2 and UN. The results indicate that Cp for the three fuel types show increasing behavior with temperature. And, UO_2 has the highest values for Cp between them.

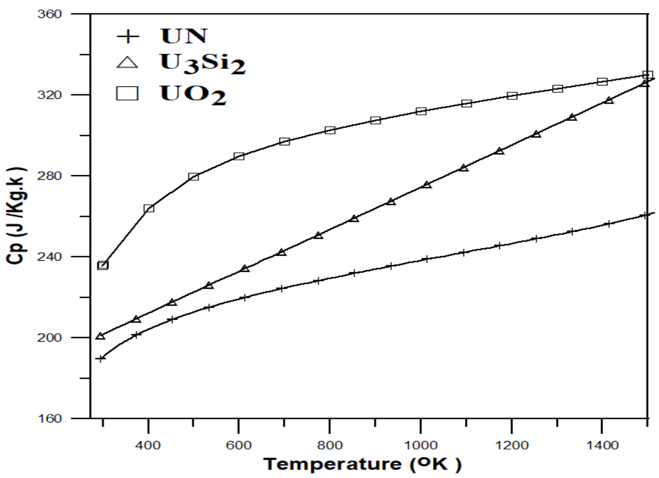

Fig (12): Heat Capacity (J/Kg. K) for fuel materials versus temperature (K)

CONCLUSION

- MCNPX computer code is used to design a computer model for an assembly of advanced PWR design to study the neutronic and thermal properties of three types of cladding Zr, SiC and FeCrAl and also three different types of fuel that are UO_2, UN and U_3Si_2.
- For Cladding materials, the FeCrAl, Ferretic steel alloy, which is an oxidation resistant, has good thermodynamic properties (high thermal conductivity in the temperature range of normal operation and accident conditions) but, has higher neutron absorption (low neutron economy).
- Silicon Carbide, SiC, clad has better thermal and neutron economy.
- UN and U_3Si_2 fuels have higher cycle length than UO_2, and better thermodynamic properties. Higher cycle length implies more economic utilization of the fuel and less nuclear spent fuel.
- UN fuel has the higher ^{235}U initial fissile concentration and more breeding than U_3Si_2 and UO_2 for the same cycle length. Pu-fissile at the end of the cycle for UN, U_3Si_2 and UO_2 are $2.77\text{x}10^{-4}$, $2.65\ \text{x}10^{-4}$ and $1.88\ \text{x}10^{-4}$ atom/barn.cm, respectively.

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