

# **A COMPARATIVE STUDY OF URANIUM AND THORIUM BASED FUEL PINS USING CODE FAIR-TFC**

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## **ABSTRACT**

**A new version of the fuel performance analysis code 'FAIR' is being developed with the capabilities of analysing thorium based fuel pins under normal operating and accidental conditions. Many important thermodynamics properties of the thorium fuel have been incorporated in this code based on the latest literature. A case study has also been shown to compare relative performance between a uranium and a thorium fuel pins.**

## **INTRODUCTION**

**The major part of the nuclear power is generated in reactors, which make use of uranium as fuel, where  $U^{235}$  is the fissile material and  $U^{238}$  is the fertile matrix. From an environmental point of view, the production of transuranium elements through neutron capture in  $U^{238}$  is a major disadvantage of the uranium fuel. Such elements, in particular plutonium, neptunium and americium, contribute significantly to the long term radiotoxicity of the high-level waste. Presently, partitioning and transmutation of the above mentioned transuranium elements is attracting much attention to achieve a considerable reduction of the radiotoxicity of the waste from nuclear power plants.**

**A different approach to this waste problem is the use of thorium based fuel. The reactors operated in a thorium fuel cycle will produce less transuranium elements per unit of fission energy. However, due to the formation of long-lived uranium isotopes ( $U^{233}$ ,  $U^{234}$ ), in significant amount, the alpha toxicity of the waste from thorium fuelled reactors is still above the level of the original ore. Moreover, as natural thorium  $Th^{232}$  is not a fissile nuclide, an external start-up material has to be added to thorium based fuel. This can be  $U^{233}$  (obtained from reprocessing of thorium fuel),  $U^{235}$  or plutonium from reprocessing of LWR fuel.**

The behaviour of nuclear fuel during irradiation is highly dependent on the physicochemical properties of the fuel material. Such properties of the fuel is not constant during the irradiation but change with temperature and burnup. The properties of thorium based fuels have been studied extensively in the past and have often not been published in easily accessible literature. As a part of our programme to develop a code for performance study of thorium based fuel, an extensive literature survey has been carried out to ascertain the thermal properties. Based on this effort, a modified version of the code FAIR is developed called FAIR-TFC. The existing version of this code has been used for a comparative performance study of high burnup uranium and thorium based fuel pins.

## THERMAL PROPERTIES OF ThO<sub>2</sub>

### Thermal Conductivity

Thermal conductivity of ThO<sub>2</sub> up to 1800<sup>0</sup>K is reasonably well established. Most of the data were derived from thermal diffusivity measurements. These data can be represented by the following equation.

$$k = 1 / (A + B T)$$

Here  $k$  (W/cm<sup>0</sup>K) is the thermal conductivity,  $A$  (cm<sup>0</sup>K /W) and  $B$  (cm/W) are the parameters. The parameter  $A$  represents the influence of phonon scattering by lattice imperfections. The parameter  $B$  describes the influence of phonon-phonon scattering.

These parameters have been determined for number of experimental data reported by many authors after correcting for 95% theoretical density. The average of these values have been found to be in close agreement with the values of Murabayashi [1], Bradshaw & Mathews [2], McElroy [3], Koenig [4] and Springer [5]. The average values are as follows [6].

$$A = 0.042 \text{ cm}^0\text{K/W} \quad ; \quad B = 0.0225 \text{ cm /W}$$

These values can be used as recommended values for 95% dense ThO<sub>2</sub> in the temperature range 300<sup>0</sup>K and 1800<sup>0</sup>K. Fig. 1 shows the variation of conductivity of ThO<sub>2</sub> with temperature as obtained by using these parameters in comparison to the conductivity of UO<sub>2</sub> quoted in MATPRO [7].

## Heat Capacity

Heat capacity is primarily used in a fuel performance code 'FAIR' for carrying out transient calculations. By fitting the equation to the values quoted by Southard [8], Hoch & Johnston [9] and Fischer et al. [10], following equation is obtained [6].

$$C_p \text{ (J /Kg}^0\text{K)} = (C_1 T^{-1} + C_2 + C_3 T + C_4 T^2 + C_5 T^3 + C_6 T^4) / (T - 298.15)$$

$$C_1 = 2.1743598 \quad ; \quad C_2 = -77960.985 \quad ; \quad C_3 = 211.97727$$

$$C_4 = 0.09707936 \quad ; \quad C_5 = -4.646742 \times 10^{-5} \quad ; \quad C_6 = 8.73534 \times 10^{-9}$$

T is the temperature in  $^0\text{K}$ . The equation has been found to be valid within the temperature range of  $300^0\text{K}$  to  $3500^0\text{K}$ . Fig. 1 shows the variation of this data with temperature. Same figure also shows the heat capacity data for  $\text{UO}_2$ .

## Melting Point and Heat Capacity of Liquid $\text{ThO}_2$

The melting point of  $\text{ThO}_2$  has been measured by several authors. The reported values vary from  $3323^0\text{K}$  to  $3808^0\text{K}$ . The recommended value is  $3651 \pm 17^0\text{K}$ , which was determined by Ronchi & Hiemaut [11] by using well defined sample (O/Th ratio 2.00) and advanced technique. No experimental data are available for heat capacity of liquid thorium dioxide. Fink et al. [12] estimated this value as  $234 \text{ J/Kg } ^0\text{K}$ .

## Linear Thermal Expansion

$\text{ThO}_2$  has face-centered cubic crystal structure from room temperature up to the melting point. The linear thermal expansion of  $\text{ThO}_2$  is well established. There is a close agreement between the experimental data quoted by number of authors. Touloukian [13] has recommended the following equation for the temperature range between  $150^0\text{K}$  to  $2000^0\text{K}$  after studying more than thirty measurements.

$$\alpha \text{ (} / ^0\text{K)} = 5.097 \times 10^{-6} + 7.464 \times 10^{-9} T - 22.782 \times 10^{-13} T^2$$

Here  $T$  is the temperature in  $^0\text{K}$ . Fig. 1 shows a comparison between thermal expansion data of  $\text{ThO}_2$  (using present equation) and  $\text{UO}_2$  (from MATPRO).

## THERMAL PROPERTIES OF $\text{Th}_{1-y}\text{U}_y\text{O}_2$

### Thermal Conductivity

Though the large experimental data are available on the measurement of thermal conductivity of  $\text{Th}_{1-y}\text{U}_y\text{O}_2$ , they lack consistency. The data reported in Murabayashi[1] have been selected keeping in mind (i) expected decrease in thermal conductivity with the increase in  $\text{UO}_2$  and (ii) temperature dependency of thermal conductivity. Following are the values of 'A' and 'B' (in the above conductivity equation) as a function of 'y', which were calculated by using the data of Murabayashi[1].

$$A = 0.042 + 111.2 y - 449.9 y^2 \quad \text{cm}^0\text{K/W}$$

$$B = 0.0225 - 0.0917 y + 0.4164 y^2 \quad \text{cm/W}$$

These data are recommended in the temperature range between  $300^\circ\text{K}$  and  $1200^\circ\text{K}$  for uranium concentration upto 10% (i.e.  $y=0.1$ ). Fig. 2 shows the variation the thermal conductivity of  $\text{Th}_{1-y}\text{U}_y\text{O}_2$  with temperature for various values of uranium concentration.

### Heat Capacity

Heat capacity of  $\text{Th}_{1-y}\text{U}_y\text{O}_2$  solid solution has been measured indirectly by enthalpy drop calorimetry by Springer[5] from  $573$  to  $2173^\circ\text{K}$  for samples containing 10.3 and 20.4 wt%  $\text{UO}_2$  and by Fischer[14] from  $2300$  to  $3400^\circ\text{K}$  for the compositions 30.0, 15.0 and 8.0 wt%  $\text{UO}_2$ . Both the results show good agreement, wherever a comparison is possible. There is not much difference between the heat capacity of  $\text{Th}_{1-y}\text{U}_y\text{O}_2$  and  $\text{ThO}_2$  upto 20 wt% of  $\text{UO}_2$  in temperature range of  $300$  to  $2000^\circ\text{K}$ . Hence heat capacity equation of pure  $\text{ThO}_2$  shown above is recommended for  $\text{Th}_{1-y}\text{U}_y\text{O}_2$  upto  $2000^\circ\text{K}$  and 20 wt% of  $\text{UO}_2$ .

### Linear Thermal Expansion

Large experimental data are available to assess the influence of uranium substitution on the linear thermal expansion. From the data of Kempter [15], Lynch [16], Springer [5] and Turner [17], it is seen that the average linear thermal expansion coefficient between  $293^\circ\text{K}$  and  $1173^\circ\text{K}$  almost decrease linearly between the values of  $\text{ThO}_2$  and  $\text{UO}_2$  within experimental accuracy.  $\text{ThO}_2$  and  $\text{UO}_2$  form an ideal solid solution in the whole composition range. The lattice parameter decreases linearly from 100%  $\text{ThO}_2$  to 100%  $\text{UO}_2$ . Considering that the vapour pressure measurements indicate an ideal solution behaviour at high temperatures, it can be assumed that this linear decrease in the lattice parameter also exists at high temperature. This linear decrease can only exist when the linear thermal expansion of  $\text{Th}_{1-y}\text{U}_y\text{O}_2$  ( $0 < y < 1$ ) equals the linearly interpolated value of that of  $\text{ThO}_2$  and

that of  $\text{UO}_2$ . This is also in reasonable agreement with the experimental data. The recommended value of linear thermal expansion of  $\text{Th}_{1-y}\text{U}_y\text{O}_2$  is shown below.

$$\alpha_Y (/ ^\circ\text{K}) = \alpha_{\text{ThO}_2} + y (4.705 \times 10^{-6} - 8.004 \times 10^{-9} T + 35.94 \times 10^{-13} T^2) \\ \text{for } 273^\circ\text{K} < T < 923^\circ\text{K}$$

$$\alpha_Y (/ ^\circ\text{K}) = \alpha_{\text{ThO}_2} + y (6.693 \times 10^{-6} - 12.322 \times 10^{-9} T + 59.352 \times 10^{-13} T^2) \\ \text{for } 923^\circ\text{K} < T < 2000^\circ\text{K}$$

Fig. 2 shows the variation of linear thermal expansion coefficient with temperature for various values of 'y'.

## DEVELOPMENT OF CODE FAIR-TFC

The above correlations have been incorporated in a new version of code FAIR called FAIR-TFC. The remaining properties, which are still undecided, have been kept same as that of uranium fuel. A case study has been done to assess the effect of above properties. A fuel pin of 235MWe Indian PHWR has been analysed up to a burnup of 10,000Mwd/T. The pin has been assumed to generate a constant power of 500w/cm. Fig. 3 shows the temperature distribution in the pin along radial direction for the two cases. In the first case, the available properties of the uranium fuel in code FAIR have been used. In the second case, the new version of the code FAIR-TFC has been used assuming a thorium fuel. It may be noted in Fig.3 that a substantial reduction in centre line temperature is obtained in thorium fuel due to better thermal conductivity. This also leads to a substantial reduction in fission gas release in thorium fuel in comparison to uranium fuel. However, such conclusions should be treated as preliminary as number of thorium fuel properties, especially transport properties, are yet to be ascertained and incorporated in code FAIR-TFC replacing the corresponding uranium fuel properties.

## CONCLUSIONS

Four important thermal properties, namely, conductivity, heat capacity, melting point and linear thermal expansion coefficient of  $\text{ThO}_2$  and  $\text{Th}_{1-y}\text{U}_y\text{O}_2$  have been assessed based on latest literature survey. These properties have been incorporated in a separate version of code FAIR. A case study has been done to show the effect of these properties in the temperature distribution of a thorium fuel pin in comparison to a similar uranium fuel pin.

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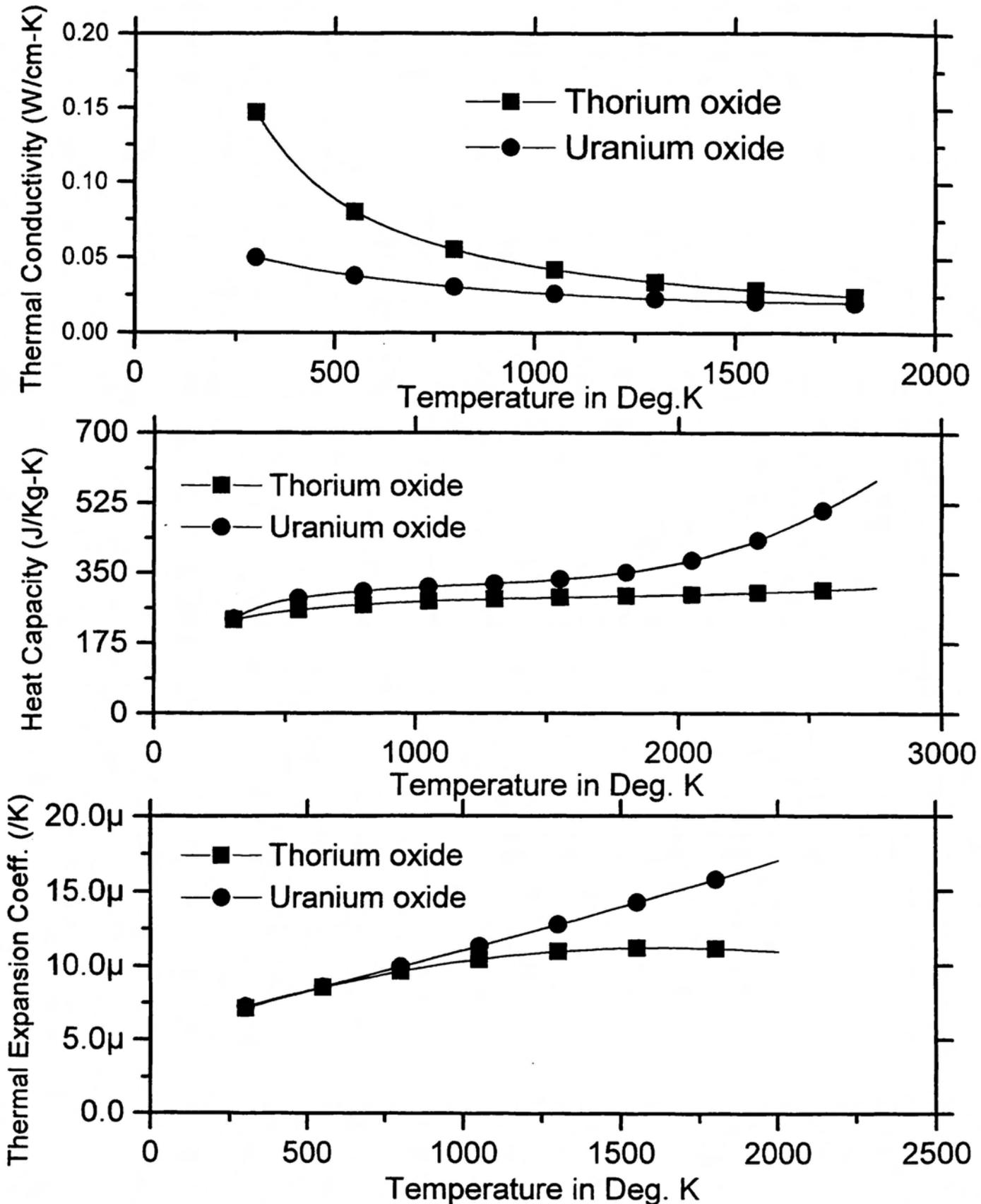


FIG.1 VARIATION of THERMO-PHYSICAL PROPERTIES of ThO<sub>2</sub>

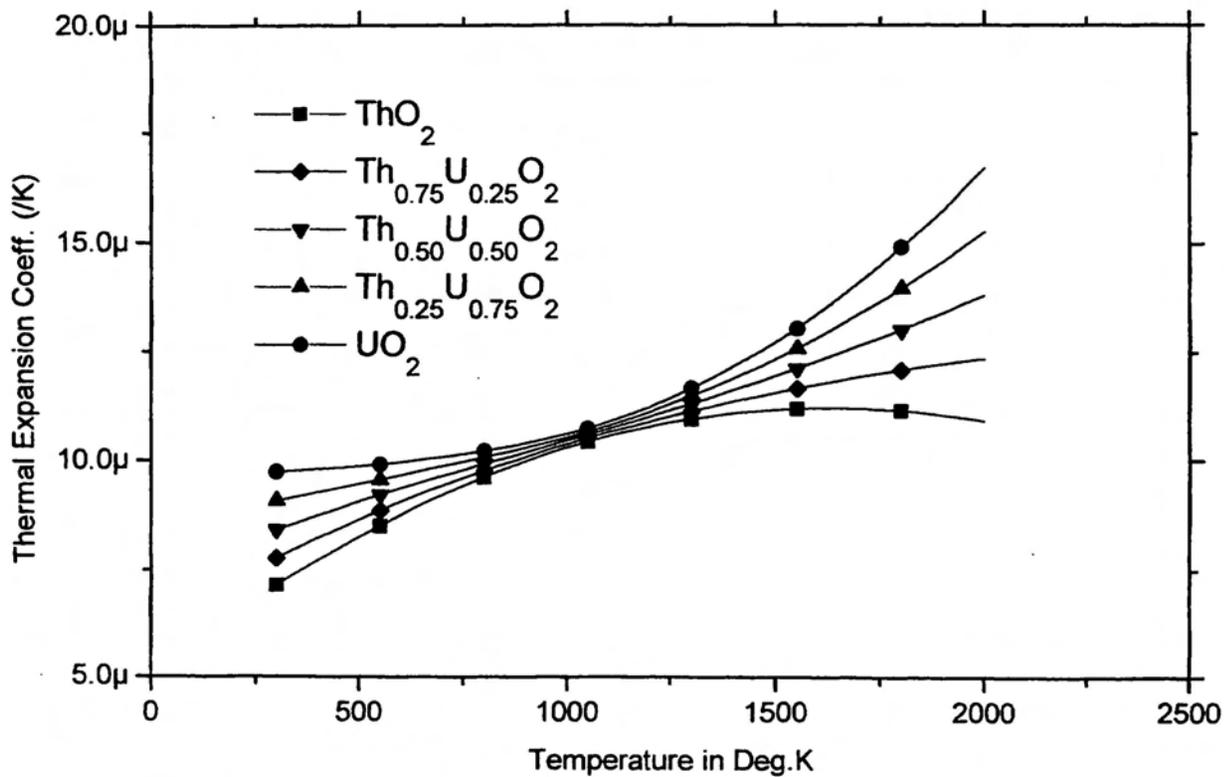
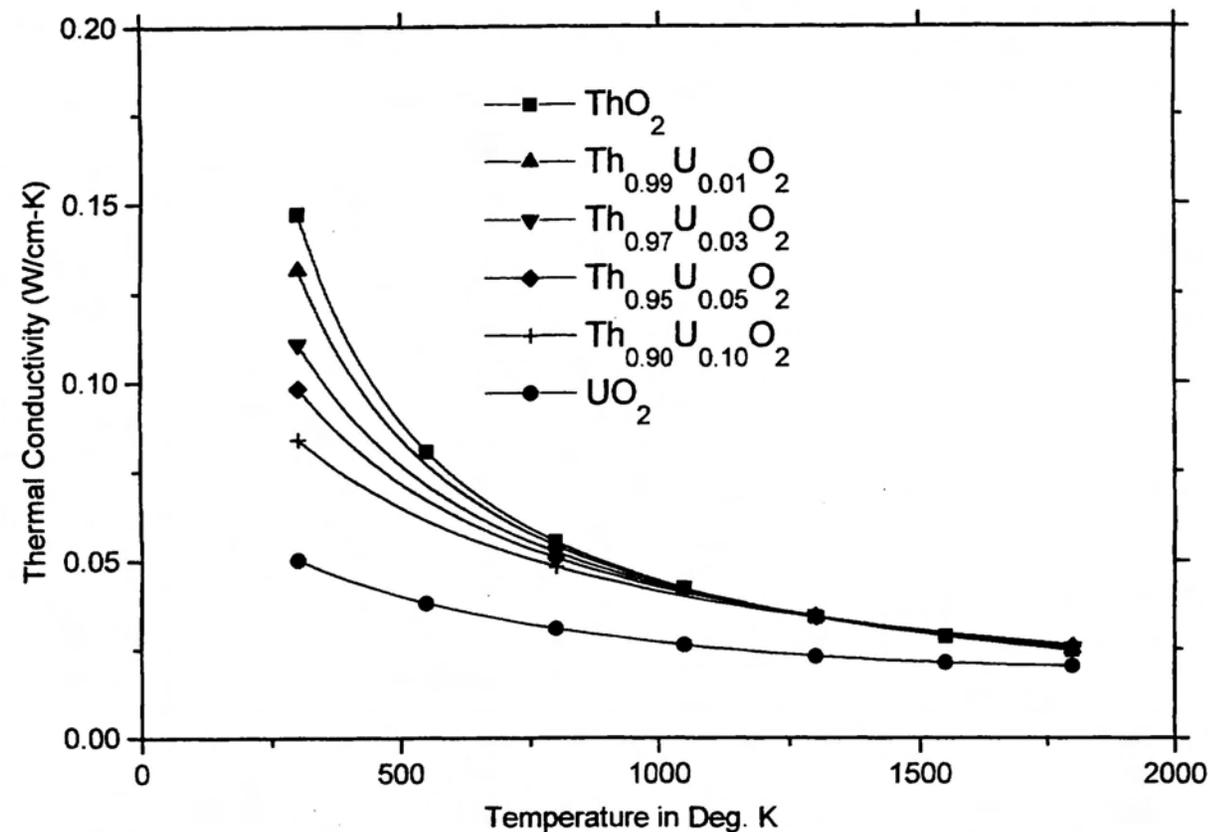


FIG. 2 VARIATION of THERMO-PHYSICAL PROPERTIES of VARIOUS ThO<sub>2</sub> - UO<sub>2</sub> SOLID SOLUTIONS

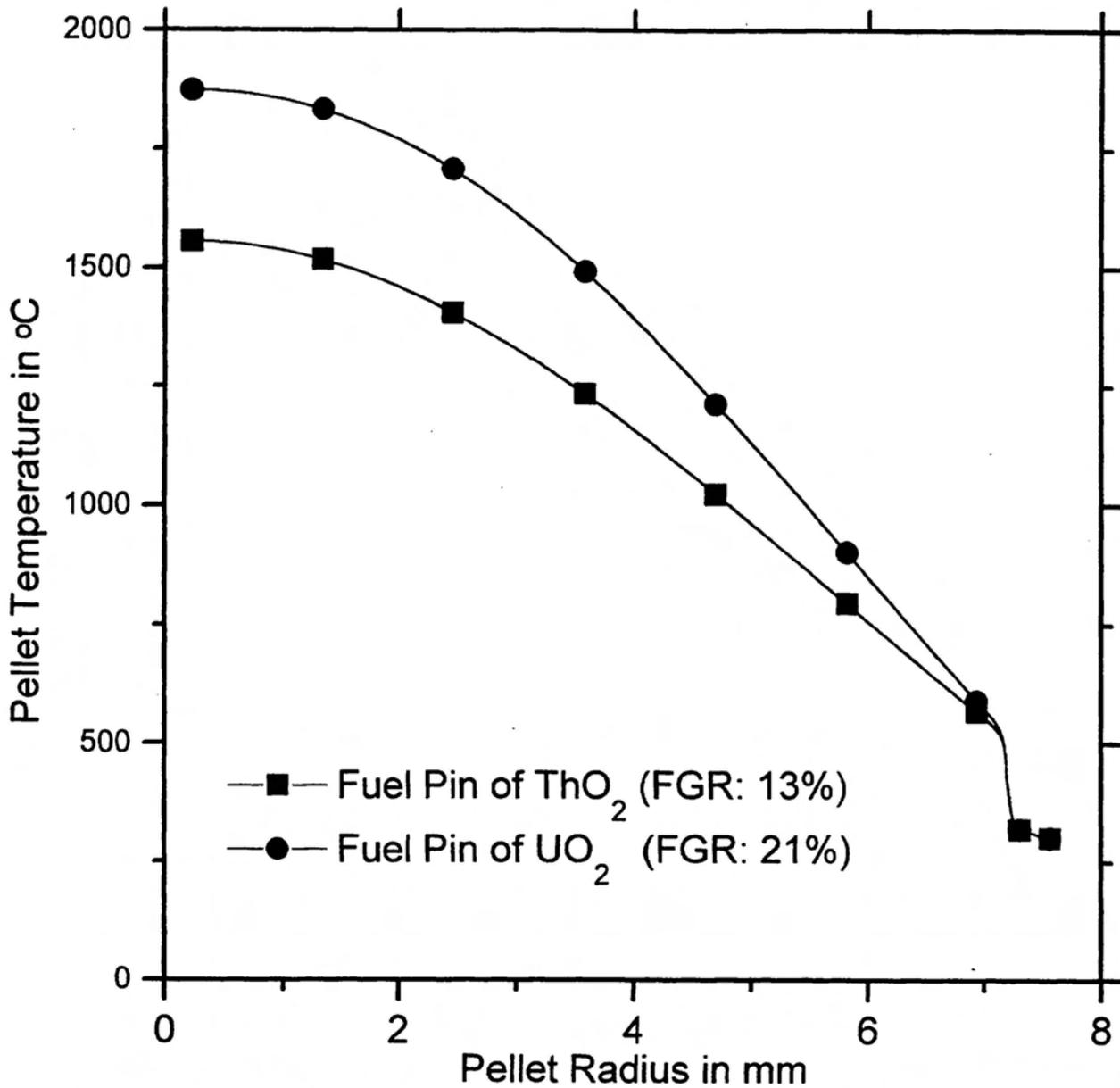


FIG.3 COMPARISON of RADIAL TEMPERATURE DISTRIBUTION  
(COMPUTED by USING CODE FAIR-TFC)