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Thermal–mechanical performance modeling of thorium–plutonium oxide fuel and comparison with on-line irradiation data

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HIGHLIGHTS

- The literature on thermal–mechanical properties of $(Th,Pu)O_2$ fuel is reviewed.
- The fuel performance code FRAPCON is modified for simulation of $(Th,Pu)O_2$ fuel.
- Subroutines for calculation of fuel material properties are modified.
- A new subroutine is written for calculation of radial power profiles.
- Calculated temperatures agree with measured temperatures for fresh fuel.

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ABSTRACT

Thorium-plutonium Mixed OXide (Th-MOX) fuel is considered for use in light water reactors fuel due to some inherent benefits over conventional fuel types in terms of neutronic properties. The good material properties of ThO_2 also suggest benefits in terms of thermal–mechanical fuel performance, but the use of Th-MOX fuel for commercial power production demands that its thermal–mechanical behavior can be accurately predicted using a well validated fuel performance code. Given the scant operational experience with Th-MOX fuel, no such code is available today.

This article describes the first phase of the development of such a code, based on the well-established code FRAPCON 3.4, and in particular the correlations reviewed and chosen for the fuel material properties. The results of fuel temperature calculations with the code in its current state of development are shown and compared with data from a Th-MOX test irradiation campaign which is underway in the Halden research reactor. The results are good for fresh fuel, whereas experimental complications make it difficult to judge the adequacy of the code for simulations of irradiated fuel.

1. Introduction

Thorium-plutonium Mixed OXide fuel (Th-MOX) is considered a promising technology for plutonium incineration in light water reactors [1–3], and also offers benefits in terms of neutronic properties compared with the traditional fuel types, Uranium OXide (UOX) and Uranium-plutonium Mixed OXide (U-MOX) [4,5]. A research program is currently addressing both the particularities of Th-MOX fuel manufacture and its irradiation behavior, through a test irradiation in the Halden research reactor [6].

In order for a new nuclear fuel type such as Th-MOX to be licensed for use in a commercially operating nuclear reactor, its material properties and thermal–mechanical behavior must be well known and predictable for all operation modes of the reactor. These predictions are normally done using a fuel performance code, in which established correlations for the various property changes are integrated. A modified version of the well-established code FRAPCON 3.4 [7] is being developed for this purpose, and the first phase of this development is described here. The modified version is referred to as FRAPCON-ThMOX, and has been used to model the Th-MOX pellets within the mentioned irradiation program, enabling a comparison between calculated and measured fuel

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temperatures.

Similar work was conducted previously in connection with the OMICO project [8], for prediction of the behavior of the experimental fuel which was irradiated within the scope of that project. We bring this work onward by using some data unavailable at the time of that study, and by comparison of calculated temperatures with experimental data. A version of FRAPCON for modeling of thorium-uranium mixed oxide fuel has also been created by Long et al. [9]. Our work has to a large extent been guided by their methodology. Other relevant studies include: Work on a more generalized FRAPCON-based code is ongoing at MIT [10], adaptations of the fuel performance code TRANSURANUS to simulations of thorium-containing fuels is ongoing at Technische Universität München [11], and the National Nuclear Laboratory in the UK is developing a thorium-capable version of the fuel performance code ENIGMA [13].

For the purpose of modifying FRAPCON 3.4 for use with Th-MOX fuel, the literature on the material properties of thorium dioxide and mixtures with plutonium dioxide was reviewed and appropriate data was incorporated into FRAPCON-ThMOX. A previous review of the literature data was done in 1997 by Bakker et al. [14], concluding that very little was known at that time. Several new findings have been published since this review was made [15,16], in particular regarding the important thermal conductivity [17]. However, for some properties, data is still lacking and in such cases a best estimate is suggested.

Since Th-MOX fuel also differs from UOX and U-MOX fuel with regard to neutronic properties, the power distribution within the fuel pellet is expected to be different, and this affects the temperature profile. To account for this, a new subroutine for prediction of power profiles has also been developed [18].

Some properties of the fuel material will change with the burnup of the fuel. Quantitative assessments of these dependencies are however very scarce. As the above-mentioned Th-MOX irradiation experiment proceeds, information is becoming available to make such assessments, but for the time being, the burnup dependence of most of the physical properties is left as they are in FRAPCON 3.4.

A brief account on the working mode of the FRAPCON code is given in Section 2. In Sections 3–9, we describe the correlations chosen for the material properties and behaviors which have been incorporated in the code. Section 10 discusses fission gas release. The subroutine for power profile prediction is described in Section 11 and a comparison between the preliminary calculated results and the experimental data is shown and discussed in Section 12. Comments on the future development and validation of the code are provided in Section 13. Finally, conclusions are drawn in Section 14.

2. The FRAPCON code

FRAPCON 3.4 iteratively calculates temperature, pressure and deformation of a light-water reactor fuel rod during long-term burnup, thereby describing phenomena such as heat conduction through the fuel and cladding to the coolant, fuel-cladding mechanical interaction and fission gas release. For this purpose, the thermal–mechanical properties of fuel and cladding materials are incorporated in the code through calls to specific subroutines, each calculating a single property. In this work, the subroutines relating to the cladding material properties are left unchanged.

The fuel rod is subdivided into nodes in the axial direction, and the total heat generation in the fuel at any axial node is normalized to the local LHGR specified by user input. Each axial node is further subdivided into concentric cylindrical radial nodes with a finer spacing towards the pellet periphery. The radial distribution of the heat generation is assumed to be proportional to the local fission rates, which are calculated as described in Section 11.

At each axial node, the temperature is calculated for every radial node using the heat conduction equation with the normalized local heat generation as the source term. The temperature dependent material properties are determined using the locally calculated temperature of the fuel material. The temperature, denoted T in the following, is always assumed to be given in units of Kelvin. SI units are used throughout the paper.

The state of the fuel rod is determined for each time step by iterative calculations which can be summarized as follows:

1. The fuel temperature and dimensional changes are calculated, then the resulting cladding mechanical response and ultimately the temperature drop over the pellet-cladding gap, which in turn affects the fuel temperature. This sequence is iterated until the pellet-cladding gap temperature drop converges. This is the only step essentially affected by the currently performed code modifications.
2. Local power, burnup and cladding properties are calculated and step 1 is carried out for each axial node.
3. The resulting gas release into the rod's free gas volume (total from all nodes) is calculated. Since the FGR affects the pellet-cladding gap temperature drop in all nodes, steps 1 and 2 are repeated until the rod internal pressure converges.
4. The state of the fuel rod resulting from step 3 is used as input to the next time step.

The fuel material is specified by user input in terms of, most importantly, (a) porosity, which in the following will be denoted P (unitless), (b) the plutonium dioxide weight fraction and (c) the oxygen to metal (O/M) ratio. The plutonium dioxide weight fraction is recalculated to give the unitless molar plutonium dioxide fraction, which we denote y. We will let x denote the negative deviation from stoichiometry, i.e. from O/M = 2.00. Since neither ThO_2 nor PuO_2 become hyperstoichiometric, x will always be a positive number [19]. It should be noted that FRAPCON 3.4 does not track stoichiometry changes, but only uses the stoichiometry value that is input from initial conditions, which need not be exactly 2.00. We will nevertheless discuss the stoichiometry dependence of the material properties, since it is foreseen that this study will be complemented with further studies in which stoichiometry is treated with more detail.

In order to improve readability in formulas, $Th_{1-y}\,Pu_yO_2$ will sometimes be simplified to (Th,Pu)O_2.

3. Thermal expansion

3.1. Thermal expansion of ThO_2

The linear thermal expansion of ThO_2 is treated by several sources [14,20–23] which all agree well. In FRAPCON, the thermal expansion is calculated in terms of percent linear dimensional change, ΔL/L0, relative to dimensions at room temperature, L_0.

The correlation recommended by Belle and Berman [23] and shown in Equation (1) is adopted in preference to the others, since it is based on several different data sets and claims the largest temperature interval of validity, 150 K < T ≲ 2500 K. This correlation is plotted in Fig. 1.

$$\left(\frac{\Delta L}{L_0}\right)_{ThO_2} = -0.243\cdot 10^{-2} + 7.84\cdot 10^{-6}T + 10.0\cdot 10^{-10}T^2. \quad (1)$$

The correlation used for the thermal expansion of PuO_2 is unchanged from FRAPCON 3.4.