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Implementation and Validation of MOX Fuel Models in FINIX

Valtteri Turkki
VTT Technical Research Centre of Finland
P.O. Box 1000, FI-02044 VTT, FINLAND
Valtteri.Turkki@vtt.fi

ABSTRACT

Uranium oxide is the most common material for nuclear fuel, especially in light water reactors. The fissile material in uranium oxide is the isotope U-235, which comprises typically around 5% of the fuel's mass. As the fuel is irradiated in the reactor, the U-235 isotope is consumed, and the amount of fissile material decreases. At the same time new fissile material is created, as U-238 transmutes to Pu-239 through neutron capture and beta decay. One way to utilize this material is to process the spent fuel and manufacture so-called MOX (mixed oxide) fuel, which is composed of uranium oxide and plutonium oxide (typically < 10 wt%). These fuels can reach higher burnups than uranium oxide fuel and thus they are more efficient in terms of fuel consumption. The improved efficiency arises from both higher burnup and the spent fuel recycling option.

This paper looks at the thermomechanical modelling of MOX fuels using VTT's FINIX fuel behaviour code. Since MOX fuels are solid solutions of two oxides, their thermal and mechanical properties differ from the standard uranium oxide fuels, which needs to be taken in to account in the fuel behaviour models. The implemented models here are based on the correlations found from the literature and other fuel behaviour codes. The changes to FINIX are validated against experimental data from Halden reactor and state-of-the-art FRAPCON-4.0 code. The results show that by implementing simple thermal and mechanical correlations to FINIX its temperature prediction accuracy of MOX fuel experiments can be improved by nearly 30%.

1 INTRODUCTION

Mixed oxide (MOX) fuels have been used in nuclear reactors since 1960s. Initially the motivation behind them was to make more efficient use of the existing resources, as uranium resources were thought to be limited, and the decrease of uranium supply was expected to increase the prices. When more natural uranium was discovered and the building pace of new nuclear power plants (NPPs) started to slow down in the 80s, the interest in MOX fuel technology dropped and it remained in use only in some countries, especially France and Japan.[1] In recent years, the interest towards MOX fuels has started to rise again as the problem of nuclear waste handling needs a solution. Manufacturing MOX is one partial solution to that as it allows both fuel recycling and more efficient fuel usage (higher burnup).

MOX fuels are usually composed of two oxides, uranium oxide (UO_2) and plutonium oxide (PuO_2) and are characterised by the enrichment (U-235 wt%) and the plutonium content (Pu-wt%). Both oxides are initially powders with grain size in the order of a few microns. To produce a homogenous material that has predictable in-reactor behaviour, one needs to mix the oxides carefully. Common techniques used for the mixing process are optimised co-milling (OCOM), micronized master (MIMAS) and short binderless route (SBR). OCOM and SBR are based on grinding the two powders, while MIMAS also utilizes a nitric acid solution in which the oxides are mixed [2]. These processes yield homogenous fuel on the pellet scale, but the solution is still heterogenous on the scale of microns. Despite the process, PuO_2 tends to form Pu-rich spots with mean size varying from 10 to 50 µm depending on the used process. The distribution of these Pu-rich spots is important when analysing the behaviour of MOX fuel especially in high temperatures.[3]

This paper introduces the main differences between conventional UO_2 fuel and MOX fuel in terms of fuel behaviour modelling. The introduced models are implemented in VTT's fuel behaviour code FINIX and the modifications are validated against experimental data. FINIX is designed for coupled calculations and the aim of the project was to make the FINIX code suitable for a larger number of fuel types, which in turn increases the applicability of VTT's reactor analysis framework KRAKEN.[4]

2 BACKGROUND & METHODS

The fact that MOX fuels are solutions affects both the thermal and mechanical properties of the fuel. On the scale of the reactor, the neutronics is also impacted as the fission cross section is different compared to UO_2 fuels and the power distribution can have notable local effects due to the Pu-rich spots.

This localization also contributes to the fission gas release (FGR) of the MOX, which is generally expected to be higher in MOX case.[5] FGR model of MOX fuels is not covered in this paper but an interested reader should see ref. [5].

2.1 Thermal Models

The thermal properties models used in fuel behaviour modelling refer to the models for fuel pellet thermal conductivity λ_{th} and heat capacity c_p. These are modelled with their theoretical models and adjusted with experimental correlations to account for the irradiation induced effects. The model for MOX fuel thermal conductivity λ_{th} [W/(m·K)] is given by equation (1) as follows

$$\lambda_{th} = 1.0789\lambda_{th,95}\frac{\rho_{TD\%}}{1+\frac{1}{2}(1-\rho_{TD\%})} \quad (1),$$

where $\rho_{TD\%}$ is the fractional density of the pellet. Equation (1) relates λ_{th} to thermal conductivity with fractional density of 0.95 $\lambda_{th,95}$. Term $\lambda_{th,95}$ can be expressed with equation (2) as

$$\lambda_{th,95} = \frac{1}{A(x)+B(x)T+h(Bu,T)} + \frac{1.5\cdot10^9\, e^{-13520/T}}{T^2} \quad (2),$$

where *T* the temperature and *Bu* the burnup of the fuel pellet. The terms *A(x)*, *B(x)* and *h(Bu,T)* are defined for MOX fuel as

$$\begin{gathered} A(x) = 2.85x + 0.035 \\ B(x) = 2.86\cdot10^{-4} - 7.15\cdot10^{-4}x \\ h(Bu,T) = 0.00187Bu + \frac{0.038Bu^{0.28}\left(1-0.9e^{-0.04Bu}\right)}{1+396e^{-6380/T}} \\ x = 2.00 - y \end{gathered} \quad (3),$$

with *y* being the oxygen-to-metal ratio of the fuel pellet.[6] Here it is worth noting that in equations (3) *y* is expected to be less than two and that burnable neutron absorbers, such as gadolinia, are generally not included in MOX fuels.

Fuel heat capacity c_p is modelled with a simple model which assumes that the heat capacity of the MOX fuel is a weighted average of the heat capacities of UO_2 and PuO_2. The weight used is the plutonium content Pu-wt%. Heat capacities of these oxides in [J/(Kg·K)] can be obtained with equation (4) as

$$c_p = \frac{K_1\theta^2 e^{\theta/T}}{T^2\left(e^{\theta/T}-1\right)^2} + K_2T + \frac{yK_3E_D}{2RT^2}e^{-E_D/(RT)} \quad (4),$$

where θ is Einstein temperature, *R* is the molar gas constant and E_D is activation energy for Frenkel defects.[7] Constants K_1, K_2 and K_3 and values for θ and E_D are shown in table 1 for both oxides. When the oxide heat capacities are known, the MOX fuel heat capacity can be calculated as

$$c_{p_{MOX}} = \gamma c_{p_{PuO_2}} + (1-\gamma)c_{p_{UO_2}} \quad (5),$$

where γ is the plutonium content as wt%/100.[6]

In addition to thermal conductivity and heat capacity the melting point of the fuel also changes. That change is not crucial for steady state modelling but should still be considered. The melting point of MOX fuel comes from weighted average like the heat capacity and yields 3017 K at zero burnup.[6]

Table 1: Values for constants in equation (4).

Constant [unit]	UO_2	PuO_2
K_1 [J/(Kg·K)]	296.7	347.4
K_2 [J/(Kg·K^2)]	0.0243	0.000395
K_3 [J/(Kg·K)]	$8.745\cdot10^7$	$3.86\cdot10^7$
θ [K]	535.285	571
E_D [J/mol]	$1.577\cdot10^5$	$1.967\cdot10^5$

2.2 Mechanical Models

The mechanical model currently used in many fuel behaviour codes is the rigid pellet model, in which the pellet is not expected to deform permanently from the effect of stress. The correlations used in FINIX for the rigid pellet model are for thermal strain, radial relocation, swelling and densification.[8]

Densification behaviour of the fuel depends on fission rate, temperature and burnup. Since MOX fuel contains Pu-rich spots, one could expect different densification between MOX and UO_2. Despite this, earlier studies show that the behaviour is similar between them.[2] Likewise, swelling is quite similar between the fuel materials. For these reasons state-of-the-art fuel behaviour code FRAPCON-3.3 implemented no changes for the mechanical model, when the MOX fuel option was introduced to it.[6]

In case of the FINIX MOX model, a different thermal strain (induced by thermal expansion) model was introduced. Thermal strain for MOX fuel is given by equation (6) as

$$\epsilon_{th} = \begin{cases} -2.66\cdot10^{-3} + 9.802\cdot10^{-6}T + 2.705\cdot10^{-10}T^2 + 4.391\cdot10^{-13}T^3, T < 923\ K \\ -3.28\cdot10^{-3} + 1.179\cdot10^{-5}T + 2.429\cdot10^{-9}T^2 + 1.219\cdot10^{-12}T^3, T \geq 923\ K \end{cases} \quad (6).[9]$$

2.3 The implementation and validation

The implementation of the MOX models to FINIX code was performed by writing the experimental correlations in equations (1-6) to the source code and adding new user input parameters needed for running the simulation with MOX fuels. The parameters include plutonium content, plutonium isotope distribution and fuel oxygen-to-metal ratio.

The validation of the new FINIX version was done against Halden HBWR reactor experimental data from cases IFA610 2&4, IFA629 1&3 and IFA648. These experiments included both lift-off and high burnup tests with the MOX fuel rods and the same data has also been used to validate FRAPCON-4.0's MOX models.[10]

FINIX input data (including physical dimensions, simulation options and operation history) for these simulations was generated from FRAPCON-4.0 validation inputs (available in [10]) using a self-written Python script. This approach further facilitates the comparisons between the two codes' results.

From the point of view of the temperature solution, the selection of boundary conditions for the fuel rod is important. The option chosen for the validation simulations was such that FINIX gets the heat transfer coefficient h_{cc} between the coolant and the cladding and the coolant bulk temperature as user-input. The used value for h_{cc} was 18 000 W/(m^2·K). This is boundary option 2 in the FINIX documentation [8].

3 RESULTS

The available validation data had fuel temperature, which was measured from the centre of the top fuel pellet with a thermocouple in the Halden experiments.[11] This data was compared to fuel rod centreline temperature calculated with FINIX in eight cases. Figure 1 shows the experimental data against the simulations run with FINIX with MOX models and FINIX without MOX models (denoted as UO_2 in Figure 1). The MOX models improve the temperature prediction significantly, but the predicted temperature is still slightly below measured even with MOX models. The mean relative error is around 5% with MOX model and 7% without it. The power drops (spikes in the Figure 1) were filtered out from the input, and therefore do not appear in the temperature predictions of FINIX. The inputs did not have the whole experiment period covered, which is why the prediction and Halden data have different ending points in Figure 1.

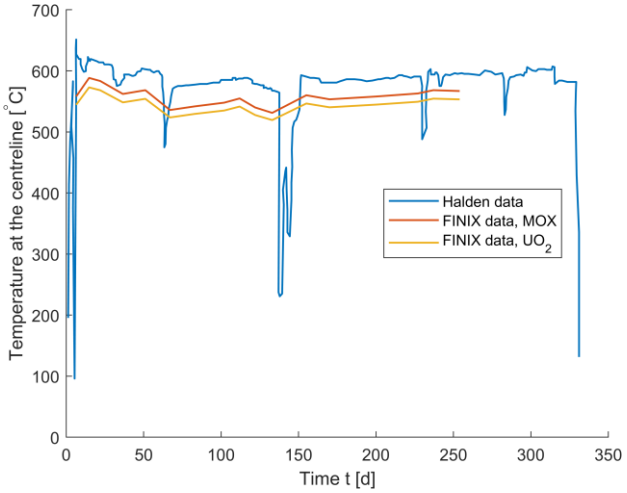

Figure 1: Simulations against experiments with IFA648 rod 2.

Figure 2 shows data from all validation cases in a measured vs. predicted graph. The results agree well in most cases, but in experiments IFA629-3 rods 5 & 6 (light blue square and green cross in Figure 3) the simulation overpredicts the temperature noticeably. The average relative error of all the data points is 7.5% and excluding the two high burnup cases yields 5.7%.

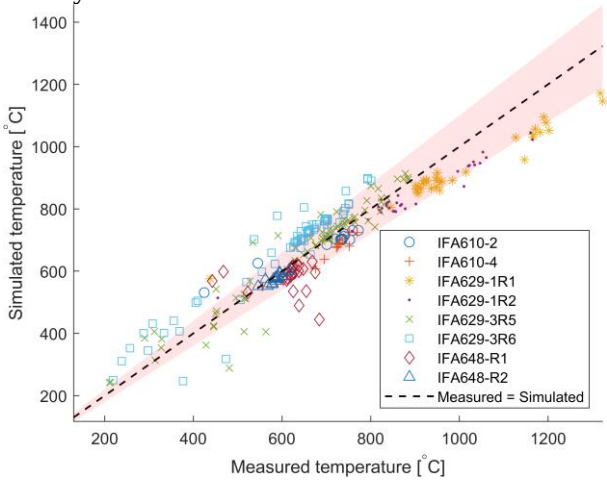

Figure 2: Predicted values plotted against the measured values from all the MOX validation cases. The red fill marks the 10% relative error.

Comparing FINIX to the state-of-the-art fuel behaviour code FRAPCON-4.0 showed that in most cases the difference was quite small, less than 8% for both. For FRAPCON-4.0 the total relative error of all cases was 5.9% and 4.9%, when excluding the high burnup cases.

In the high burnup experiments the difference increased significantly, as can be seen from Figure 3 FINIX and FRAPCON temperature predictions. Both codes over-predict the temperature noticeably: The relative error is around 22% for FINIX and 11% for FRAPCON. The starting burnup

in this experiment was 52.2 MWd/kg, which is rather high. Since both of the codes use the same thermal model, it is possible that the MOX correlations fail to take into account some high burnup phenomena.

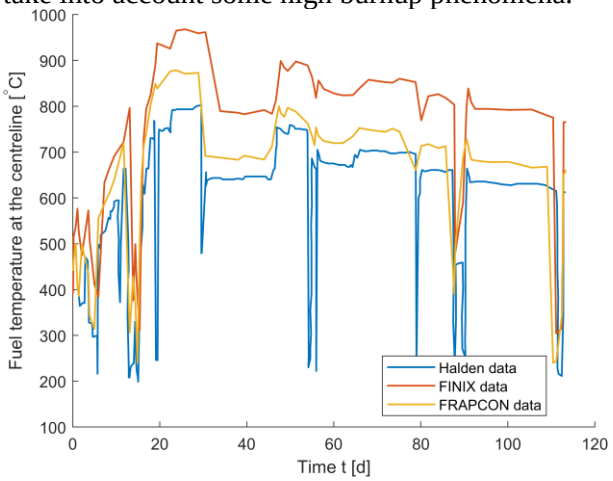

Figure 3: FINIX and FRAPCON-4.0 temperature predictions against experimental data from Halden experiment IFA629-3 rod 6.

4 CONCLUSIONS

The implementation of MOX models improves the accuracy of the temperature prediction for MOX fuel experiments by nearly 30%, as seen in the example of Figure 1. On the other hand, Figures 2 & 3 shows that the predictions deviate from the measurements more on high burnup, which means that for those cases one would likely need additional correlations.

The only discussed quantity here was fuel temperature, which is the most valuable output from a fuel performance code, especially for coupled applications. Other quantities of interest, such as fission gas release in these MOX experiments, can now be studied using this research as the basis. In upcoming improvements of FINIX the high burnup behaviour as well as prediction capability of quantities beyond temperature can be assessed further.

ACKNOWLEDGEMENTS

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REFERENCES

[1] J. Hales, W. Li, R. Williamson, G. Rossiter, P. Van Uffelen, “A review of fuel performance modelling”, Journal of Nuclear Materials, 516(INL/JOU-18-45934-Rev000), 2018

[2] A.R. Massih, “Models for MOX fuel behaviour A selective review”, Technical Report SKI-R06-10, Sweden, 2006

[3] P. Van Uffelen, “Modelling of nuclear fuel behaviour”, Report EUR 22321 EN, 2006

[4] J. Leppänen, V. Valtavirta, A. Rintala, V. Hovi, R. Tuominen, J. Peltonen, M. Hirvensalo, E. Dorval, U. Lauranto, R. Komu, “Current Status and On-Going Development of VTT’s Kraken Core Physics Computational Framework”, Energies 2022, 15, 876

[5] L.O. Jernkvist, “A model for fission gas release from mixed oxide nuclear fuel”, Technical Report SKI-R08-30, Sweden, 2007

[6] D.D. Lanning, C. E. Beyer, K.J. Geelhood, “FRAPCON-3 Updates, Including Mixed-Oxide Fuel Properties”, Technical Report PNNL-11513, Pacific Northwest National Laboratory, 2005

[7] D.L. Hagrman, A. Reymann, R.E. Mason, “MATPRO-Version II (revision 2): A Handbook of Materials Properties for Use in the Analysis of Light Water Reactor Fuel”, NUREG/VR 0497 (TREE-1280), Rev.2, 1981

[8] H. Loukusa, J. Peltonen, V. Valtavirta, “FINIX - Fuel behavior model and interface for multiphysics applications - Code documentation for version 1.19.1”, VTT Research Report, No. VTT-R-00052-19, 2019

[9] J.J. Carbajo, G.L. Yoder, S.G. Popov, V.K. Ivanov, “A review of the thermophysical properties of MOX and UO2 fuels”, Journal of Nuclear Materials, 299(3), 181-198, 2001

[10] K.J. Geelhood, W.G. Luscher, “FRAPCON-4.0: Integral Assessment”, Technical Report PNNL-19418, Vol. 2, Rev. 2, Pacific Northwest National Laboratory, 2015

[11] R.J. White, “The Re-Irradiation of MIMAS MOX Fuel in IFA-629.1”, HWR-586, OECD Halden Reactor Project, Norway, 1999