Analysis of Fuel Centre Temperatures with the TRANSURANUS Code

A. Schubert, C. Györi¹, D. Elenkov², K. Lassmann and J. van de Laar

European Commission Joint Research Centre Institute for Transuranium Elements P.O. Box 2340 76125 Karlsruhe, Germany

¹KFKI Atomic Energy Research Institute P.O. Box 49 1525 Budapest 114, Hungary

²Bulgarian Academy of Sciences Institute for Nuclear Research and Nuclear Energy Tsarigradsko shousse 72 1784 Sofia, Bulgaria

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Abstract

At present a comprehensive verification of the fuel rod performance code TRANSURANUS is being performed using irradiation data from the "International Fuel Performance Experiments (IFPE) Database" and the OECD Halden Reactor Project. For this verification standard models and options are applied. Recent developments have concentrated on high-burn-up phenomena, such as the local thermal conductivity and the local porosity in the High Burn-up Structure (HBS).

In this paper, fuel centre temperatures are calculated by the TRANSURANUS code with standard options and compared with measured temperatures, under steadystate conditions. More than 40000 data points have been analyzed in total. They cover UO_2 fuel (both for Western-type LWR and for Russian-type VVER) and MOX fuel for LWR.

It is shown that the vast majority of fuel centre temperatures predicted by the TRANSURANUS code deviates from the measured values by less than 10%. For all standard fuel configurations the actual deviations are considerably smaller. The spread is of the same order of magnitude as the uncertainties in the measurements (due to power calibration and thermocouple calibration). The present analysis does not reveal any general bias. It can be concluded that under the studied conditions the TRANSURANUS code predictions of the fuel centre temperatures are very satisfactory.

1. Introduction

The TRANSURANUS code is a computer program for the thermal and mechanical analysis of fuel rods in nuclear reactors [1, 2]. An actual overview of the whole TRANSURANUS project can be found in Ref. [3] and on the Internet page of the Institute for Transuranium Elements (ITU). Since 1992 high burn-up models for Light Water Reactors (LWR), a version for Russian VVER reactors and a MOX version have been developed.

In this paper we outline the general approach for code verification. Emphasis is put on comparisons with fuel centre temperatures obtained from a large set of irradiation experiments. They cover:

- UO₂ fuel for Western-type LWR in the following referred as "standard UO₂"
- UO₂ fuel applied in Russian type fuel rods as used in VVER reactors in the following referred as "UO₂-VVER"
- MOX fuel for Western-type LWR

2. Verification of the TRANSURANUS Code

2.1. General Approach

The verification of TRANSURANUS is performed in three phases: comparison with analytic solutions, code-to-code comparisons and - most importantly - comparisons with irradiation experiments.

Extensive work has been done in the first two phases. For a large number of physical models and specific conditions an analytic solution is available. In almost all cases different numerical methods were compared to each other. The results of code-to-code comparisons – as the IAEA-FUMEX exercise [4] - emphasized the advantage of applying models of "adequate complexity" rather than highly mechanistic models.

So far approximately 400 irradiations have been compiled in the "International Fuel Performance Experiments" (IFPE) Database [5, 6], allowing a comparison of code calculations with a comprehensive set of irradiation experiments. From this source approximately 70 irradiations have been analyzed by means of the TRANSURANUS code up to now. In addition, six major irradiation experiments from the OECD Halden reactor project have been analyzed, including UO₂ fuel at high burn-up as well as MOX fuels. These two pools of experimental information together constitute the basis for the TRANSURANUS verification database.

2.2. Standard physical models

The primary goal of the verification work is to verify models and correlations on a broad basis. We consider the present work as the first phase, in which we apply standard models and options. All irradiations analyzed are interpreted as far as possible with identical models and input parameters, i.e. as if they were blind predictions. Emphasis is put on all phenomena and quantities that affect the temperature in the fuel, i.e. densification and swelling, relocation, fission gas release and the thermal conductivity of the fuel.



Figure 1: Sinterable porosity as a function of the initial grain size according to [7]

For most of the fuels analyzed the prediction of densification is a severe problem since microstructural details are often completely unknown. If no other information is available, we follow a recommendation given in ref. [7] and adjust our empirical densification model to:

$$\Delta \mathsf{P} = \frac{2.23}{\mathsf{d}} \mathsf{P}_0 \tag{1}$$

where ΔP is the sinterable porosity, P_0 is the fabrication porosity and d the mean linear intercept (diametric) grain size in μm . However, Figure 1 shows that the deviations from this general trend may be rather large.

Swelling is formulated as a rate equation; relocation is very similar to the model of Lanning et al. [8] incorporated in the FRAPCON code; fission gas release is based on an effective diffusion model in the grain plus a grain boundary model.

The thermal conductivity of the fuel has been derived from data obtained at ITU as well as from the open literature. The correlation takes into account the High Burn-up Structure (HBS), as well as the influence of gadolinium:

$$\lambda = \left(\frac{1}{a + a_1 b u + a_2 G d + b_1 b u T_p + b_2 G d T_p + bT} + \frac{c}{T^2} e^{\frac{d}{T}}\right) (1 - P)^{2.5} \quad (2)$$

Here a, b, c and d are fitting constants, bu is the local burn-up (MWd/kgU), Gd the local gadolinium content (wt%), T the local absolute temperature (K), $T_p = min (1923,T)$ and P the local porosity. For UO₂ fuels, the constants a, b, c and d follow the recommendation of Harding and Martin [9]. The remaining parameters were fitted using the data of [10-14] for UO₂ and (U,Gd)O₂:

a = 0.0375	$b = 2.165 \times 10^{-4}$	$c = 4.715 \times 10^9$
$a_1 = 0.38360 \times 10^{-2}$	$b_1 = -0.90849 \times 10^{-6}$	d=16361
a ₂ = 0.84476×10 ⁻²	$b_2 = 0.22149 \times 10^{-5}$	

One important result of our analysis was that data from SIMFUEL are not representative for irradiated UO_2 fuel since SIMFUEL gives a significantly lower parameter a_1 , and thus a higher thermal conductivity than irradiated UO_2 [15].



Figure 2a, b: Measurements of the Xe concentration (C.T. Walker) and the porosity in the outer regions of different fuel rods as a function of the calculated local burn-up. Clearly, from both figures it can be concluded that around a local burn-up of 60-80 MWd/kgU the Xe concentration in the fuel matrix decreases whereas the porosity increases. This has been identified as consequence of the formation of a new microstructural fuel zone, the so-called "High Burn-up Structure", HBS [15].

It is important to note that the local porosity is used in Eq. (2) which is especially relevant in the outer parts of the fuel where the heat flux density is highest and the porosity is increased due to the formation of the HBS. (This aspect is not always considered in all correlations that have been developed for irradiated fuel). Evaluations of ITU data have shown that not only the local Xe concentration but also the local porosity can be correlated to the local burn-up [15]. Both trends are shown in Figure 2 and are part of the high burn-up models of the TRANSURANUS code. Hence, we have used the porosity given by Figure 2b for the fitting of the parameters. Consequently, Eq. (2) should not be used with other models for the local porosity. The correlation must be considered as preliminary and will be replaced by a more comprehensive correlation of C. Ronchi et al. [16, 17] which is presently under development.



Figure 3: Comparison between measured thermal conductivities and those of Eq. (2). Note that this correlation is only valid at high burn-up if the porosity dependence according to Figure 2b is taken into account.

Figure 3 shows the comparison between measured and calculated thermal conductivities for UO_2 and UO_2 -Gd₂O₃ fuels. For irradiated UO_2 fuel 419 data, and for fresh UO_2 and UO_2 -Gd₂O₃ fuels 688 data were used for the fitting of parameters.

Specific models have been developed to allow the application of the TRANSURANUS code to MOX fuels. The fuel is treated as homogeneous material. Recently the MOX version has been extended:

- 1. The burn-up model TUBRNP [18, 19] has been modified in order to better predict the radial distribution of all relevant Pu isotopes.
- 2. The standard correlation for the thermal conductivity of UO_2 fuel (eq. (2)) has been adopted by:

- modified coefficients recommended by Duriez et al. [20] for fresh MOX fuel

- a simple burn-up dependence deduced from original experimental data of irradiated MOX fuel obtained at ITU [21].

In the TRANSURANUS-VVER version [22] specific correlations are applied for densification and swelling of the fuel. For the VVER-specific Zr1Nb cladding material, the following thermal and mechanical properties are implemented:

- Thermal linear expansion coefficient
- Thermal conductivity
- Specific heat
- Effective creep rate with suitable anisotropy coefficients
- Irradiation growth
- Young's modulus and Poisson's ratio

2.3. Irradiation experiments - discussion of fuel centre temperatures

In this paper the analysis focuses on the verification of fuel centre temperatures under steady-state conditions. More than 40000 predictions are plotted against measured values in Figures 4-5 and 7-10. The data points have been grouped according to fuel types (standard UO_2 , UO_2 -VVER and MOX) and irradiation conditions (OECD Halden reactor and SOFIT programme). All graphs show good agreement between measured fuel centre temperatures and those calculated with the TRANSURANUS code. The vast majority of calculated points deviates less than 10 % from the measured data. No overall bias can be seen. The standard deviation of the total dataset is below 4%.



Figure 4a, b: Comparison of measured and calculated fuel centre temperatures for standard UO₂ fuel rods irradiated in different configurations in the OECD Halden reactor: a) small-gap rod, b) large-gap rod



Figure 4c, d: Comparison of measured and calculated fuel centre temperatures for standard UO₂ fuel rods irradiated in different configurations in the OECD Halden reactor: c) small-diameter rod, d) special UO₂ rod irradiated as reference together with Gd-doped fuel



Figure 5a, b: Comparison of measured and calculated fuel centre temperatures for UO₂ -VVER fuel rods irradiated in the OECD Halden reactor: a) small-gap rods, b) large-gap rods



Figure 6a, b: Ratio of calculated versus measured fuel centre temperatures for UO₂ -VVER fuel rods irradiated in the OECD Halden reactor: a) small-gap rods, b) large-gap rods

In a further analysis we can search for systematic deviations emerging for selected fuel types or different irradiation conditions. The ratio of calculated and measured temperatures can be plotted as function of irradiation time or burn-up. This step allows specific trends to be investigated. Examples are discussed later on (Figure 6). It should be noted that any trend can arise from the limitation of a basic physical model as well as from a systematic experimental error. In particular, step-like changes of the temperature ratio are most likely due to shifts in the calibration of the applied linear heat rate and/or the measured fuel temperatures.

Standard UO₂ fuel for Western-type LWR

Figure 4 shows the excellent agreement between measured and calculated fuel centre temperatures for standard UO_2 fuel. The individual graphs (a-d) illustrate that the behaviour is practically identical for a rather wide range of different irradiation configurations in the OECD Halden reactor. The irradiation experiments cover different pellet and gap sizes as well as different initial enrichments. The consistent picture obtained for the large amount of available data emphasizes that modelling of in-pile temperatures of standard UO_2 fuel is now mature and well verified.

Most deviations are clearly below 10%. Larger deviations are found only in the burnup region above 60 MWd/kgHM (see the shaded area in Figure 4c). This area needs further consideration. It reflects the remaining limitations of material-property data, in particular after the formation of the high burn-up structure (HBS).

UO2 fuel for VVER reactors

The TRANSURANUS code has been successfully applied for post-irradiation computations of VVER fuel. Details of the TRANSURANUS-VVER version can be found in [22]. Very good agreement between measured and calculated fuel centre temperatures is seen in the two small-gap rods (Figure 5a). For the two large-gap rods the agreement is still fair (Figure 5b) but points at a systematic underestimation, increasing with burn-up. This behaviour is confirmed by the analysis of the ratio of calculated and measured fuel centre temperatures, as shown in Figure 6a, b. In the context of the large fuel-cladding gap (270 μ m) this trend is expected to arise mainly from the application of a constant fuel swelling rate. The figures confirm the consistency between the two rods of the same gap size.



Figure 7: Comparison of measured and calculated fuel centre temperatures for UO₂ -VVER fuel rods irradiated in the SOFIT programme

Experimental data on VVER fuel had also been obtained from the Finnish-Russian SOFIT programme and compiled in the IFPE database. This data enables an investigation of calculated and measured temperatures under completely independent irradiation conditions.

Figure 7 shows the corresponding scatter plot for two different irradiation phases of SOFIT, illustrating good agreement over a wide range of temperatures. Figure 8 compares the data of the SOFIT programme to those obtained from the OECD Halden reactor project. The consistent behaviour of fuel centre temperatures from the two independent data sources is an important contribution to the verification of the TRANSURANUS-VVER version. The overall range of deviations between measured and calculated fuel centre temperatures is almost identical for standard and VVER-type UO_2 fuel (see also Figure 10a).



Figure 8: Comparison of calculated and measured fuel centre temperatures for UO₂-VVER fuel rods in different irradiation conditions: SOFIT programme (triangles), compared to those irradiated at Halden (crosses)

MOX fuel

In parallel to the analysis of UO₂ fuel, first verification work for the TRANSURANUS-MOX version was carried out using in-pile temperature measurements obtained at the OECD Halden reactor. The agreement between measured and calculated temperatures is good although the overall spread is larger than in the case of UO₂ fuels (Figure 9 and Figure 10b). Systematic deviations can be seen already at burnup values above 25 MWd/kgHM. Further investigations are required, including the enhanced generation and release of He in MOX fuels - originating mainly from alpha decay of ²⁴²Cm. Its modelling is not straightforward and not covered in the present TRANSURANUS calculations. There is also a need for a larger scope of data to be obtained from independent in-pile measurements.



Figure 9: Comparison of measured and calculated fuel centre temperatures for MOX fuel rods irradiated in the OECD Halden reactor

3. Summary and Conclusions

A large set of temperature data from instrumented irradiation experiments performed at the OECD Halden reactor and within the SOFIT programme has been analyzed with the TRANSURANUS code applying standard options. These irradiations include high burn-up UO₂, UO₂ fuel for Russian-type VVER reactors as well as MOX fuels. The experimentally obtained fuel centre temperatures are well predicted by the TRANSURANUS code, with most deviations below 10%. The overall spread is of the same order as the experimental uncertainties, in particular the power calibrations and thermocouple calibrations. The spread between measured and calculated fuel centre temperatures is consistent for all analyzed fuel types and irradiation conditions. No general trends or biases are seen. There is also no bias when comparing the measured and calculated temperatures of the non-standard fuel types (UO₂-VVER and MOX) to those for standard UO₂ fuel (Figure 10).

For selected irradiation phases a detailed analysis of fuel centre temperatures allows specific deviations and systematic trends to be identified. It should be noted that the maximum spread is still within +/-15%. The observed trends concern:

- UO₂ fuel at high burn-up (above 60 MWd/kgHM)
- irradiation-induced swelling of UO2-VVER fuel
- He production and release in MOX fuel (above ~ 25 MWd/kgHM)

These areas belong to the priorities for further development in modelling of fuel rod performance. They are in agreement with the conclusions of the first IAEA-FUMEX exercise [4]. The needs for further investigation are also reflected in the ongoing and future experiments of the OECD Halden reactor project and in the permanent extension of the IFPE database.

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Figure 10: Measured and calculated fuel centre temperatures for different fuel types irradiated in the OECD Halden reactor: a) UO₂–VVER fuel, b) MOX-LWR fuel, both compared to standard UO₂ fuel

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