Verification calculations for the WWER version of the TRANSURANUS code

D.Elenkov, St.Boneva, M.Georgieva, St.Georgiev

Institute of Nuclear Research and Nuclear Energy,
Bulgarian Academy of Sciences,
Sofia, Bulgaria

A. Schubert, P. Van Uffelen

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

1. Introduction

The paper presents part of the work performed in the study project "Research and Development for Licensing of Nuclear Fuel in Bulgaria". The main objective of the project is to provide assistance for solving technical questions of the fuel licensing process in Bulgaria. One important issue is the extension of the predictive capabilities of fuel performance codes for Russian-type WWER reactors. In the last decade, a series of international projects has been based on the TRANSURANUS fuel performance code [1]: Specific models for WWER fuel have been developed and implemented in the code in the late 90's [2]. In 2000-2003, basic verification work was done by using experimental data of nuclear fuel irradiated in WWER-440 reactors [3, 4].

While the present paper focuses on the analysis of WWER-1000 standard fuel under normal operating conditions, the above study project covers additional tasks:

- Post-irradiation calculations of ramp tests performed in the DR3 test reactor of the Risoe national laboratory (five instrumented fuel rods of the Risoe3 dataset contained in the IFPE database [5]) using the TRANSURANUS code

- Compilation of cross-section libraries for isotope evolution calculations in WWER-440 and WWER-1000 fuel assemblies using the ORIGEN-S code [6]
- Analysis of current situation and needs for an extension of the curriculum in Nuclear Engineering at the Technical University of Sofia.

The project involves five Bulgarian organisations - the Nuclear Regulatory Agency, the Institute for Nuclear Research and Nuclear Energy, the Technical University of Sofia, the Physics Department of Sofia University, and the Kozloduy Nuclear Power Plant.

In this paper we present post-irradiation calculations of steady-state irradiation experiments with nuclear fuel for Russian-type WWER-1000 reactors [7,8,9,10], using the latest release of the TRANSURANUS code (v1m1j03). Regarding a comprehensive verification of modern fuel performance codes, the burn-up region above 40 MWd/kgU is of increasing importance. A number of new phenomena emerge at high fuel burn-up, implying the need for enlarged databases of post-irradiation examinations (PIE). For one fuel assembly irradiated in a WWER-1000 reactor with a rod discharge burn-up between 50 and 55 MWd/kgU, comprehensive PIE data had been produced in the experimental facilities of RIAR Dimitrovgrad (Russian Federation) and recently released to the IFPE database [5]. For this fuel assembly we analyse the calculated geometrical parameters (fuel rod elongation, outer cladding diameter, fuel-to-cladding gap), as well as calculations of fission gas release at end of irradiation.

2. Experimental data of WWER–1000 fuel rods

2.1. Operational conditions

The fuel assembly FA0325 was operated in the first unit of Zaporoshye NPP during the 4-th to 8-th fuel cycles. It was irradiated for 1142.1 effective days to a burn-up of 48.9 MWd/kgU (average for the whole FA), corresponding to 51.3 MWd/kgU in the "hottest" fuel rod. The maximum local linear power in a fuel rod was 29 kW/m. The average linear power for the whole operational period of the fuel assembly varied within the limits of 7.1 kW/m and 26.6 kW/m. After the base irradiation, the FA0325 was subjected to PIE at the hot cells of RIAR, Dimitrovgrad.

In the IFPE database [5] detailed irradiation histories and axial power distributions of the individual fuel rods are available. The fast neutron fluence (E > 0.1 MeV), the local burnup and the temperature of the outer cladding surface are given for 10 axial nodes. The given neutron flux was multiplied by a factor of 0.7, required by the creep correlations of the TRANSURANUS to represent the flux of fast neutrons with energy above 1 MeV. The factor 0.7 is obtained from the expression $\frac{N_{1MeV}}{N_{0.1MeV}} = 0.7$, where $N_p = 0.484\int_p^{\infty} sinh\left(\sqrt{2E}\right)exp(E)dE$, for $p = 0.1$ *MeV* and $p = 1$ *Mev* [11].

The geometrical parameters of fresh WWER-1000 and WWER-440 fuel rods have no significant differences, except for the diameter of the central hole - corresponding to 2.4 mm for WWER-1000 and 1.2 mm for WWER-440. However, the operational conditions of the two types of reactors are different (Table 1).

Table 1. Comparsion of operational parameters of WWER-440 and WWER-1000 reactors relevant for fuel rod performance calculations

	WWER-440	*WWER-1000*
Initial fill pressure (He)	0.6 MPa	2.25 MPa
Average linear power	12.9 kW/m	16.7 kW/m
Coolant temperature at the highest power density	312 ^{o}C	335 ^{o}C

Coolant pressure	12.5 MPa	16.0 MPa

2.2. Post irradiation examination

The fuel rods were examined in hot cells at RIAR [7 - 10]. For 59 fuel rods, the available experimental data from the post-irradiation examination (PIE) cover the final fuel burn-up and at least one of the following quantities:

- change of the outer cladding diameter (creep down);
- change of the rod length (cladding elongation);
- size of the fuel-to-cladding gap;
- fractional fission gas release.

For the first time, this data set provides a possibility to validate the TRANSURANUS-WWER code predictions for the rod geometrical changes of standard WWER-1000 fuel.

Although the operational conditions of the WWER-1000 fuel rods are more challenging than those for WWER-440 fuels, the post irradiation examinations at RIAR do not reveal any considerable difference in the geometrical parameter changes of the fuel components. As it was mentioned in [8], the difference between WWER-1000 and WWER-440 fuel rods becomes apparent at a burnup higher than 40 MWd/kgU, in the fourth year of operation. This difference was confirmed by the results of fuel rod testing at high burn-up in the MIR reactor under transient conditions.

3. Analysis of selected fuel rods by TRANSURANUS

3.1. Methodology

For the post-test computations with the TRANSURANUS fuel performance code, each of the 59 available fuel rods is modelled as a stack of 10 axial slices. The height of each slice is prescribed by the supplier in the IFPE database.

Previous calculations of WWER-440 fuel rods (KOLA-3 experiment [3]) revealed a satisfactory agreement between measured and calculated values. Hence, the same standard options, models, and correlations of the fuel and cladding material properties are applied for the WWER-1000 calculations (Table 2).

Table 2. Physical models and material properties used in TRANSURANUS calculations

Model	*Description*
Fission gas release	URGAS algorithm with thermal diffusion coefficients of Matzke [12] and constant athermal diffusion coefficient [13]. Athermal fission gas release is simulated by linear dependence on the burn-up (bu - in MWd/kgU): f^{ath}=6.17*10^{-5} bu
Fuel Densification model	Simple empirical model using a generic densification of 1.2. vol.%
Cladding material properties	Specific correlations for Zr1%Nb [4]
Cladding strain due to swelling	Irradiation growth correlation. of Zr1%Nb, based on data from Bibilashvili at al. [14]
Texture factors for irradiation growth (swelling) of Zr1%Nb	Recommendation for the Kola3 data cases (WWER-440): f_r = 0.52, f_t = 0.38, f_a = 0.10
UO_2 material properties	Standard TU models for the LWR [15]
Thermal conductivity of the fuel	The new standard correlation for UO_2 and $(U,Gd)O_2$, accounting for the local porosity [15]
Saturation limit for concentration of grain boundary gas	Constant value: 1.10^{-4} µmol/mm^2 (saturation limit is not depending on temperature)

A generic densification of 1.2 vol% is recommended in the IFPE data base (additional information on the WWER-1000 assembly FA325 [5]). This value was applied as maximum fuel densification in the standard empirical densification model.

Since appropriate information on the relocation of the hollow WWER pellets is not accessible, the effect of the early-life fuel relocation on the overall fuel rod performance has been investigated by using two different relocation models :

a) an adapted model used in the FRAPCON fuel performance code [16];

b) an alternative model proposed by the German suppliers (former KWU) [17].

Option (a) has been applied to all 59 rods. For testing option (b), 22 fuel rods were selected. These rods cover all measured parameters of the final rod geometry in the whole range of the discharge burnup (42.5 to 51.3 MWd/kgU).

3.2. Results and discussion

For the burnup range from 42.5 to 51.3 MWd/kgU the measured and calculated results are presented in Figures 2-5. Each point represents one individual fuel rod. The fuel rod burn-up generated by the TRANSURANUS code is systematically larger than the measured values, with differences between 3 and 14 %. Similar differences are found from independent simple burn-up computations using the power history given in the IFPE database. A correction factor will have to be introduced and is still subject to clarification. Hence, the calculated and the measured quantities are compared as a function of the rod averaged burn-up measured by PIE.

3.2.1. Fuel central temperature

No temperature measurements were made for the considered WWER-1000 fuel rods. On the basis of the TRANSURANUS analyses, the hottest fuel temperature of about 1000 ^{o}C was reached in the 2nd cycle of fuel rods No. 001 and 287, at the burn-up level of 16 and 10 MWd/kgHM, respectively. The discharge burn-ups of these rods are 51 and 44 MWd/kgU, respectively. The applied linear heat rates and the calculated fuel temperatures of these “hottest” slices are presented in Figure 1.

Nevertheless, these temperatures remain below the empirical (Vitanza) threshold for fission gas release. In this phase the rod averaged burnup is 10 to 20 MWd/kgU. Close to the end of irradiation (EOL), the reactor power is about 60% of the nominal power and the fuel temperatures are low.

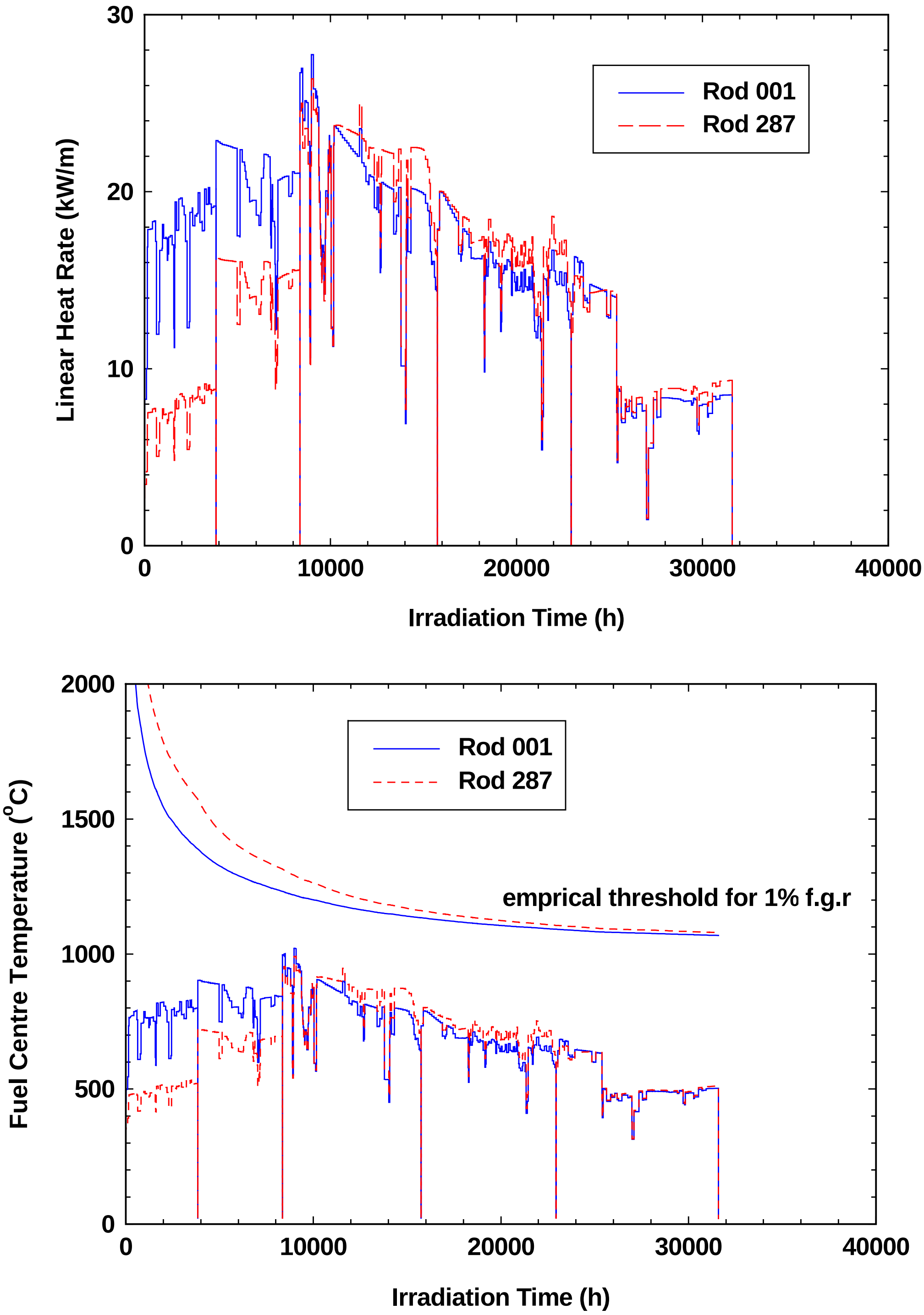

Fig. 1: Maximum linear heat rates (top) and maximum fuel central temperatures (bottom) for two fuel rods from assembly FA 0325.

3.2.2. Change of fuel rod diameter and length

The residual geometrical changes of the fuel rod are mainly influenced by two phenomena:

- the creep-down of the cladding tube due to overpressure of the coolant
- the axial growth of the cladding due to irradiation

The axial profile of the cladding outer diameter change reflects the axial distribution of the neutron flux density and the distribution of the cladding temperature up to the moment of the fuel-to-cladding contact (gap closure). For this reason, the maximum change of the cladding diameter is observed in the central (most loaded) part of the fuel rod. Thus, the difference in the average diameters of the cladding in the region of the gas plenum and the central part of the rod is used to estimate the diameter decrease. Details for the measurement techniques can be found in [18].

A wide range of examinations of geometrical rod parameters was presented at the last International Conference on WWER Fuel Performance, Modelling and Experimental Support, 2001 and 2003 [7 – 10]. The main conclusions were:

a) if the average gap is less than 12 μm in cold state, there is a tight fuel-to-cladding contact at operating temperature in the middle part of fuel rod;

b) in the fuel rods with higher discharge burn-up, pellet-cladding mechanical interaction (PCMI) considerably increases the claddding elongation.

In Figure 2 the change of the fuel rod diameter predicted by TRANSURANUS at EOL is compared with the measured value of each fuel rod. In Figure 3 we compare the predictions of the fuel rod length with the corresponding quantity measured at EOL. The experimental results for the assembly FA0325 do not show a trend as mentioned in [10]. In any case a trend is very difficult to be quantified in the available limited burn-up interval - 42.5 to 51.3 MWd/kgU. In [10] the conclusions had been made for a much larger burn-up interval – from 10 to 50 MWd/kgU.

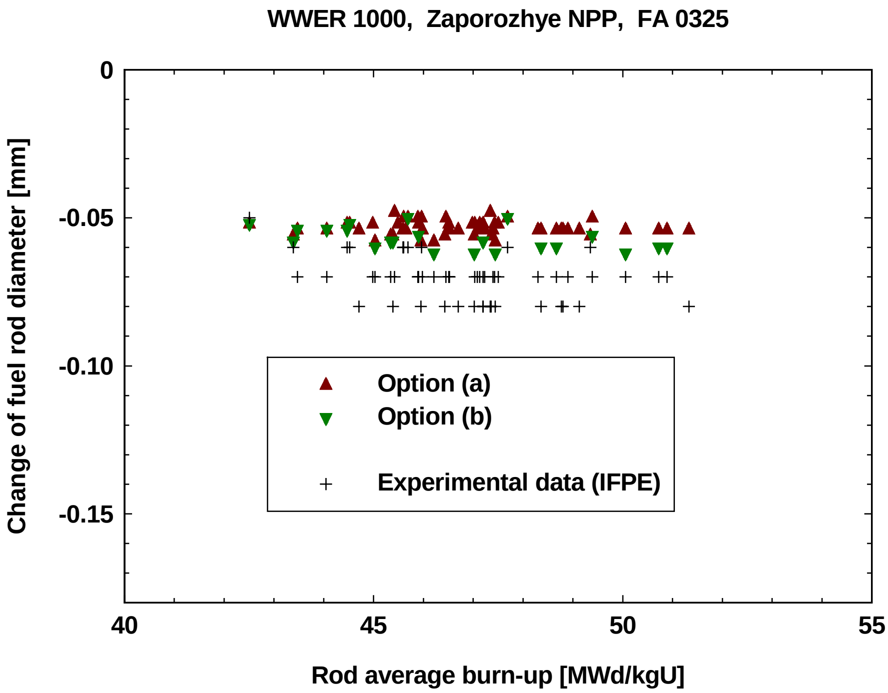

Fig. 2: Comparison of the measured change of cladding outer diameter with the corresponding calculations by the TRANSURANUS code. Two different options for fuel relocation are shown. See text for details.

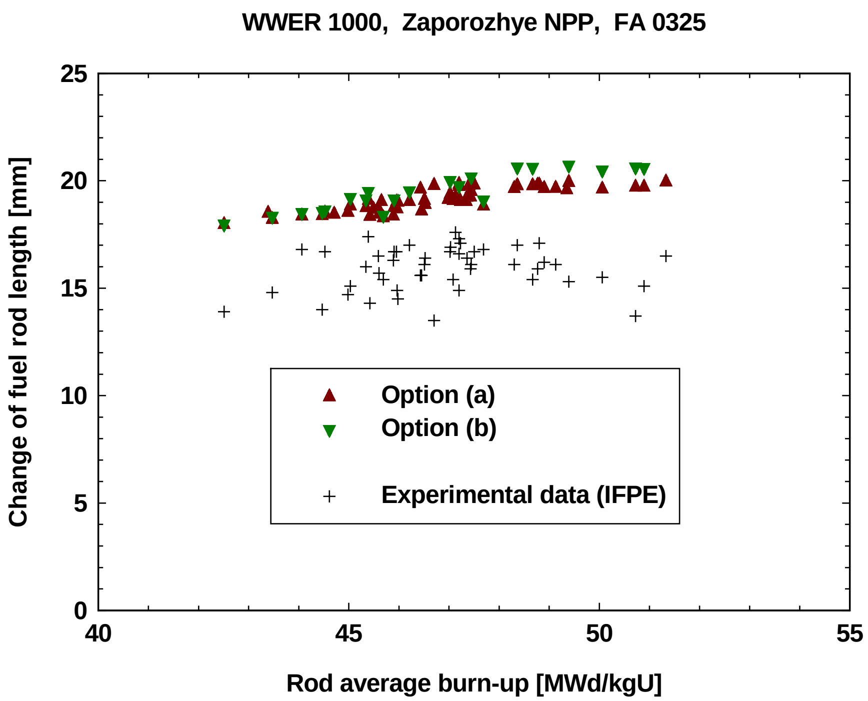

Fig. 3: Comparison of the measured cladding elongation with the corresponding calculations by the TRANSURANUS code. Two different options for fuel relocation are shown. See text for details.

Figures 2 and 3 reveal systematic differences between the measured outer fuel rod geometry and the first computations. On one hand, the calculated changes of the fuel rod outer diameter can be regarded as satisfactory, although a slight under-prediction of the diameter decrease by the TRANSURANUS code can be observed. On the other hand, an analysis of the fuel rod elongation indicates the need for further investigating the mechanical behaviour of the WWER fuel rods:

- There are considerable uncertainties in densification and swelling of the WWER-type fuel.
- The application of the standard relocation models to annular fuel needs further consideration.
- More independent experimental data are needed to test the correlation for the irradiation induced creep of the WWER-specific (Zr1%Nb) cladding. In particular, the anisotropy parameters, that are used for transforming the effective strain into the radial, tangential and axial components, could so far not be fully clarified.

3.2.3. Fuel-to-cladding gap

The diametrical fuel-to cladding gap was measured by the compression technique, with an error of $\pm$10 μm [18]. The technique does not allow measurement of gaps bigger than 130 μm. The axial distribution of the fuel-to-cladding gap shows the biggest decrease of the gap in the region of 500 to 3000 mm from the bottom of the fuel rod.

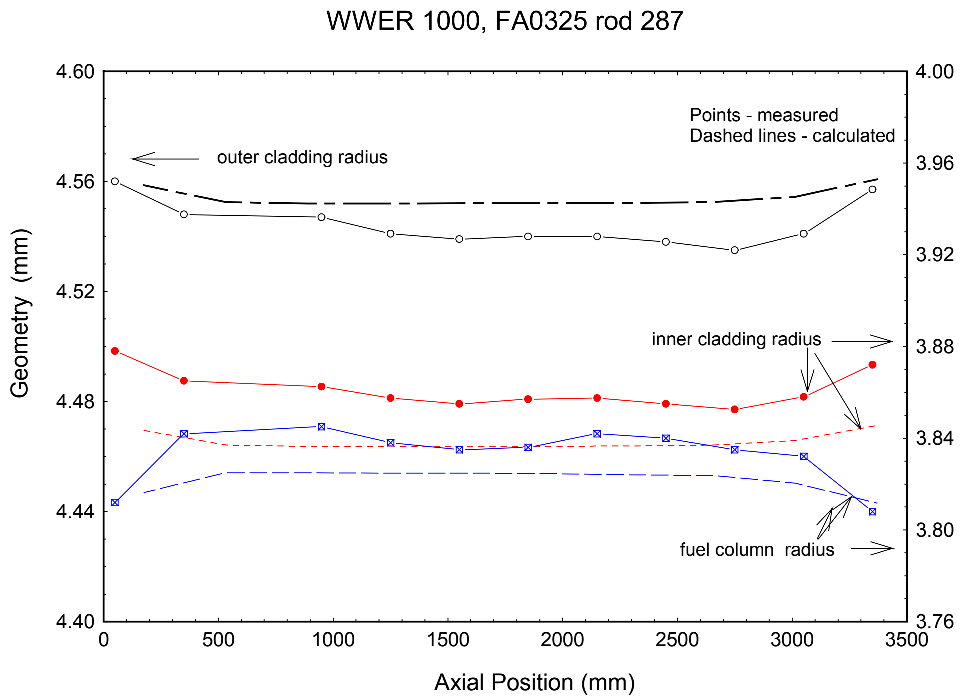

Fig. 4: Axial distribution of the fuel-to-cladding gap of one WWER-1000 fuel rod. The dots mark the experimental values, the dashed lines represent the TRANSURANUS calculation.

For illustration, the axial distributions of the fuel and cladding radii measured for one (unspecified) fuel rod [18] are given in Figure 4. They are compared with the TRANSURANUS calculations for rod No. 287, having the same averaged burnup at EOL. Considering the experimental uncertainties, the agreement is satisfactory.

Figure 5 illustrates that the final gap size at end of irradiation can be qualitatively reproduced by the TRANSURANUS code. The calculated values are averaged over the fuel rod, excluding the bottom and the top slices. The scatter of the experimental data is comparable to the above mentioned uncertainty of the gap size measurements. The dependence of the final gap size on the final rod average burn-up has a larger slope than the values calculated by the fuel performance code. However, in view of the uncertainties discussed above, any quantitative conclusion first requires a better understanding of the dependence of the final cladding geometry on the final burn-up (cf. Section 3.3).

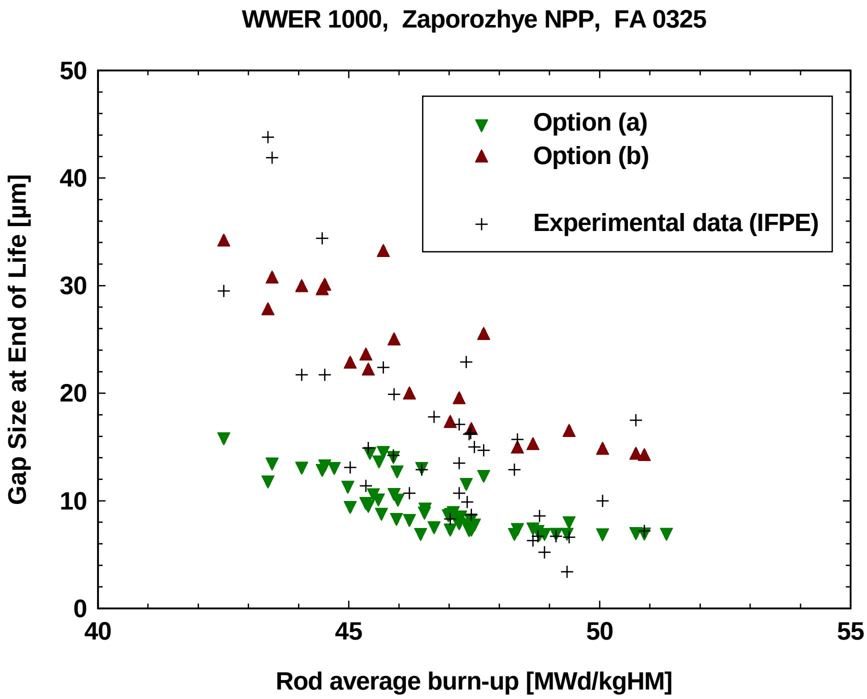

Fig. 5: Comparison of the measured size of the fuel-to-cladding gap with the corresponding calculations by the TRANSURANUS code.

3.2.4. Fission Gas Release

Figure 6 shows the measured and calculated fission gas release in the 36 WWER fuel rods for which PIE data became available. The data indicate an enhanced athermal gas release above rod averaged burn-up of 40 MWd/kgHM. This phenomenon is modeled in the TRANSURANUS code through an optional threshold for the onset of the enhanced release. The threshold is expressed in terms of local burn-up and was tuned on the basis of the Kola-3 data set. With this option, however, the TRANSURANUS code tends to under-predict the fission gas release in the high-burn-up WWER-1000 fuel.

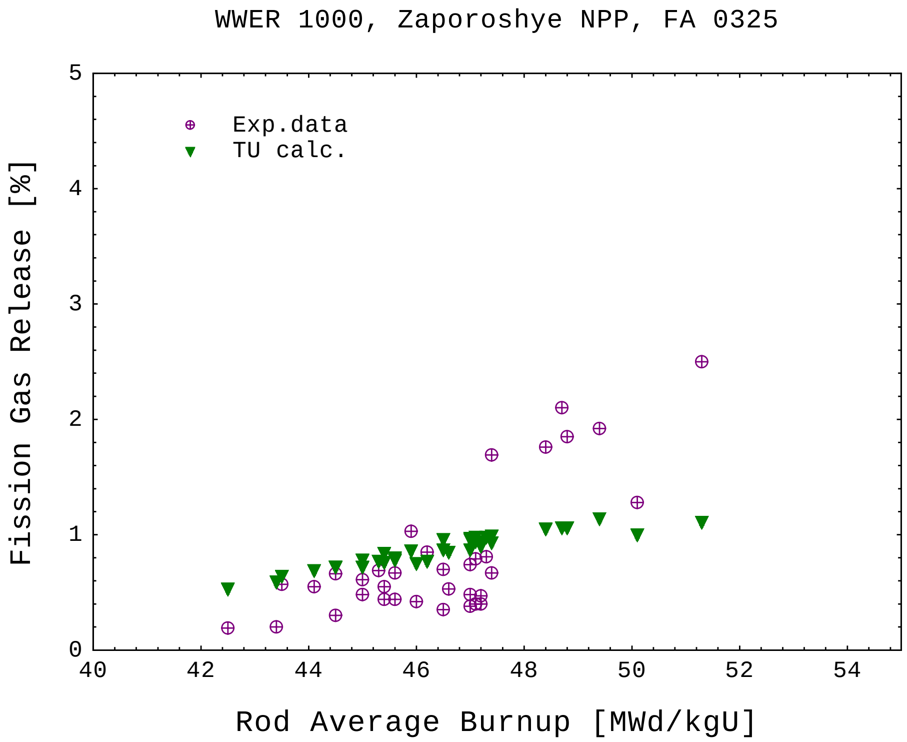

Fig. 6: Comparison of the measured fission gas release with the corresponding calculations by the TRANSURANUS code

3.3. Tests of a modified cladding deformation

The initial fuel performance computations of the WWER-1000 fuel lead to a slight systematic underestimation of the radial deformation of the fuel rods (Figure 2) and at the same time to a systematic overestimation of the axial deformation (fuel rod elongation, Figure 3). A first analysis has therefore focused on the anisotropy of the cladding deformation. Two groups of parameters are related to the transformation from the effective strain to its radial, tangential and axial components: a) the texture factors (used in the swelling correlation) and b) the anisotropy coefficients for creep (used in the flow law).

From the IFPE database, specific fuel rods could be selected where the evolution of the cladding geometry is not or only weakly influenced by the fuel column. This condition is fulfilled for the fuel rods with a final average burn-up below approx. 45 MWd/kgHM: In these cases the two different fuel relocation options shown in Figures 2 and 3 - and even a total switch-off of the relocation (not shown) - have only a negligible influence on both fuel rod elongation and fuel rod diameter. Out of this domain we have hence selected four fuel rods to be applied for parametric tests of the quasi-independent evolution of the cladding geometry.

In a first step, the response of the calculated cladding deformation (in radial and axial dimension) for the four selected fuel rods has been approximated by assuming a local linear dependence on the anisotropy parameters. For each of these rods, the "optimum" cladding texture factors (f_r, f_t, f_a) and creep anisotropy coefficients (F, G, H) have been determined by a simple fit. A mean set of anisotropy parameters is derived from the four considered rods and proposed as alternative to the parameters given in the IFPE database (Table 3).

Table 3. Proposed test option of cladding texture factors and cladding creep anisotropy coefficients derived from the experimental data of the four selected fuel rods. For comparison, the coefficients given in the IFPE database are listed as "standard" option.

Option	f_r	f_t	f_a	*F*	*G*	*H*
Standard (IFPE)	0,52	0,38	0,10	0,18	0,62	0,38
Test	0,37	0,33	0,30	0,43	0,53	0,47

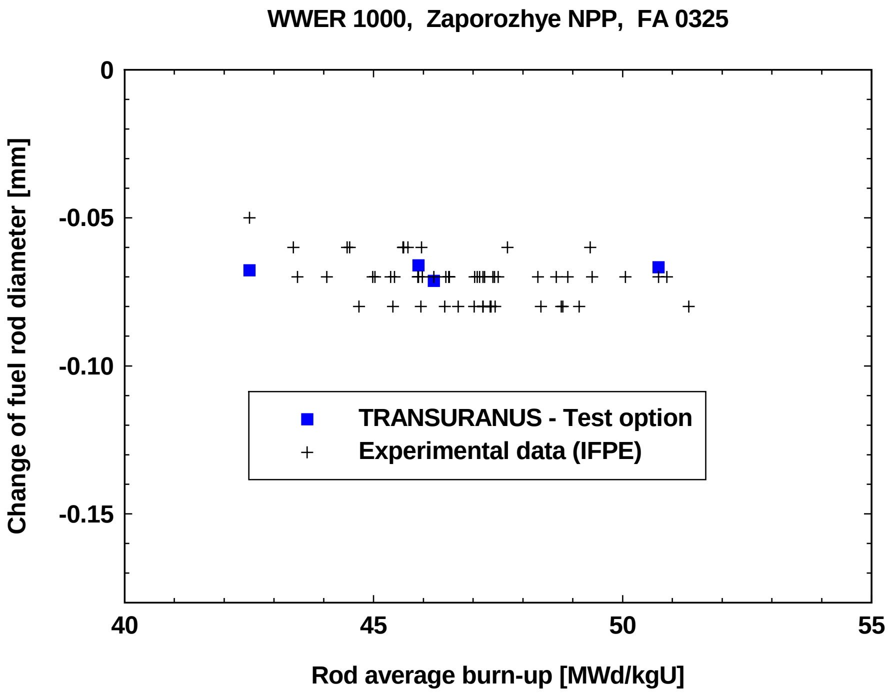

Fig. 7: Comparison of the measured decrease in fuel rod outside diameter to the quantities calculated by TRANSURANUS when applying the test option for the cladding anisotropy coefficients. See text for details.

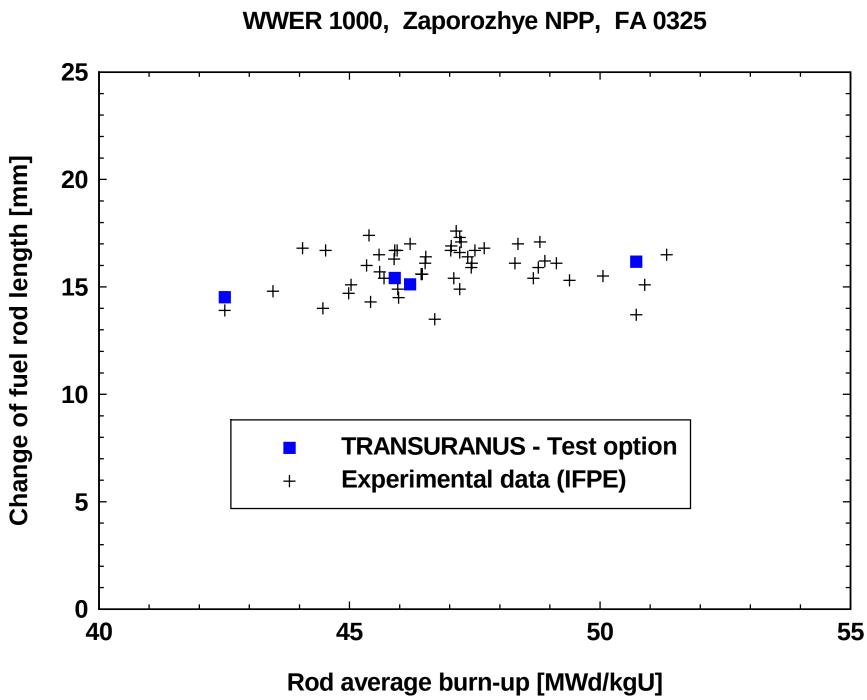

Fig. 8: Same as Fig. 7, but for the increase in fuel rod length (elongation).

The test option has been applied to the “low burn-up” fuel rod and to three additional rods of the fuel assembly FA 325 with a higher final burn-up. The results are shown in Figures 7 and 8 and compared to the same experimental data as in Figures 2 and 3. A first comparison is encouraging, although surprisingly the fit results are more close to an isotropic behaviour. Nevertheless, one should keep in mind that the present approach is purely empirical. For profound verification, further calculations will have to be based on independent experiments.

4. Summary and conclusions

Recently released experimental data on irradiated WWER-1000 fuel rods of the IFPE database [5] provide a valuable pool of information for verification and refinement of the WWER version of the TRANSURANUS fuel performance code. A first comparison between the measured and calculated geometry of selected WWER-1000 fuel rods at end of irradiation can be summarized as follows:

The experimentally observed trends for the dependence of rod outer diameter change and final gap size on the final burn-up can be satisfactorily reproduced. However, a comparison of the measured and calculated fuel rod elongation underlines the need for further investigating the material properties of the WWER-specific (Zr1%Nb) cladding. Tests have confirmed the feasibility for a self-consistent empirical adjustment of the cladding anisotropy coefficients. Although the results are encouraging, it should be critically reviewed to which extent this approach is compatible with material theory.

Evidently the deformation of the cladding is a key factor for the correct simulation of the fuel-to-cladding gap. Any revision of the anisotropy factors will have a direct impact on the slope of the calculated gap sizes. After completion of this step, the relocation and swelling of WWER fuel will have to be further analyzed.

For extending the verification, further WWER-1000 as well as WWER-440 fuel rods will have to be simulated. The simulations should include independent irradiation experiments. As complement to the information available from the IFPE database, we will apply the original datasets of WWER fuel irradiated at the OECD Halden reactor.

Acknowledgements

The authors would like to thank Klaus Lassmann, author of the TRANSURANUS fuel performance code, for many interesting discussions and critical comments. The manuscript has benefited considerably from a critical review by Csaba Györi (ITU Karlsruhe)

References

1 K. Lassmann, "TRANSURANUS: a fuel rod analysis code ready for use", Journal of Nuclear Materials, Vol. 188, pp. 295-302, 1992.

2 D. Elenkov, K. Lassmann, "The development of the TRANSURANUS-WWER version", Third International Seminar on WWER Fuel Performance, Modelling and Experimental Support, Pamporovo, Bulgaria, 4-8 October 1999, pp. 245.

3 E K. Lassmann, A. Schubert, J. van de Laar, C. Györi, D. Elenkov, M. Cvan, B. Hatala, "The Status of the TRANSURANUS-PECO Co-operation (PECO-1 Project)", March 2002, ITU-report JRC-ITU-TN-2002/10.

4 P. Van Uffelen, K. Lassmann, A. Schubert, J. van de Laar, C. Györi, D. Elenkov, B. Hatala, "Review of Operational Requirements with Respect to PCMI in a VVER and the Corresponding Developments in the TRANSURANUS Code", International Seminar on Pellet-Clad Interaction in Water Reactor Fuels (PCI-2004), CEA Cadarache/DEN/DEC, Hôtel Novotel Pont-de-L'Arc, Aix en Provence, France, 9-11 March 2004.

5 The Public Domain Database on Nuclear Fuel Performance Experiments for the Purpose of Code Development and Validation, International. Fuel Performance Experiments (IFPE) Database, in: http://www.nea.fr/html/science/fuel/ifpelst.html (2005).

6 SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, NUREG/CR-0200, Rev. 6 (ORNL/NUREG/CSD-2/R6), December 1999.

7 D. Markov et al., "Validation of WWER-1000 fuel rod efficiency at operation during four fuel cycles", Third International Seminar on WWER Fuel Performance, Modelling and Experimental Support, Pamporovo, Bulgaria, 4-8 Oct. 1999, pp. 147.

8 B. Kanashov, S. Amosov, G. Lyadov, D. Markov, V. Ovchinnikov, V. Polenok, A. Smirnov, A. Sukhikh, E. Bek, A. Yenin, V. Novikov, "Change in Geometrical Parameters of WWER High Burnup Fuel Rods under Operation Conditions and Transient Testing", 4th International Conference on WWER Fuel Performance, Modelling and Experimental Support, Albena, Bulgaria, 1-5 October 2001, pp. 88.

9 A. Smirnov et al., Int. Conference on WWER Fuel Performance, Modelling and Experimental Support, Albena, 2001, p. 63.

10 A. Smirnov et al., Int. Conference on WWER Fuel Performance, Modelling and Experimental Support, Albena, 2003, p. 267.

11 F. Ovchinnikov et al., in "WWER in operation", M., Atomizdat, 1977.

12 H. Matzke, "Gas release mechanisms in UO_2 - a critical overview", Radiation Effects, Vol. 53, pp. 219-242, 1980.

13 R. J. White, M. O. Tucker, "A new mechanistic model for the calculation of fission gas release", International Topical Meeting on LWR Fuel Performance, West Palm Beach, Florida, 1994, pp. 196-202.

14 Y. K. Bibilashvili et al., "Main examination results of WWER-1000 fuel after its irradiation in power reactors", International Seminar WWER Reactors Fuel Performance, Modelling and Experimental Support, Varna, Bulgaria, 7-11 November 1994, pp. 175.

15 A. Schubert, C. Györi, D. Elenkov, K. Lassmann, J. van de Laar, "Analysis of Fuel Centre Temperatures with the TRANSURANUS Code", International Conference on Nuclear Fuel for Today and Tomorrow - Experiences and Outlook, ENS TopFuel 2003 / ANS LWR Fuel Performance Meeting, Track 1 (proceedings available on CD only from Inforum GmbH, Bonn), Würzburg, Germany, 16-19 March 2003.

16 FRAPCON-3: A Computer Code for the Calculation of Steady-State, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup, NUREG/CR-6534-V2, (PNNL-11513-V2), December 1997.

17 R. Eberle, D. Stegemann, W. Wiesenack, "Comparison of HBWR fuel rod experiments to calculations with SATURN-L (paper 18, HPR 195)", 1976, pp. 7.

18 A. V. Smirnov, B. A. Kanashov, S. V. Amosov, "Geometrical parameters of the fuel rod claddings of WWER-440 after 4 and 5 cycles and of WWER-1000 after 3 and 4 cycles of operation", Technical Committee Meeting on Fuel Behavior under Transient and LOCA Conditions, Halden, Norway, 10-14 September 2001.