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APPLYING THE TRANSURANUS CODE TO VVER FUEL UNDER ACCIDENT CONDITIONS

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ABSTRACT

The TRANSURANUS code development started in 1973 and initially focused on fuel pins for fast breeder reactors. There was a shift in 1992 towards LWR applications. The VVER version of the code has been under development since the mid 90s. Specific thermal and mechanical properties for Nb-containing cladding and specific correlations for annular UO_2 fuel pellets were implemented to simulate fuel rod performance under normal operating conditions.

Simulation of accident conditions came to the front in the EXTRA project, which was completed in 2003. The project focused on the development of a data-base for Zr1%Nb cladding and on the elaboration of new models and correlations for plastic deformation, high-temperature oxidation and cladding failure. The new models were incorporated into the TRANSURANUS code and validated against burst tests for as-received, oxidised, and irradiated cladding specimens. Furthermore, the upgraded version of the code was applied for assessing the fulfilment of safety acceptance criteria in design basis accidents. An example for the modelling of fuel rod performance in large break LOCA is presented.

In the follow-up project of EXTRA it is intended to account for the hydrogen uptake by the cladding material under accident conditions, which have detrimental effects on the mechanical properties of the cladding. New experiments concerning the oxidation kinetics, the mechanical strength and the embrittlement of hydrogen charged cladding are carried out at the AEKI (KFKI Atomic Energy Research Institute) in Hungary. The experimental program and its recent results are demonstrated.

Finally, an outlook is given about the planned activities for code development. The experimental data of the new tests are to provide background for the development of new correlations and the improvement of the present models.

Keywords: Zr1%Nb cladding, oxidation, plastic deformation, hydrogen uptake, TRANSURANUS code, safety analysis

1. INTRODUCTION

Due to its flexibility, the TRANSURANUS fuel performance code [1] developed at the JRC Institute for Transuranium Elements (ITU) is widely used in the safety evaluation of fuel rods for various types of nuclear reactors in Europe. The code has a materials data bank for oxide, mixed oxide, carbide, and nitride fuels, Zircaloy and steel claddings, and different coolants. The scope of the covered phenomena and the numerical solution methods enable the code to simulate both long fuel cycles and hypothetical accidents. Options for probabilistic analysis are also involved in order to provide the possibility of a statistics-based evaluation.

New fuel licensing procedures established in the East-European countries entail the utilization of the TRANSURANUS code for VVER reactors as well. The VVER version of the code has therefore been developed since 1995 in the framework of international co-operations in different EU founded projects [2]. The present status for steady-state applications has already been summarised [3].

In one of the recent projects – accomplished in the EURATOM 5th framework program – emphasis was put on the nuclear fuel performance during design basis accidents. This project, called EXTRA (***EX**tension of **TR**ANSURANUS Code **A**pplicability with Niobium Containing Cladding Models*) [4] focused on the simulation of the Zr1%Nb cladding performance under accident conditions. The project had two main objectives: (1) the compilation of a new database containing VVER-specific experiments to provide an appropriate background for model development and code validation and (2) the improvement of the TRANSURANUS fuel performance code via the incorporation of newly developed correlations for off-normal conditions. Extensive code validation computations and the applications in the safety analyses of VVERs were also carried out in the project. The main results of this project are summarised in the second part of the present paper.

A follow-up project, involving the ITU and the AEKI, has been in progress since December 2004 to model the effects of hydrogen uptake on cladding oxidation and mechanical strength. The need to launch this project stems from the observations during the cleaning incident at the Paks NPP in April 2003 [5], indicating that hydrogen uptake played a significant role in the mechanical deterioration of the cladding material. This effect, however, was not accounted for in the thermo-mechanical computations of the fuel performance code. In order to tackle this problem, both an experimental program and a plan for model developments were launched. In this paper, we report on the first part of the experimental program, and subsequently summarise the perspectives of the project.

2. INCLUSION OF CLADDING OXIDATION UNDER ACCIDENT CONDITIONS

2.1 *Experimental database*

Since the beginning of the 90s several experimental series have been performed at the AEKI to map and to compare the oxidation kinetics and the mechanical properties of Zr1%Nb and Zircaloy-4 claddings in the temperature range of 20-1200^{o}C. The experimental program has covered ballooning tests with single rods and small bundles, tensile tests, ring compression tests and steam oxidation tests. The released database finally comprised the data of nearly 400 individual separate effect tests [6].

The most important results of the oxidation and mechanical experiments can be summarized as follows:

- The measured data confirmed the square root relationship between oxidation rate and time, indicating a diffusion-controlled process. The oxidation kinetics of the Zircaloy-4 and the Zr1%Nb alloys are very similar. However the microstructures of the oxide layers are different. The oxidation of Zr1%Nb below 1100^{o}C results in a multilayer ZrO_2 structure due to a periodic break-away phenomenon. A compact oxide layer evolves on this alloy if the oxidation temperature exceeded 1100^{o}C. The hydrogen uptake during the oxidation strongly depends on the oxide layer morphology: a compact ZrO_2 layer impedes the H_2 absorption of the Zr1%Nb only above 1100^{o}C. On the other hand, the oxidation of Zircaloy-4 indicates more compact oxide layer and consequently only limited H_2 absorption in the temperature range of 900-1100^{o}C. These results are consistent with Böhmert's observations [7].
- The mechanical behaviour of the Zircaloy versus Zr1%Nb alloys is also comparable. However, the burst experiments revealed that in the temperature range of 800-1000^{o}C the mechanical strength of the Zr1%Nb cladding is lower than that of the Zircaloy-4 tube. This can be explained by the different α-β crystallographic phase transition temperatures of these alloys, since the Nb content decreases the transition temperature by about 100^{o}C.

- Absorbed oxygen stabilizes α-Zr, causing a multilayer structure and increasing the hardness in the outer region of the cladding. At low oxygen concentration this phenomenon results in a slight increase in cladding strength in general. On the other hand, the growth of the α layer with further oxidation and the incursions of α-phase structures in the β layer result in a cladding embrittlement. The cladding oxidation process is often characterised in terms of the so-called Equivalent Cladding Reacted (ECR), which corresponds to the quotient of the weight of the instanteneous mass increment and the mass increment after the total oxidation of the cladding. The experiments clearly prove that the strength of the alloy increases for up to about 15 µm oxide layer thickness, corresponding to an ECR ≈ 2 %, but considerably decreases with further oxidation. This phenomenon was observed consistent in both tensile and the burst tests performed at low and high temperatures, respectively (Fig. 1 and 2).

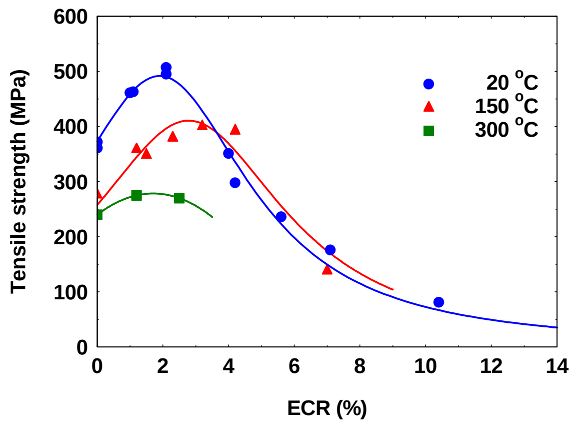

Fig. 1: Effect of cladding oxidation on tensile strength of Zr1%Nb specimens.

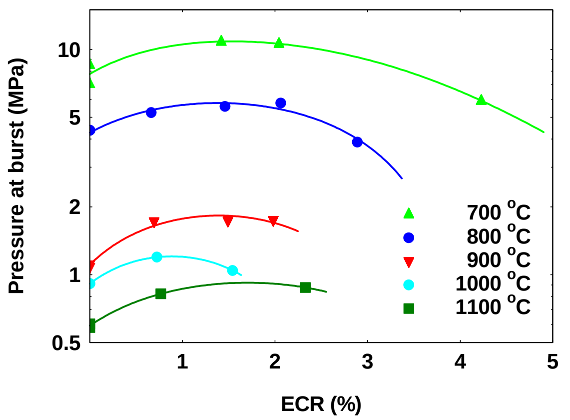

Fig. 2: Effect of cladding oxidation on burst pressure of Zr1%Nb tubes.

2.2 *New models for Zr1%Nb cladding*

The prediction of the plastic deformation, the extent of oxidation and the rupture of the cladding tube overheated under LOCA conditions is a key issue in safety analyses of pressurized water reactors. In order to assist the safety evaluation of VVER nuclear fuels, new deformation and oxidation rate correlations as well as adequate failure criteria were developed for the Zr1%Nb cladding, and were incorporated into the TRANSURANUS fuel performance code.

2.2.1. Deformation rate

The one-dimensional mechanical model of the TRANSURANUS code is based on a semi-analytic solution of the principal mechanical equations for the radial deformation (i.e., the expressions of the non-elastic strains involved in the analytic formula are integrated numerically along the radius). The non-elastic strain components are calculated incrementally in time. The increments of the equivalent (or effective) creep or plastic strain can be defined through an optional non-linear function of the equivalent stress. In conformity with this model, the large plastic deformation (i.e., ballooning) of the cladding in the temperature range of 600 – 1200°C was handled by means of a new strain rate correlation in the form of a modified Norton power equation (Eq. 1). This correlation expresses the equivalent strain rate of the Zr1%Nb cladding as a function of temperature, the equivalent stress, the weight fraction of α-zirconium and the absorbed oxygen in the cladding. In this manner, the relevant effects of both the crystallographic phase transition and the cladding oxidation produced on the strength and deformation of the cladding can be simulated in an accurate way:

$$\dot{\bar{\varepsilon}} = \varphi_\alpha k_\alpha \exp\left(\frac{-Q_\alpha}{RT} + b_\alpha(x)\right)\bar{\sigma}^{n_\alpha} + (1-\varphi_\alpha) k_\beta \exp\left(\frac{-Q_\beta}{RT} + b_\beta(x)\right)\bar{\sigma}^{n_\beta} \qquad (1)$$

where $\dot{\varepsilon}$ is the effective strain rate (1/s), $\overline{\sigma}$ is the effective stress (MPa), φ_α is the weight fraction of the α zirconium, R is the universal gas constant in $Jmol^{-1}K^{-1}$, T is the temperature in K, k_α and k_β are the strength coefficients, Q_α and Q_β are the activation energies for the plastic deformation, n_α and n_β are the stress exponents and $b_\alpha(x)$ and $b_\beta(x)$ are the oxygen concentration (x) terms for the α and β crystallographic phases of the Zr1%Nb alloy, respectively.

The so-called Norton parameters (k, Q, n) were fitted to the data of isothermal cladding burst tests through an advanced multidimensional minimization procedure based on the Levenberg-Marquardt algorithm [8]. The tests were performed at the AEKI [9] and at the Kurchatov Institute (Russia) [10] simulating linear pressure increase rate in inert (argon) atmosphere. The χ^2 merit function of the minimization was based on the comparison of measured and calculated times to cladding burst in the following form:

$$\chi^2(\underline{a}) = \sum_{i=1}^{N} \left[\log(\tau_i) - f(\underline{w}_i, \underline{a})\right]^2 \qquad (2)$$

where τ is the measured time to burst, $f(\underline{w}, \underline{a})$ is an appropriate analytic model for the logarithm of the time of failure as a function of the experimental constants ($\underline{w}$) and the Norton parameters ($\underline{a}$) [11], and N is the number of the tests.

The optimization process was carried out in two temperature intervals, 600-800°C and 900-1200°C, corresponding to the different crystallographic phases of the Zr1%Nb alloy. The two resulting sets of Norton parameters for the α and β-phases, as well as their standard deviations are summarized in Table 1.

Table 1. Norton parameters for unoxidised Zr1%Nb cladding. Results of Levenberg Marquardt optimization.

	Norton parameter		Standard deviation
α-phase (600 - 800 °C)	k_α	$6.1 \cdot 10^6$	$7.8 \cdot 10^6$
	Q_α	$3.6 \cdot 10^5$	$1.1 \cdot 10^4$
	n_α	5.18	0.34
β-phase (900 - 1200 °C)	k_β	1.4	1.4
	Q_β	$1.8 \cdot 10^5$	$1.1 \cdot 10^4$
	n_β	5.82	0.47

The effect of the cladding oxidation on the ballooning process is represented through the oxygen concentration terms $b_\alpha(x)$ and $b_\beta(x)$ in Eq. (1). These terms were evaluated by sensitivity analysis on the Norton parameters by using a perturbation function $\psi(x)$ on the relative strength of the cladding. $\psi(x)$ was fitted to experimental data as indicated in Fig. 3. The perturbation resulted in the variation of the strength coefficient (k) described by polynomial approach as follows:

$$b(x) = \ln(k'/k) = c_3x^3 + c_2x^2 + c_1x + c_0 \qquad (3)$$

where x is the oxygen weight concentration in the cladding and k' and k indicate the strength coefficient of the oxidised and unoxidised claddings, respectively. The $c_0 \dots c_3$ coefficients of the polynomial are reported in Table 2. Figure 4 shows the oxygen concentration terms for the α and β crystallographic phases of the cladding, and shows the relationship between x and the ECR.

Table 2. Polynomial coefficients for the oxygen concentration term of the Zr1%Nb-specific strain rate correlation.

		c_3	c_2	c_1	c_0
α-phase	$0 < x < 0.02$	$-6.7 \cdot 10^5$	$4.9 \cdot 10^4$	$-5.7 \cdot 10^2$	0
	$0.02 \le x < 0.1$	$2.3 \cdot 10^4$	$-6.4 \cdot 10^3$	$7.4 \cdot 10^2$	-9.5
β-phase	$0 < x < 0.02$	$-7.4 \cdot 10^5$	$5.5 \cdot 10^4$	$-6.3 \cdot 10^2$	0
	$0.02 \le x < 0.1$	$2.6 \cdot 10^4$	$-7.1 \cdot 10^3$	$8.2 \cdot 10^2$	-10.5

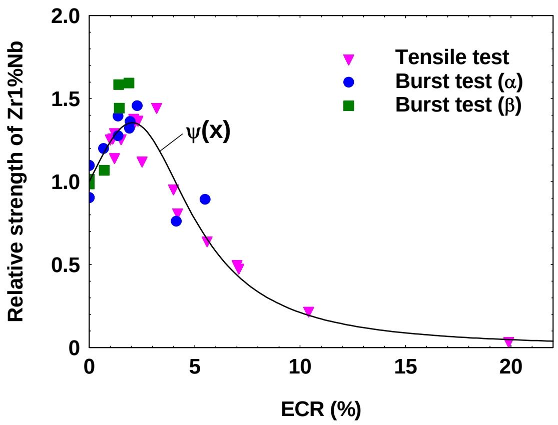

Fig. 3: Effect of cladding oxidation on the relative strength of Zr1%Nb. Experimental data are indicated by symbols.

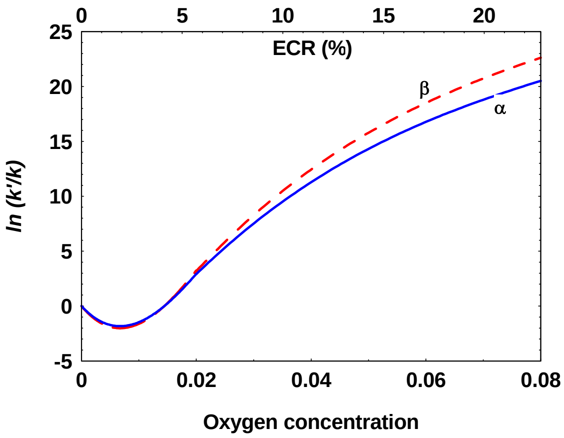

Fig. 4: Effect of oxygen concentration on the strength coefficient. Results of sensitivity analyses.

On the other hand, the strain-rate correlation does not contain any dependence on neutron flux to simulate irradiation effects. Due to limited cladding corrosion in VVER reactors and because of thermal annealing, the ductility of the irradiated Zr1%Nb cladding above 600°C is similar to that of the un-irradiated cladding. Therefore, the mechanical performances of the irradiated and the un-irradiated Zr1%Nb cladding tubes under accident conditions are very similar, as it has been proved by Russian experiments [10].

2.2.2. Oxidation rate

The cladding-steam reaction model of the TRANSURANUS code is based on parabolic kinetic correlations for both the oxygen mass gain and ZrO_2 layer thickness growth. The extent of oxidation is computed by the well-known recursive formula:

$$X_i = \sqrt{X_{i-1}^2 + K^2 \, \Delta\tau} \qquad (4)$$

where X_i and $X_{i\text{-}1}$ represent the extent of oxidation (mass gain or oxide layer thickness) in the actual and in the previous time steps, respectively. $\Delta\tau$ is the time step and K is the actual reaction rate constant which is defined as a function of the temperature through an Arrhenius relation.

The oxygen concentration used in the strain-rate equation is to be calculated with a best estimate formula of the oxygen mass gain rate derived by least–square fitting to experimental data of Zr1%Nb cladding in the temperature range of 500 – 1200°C:

$$K_m = 658 \exp(-10200/T) \qquad (5)$$

where K_m is the oxygen mass gain rate in mg/cm^2/s$^{0.5}$ and T is the cladding temperature in K.

In addition to the AEKI best-estimate relation, optional correlations like the Zr1%Nb-specific Solyany model [12], the Baker-Just correlation [13], the Leistikow correlation [14] and the Cathcart-Pawel model [14] were also incorporated into the TRANSURANUS code.

2.2.3. Cladding failure criteria

For the simulation of complex fuel rod performance under postulated accidents, the implementation of an appropriate cladding failure criterion is essential. The cladding failure is generally predicted on the basis of a stress assessment, i.e., the comparison of the calculated tangential stress with a distinct failure threshold. On the other hand, due to the significant uncertainty of the stress computation at large cladding deformation, a strain-based failure criterion can be appropriate for LOCA conditions. By considering both of these possibilities, two optional criteria were incorporated into the TRANSURANUS code:

The **first criterion** is a typical stress-based evaluation: cladding failure is indicated when the true tangential stress (σ_{tB}) exceeded the threshold stress defined on the basis of experimental data:

$$\sigma_{tB}[MPa] = \begin{cases} \kappa(3.05\cdot 10^{-4}\ T^2 - 1.13\,T + 922) & T \le 1179K \\ \kappa(4.97\cdot 10^{-5}\ T^2 - 0.15\,T + 126) & 1549K > T > 1179K \\ \kappa\, 6.70 & T \ge 1549K \end{cases} \qquad (6)$$

The effect of cladding oxidation on the true burst stress is considered through the multiplication factor κ:

$$\kappa = \exp(-32.5\,x) \qquad (7)$$

where x is the oxygen weight concentration in the cladding.

As the threshold stress can be handled in the TRANSURANUS code as a statistical variable with a given distribution, similarly to other material properties, the likelihood of the fuel rod failure can be analysed on a statistical basis, as well.

The **second failure principle** is a simple plastic instability criterion based on the simultaneous assessment of the effective true strain and the strain rate. When both the strain and the strain rate exceed the threshold values of 0.02 and 100 1/h, respectively, the cladding is assumed inhermetic. This failure criterion was introduced particularly for LOCA conditions and the threshold values of the strain and the strain rate were derived from data of cladding ballooning tests.

2.3 Validation of the extended TRANSURANUS code

The validation of the extended TRANSURANUS code has covered the comparison of the code results with analytic solutions for simplified cases (e.g., isothermal conditions), and the post-test analyses of high temperature cladding oxidation experiments and cladding burst test performed with Zr1%Nb tubes under different conditions. For the sake of brevity, only the results of the TRANSURANUS post-test analyses are summarized here.

2.3.1. Simulation of cladding oxidation tests

Altogether 122 cladding oxidation tests performed in a steam atmosphere in the temperature range of 500 – 1200^{o}C were simulated by the TRANSURANUS code. The oxidation of the Zr1%Nb specimens was calculated using both the AEKI best-estimate and the Solyany reaction rate correlations. The evaluation of the simulations was based on the comparison of the calculated and the measured oxygen mass gain data. The results are presented in Fig. 5 and 6. The satisfactory agreement between the calculations and the measurements is evident; however, two tendencies can be observed: (1) The Solyany reaction rate correlation results in over-predicted mass gain as compared to the experimental data, as well as to the results of the AEKI model. This indicates the conservatism of the Solyany model in the computation of the equivalent cladding oxidation. (2) The computation with the AEKI correlation slightly over-predicts the mass gain at moderate oxidation, when the cladding temperature is below 900°C, or the exposition time is very short.

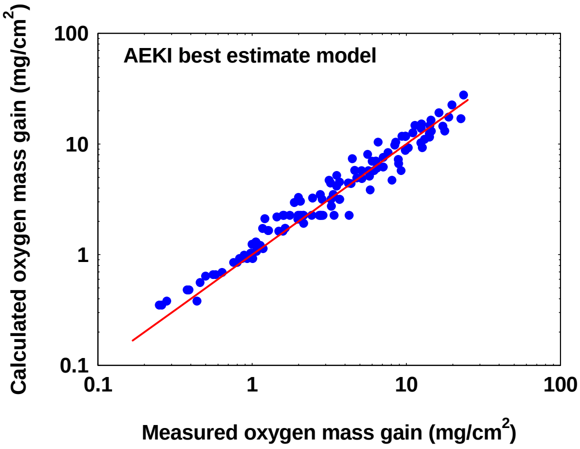

Fig. 5: Calculated versus measured oxygen mass gain. The TRANSURANUS computations were carried out with the AEKI oxidation rate correlation.

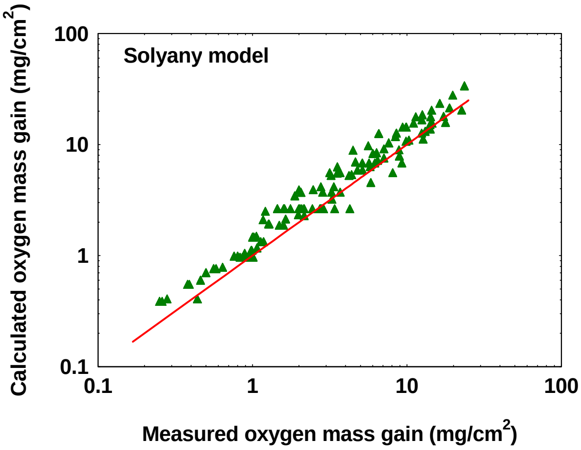

Fig. 6: Calculated versus measured oxygen mass gain. The TRANSURANUS computations were carried out with the Solyany oxidation rate correlation.

2.3.2. Simulation of cladding burst tests

The analysis of cladding ballooning tests of the AEKI, the Kurchatov Institute (KI) and the Forschungszentrum Karlsruhe (FZK) [15] constituted the kernel of the TRANSURANUS code validation for LOCA conditions. These test series covered a wide scope of simulated LOCA conditions concerning pressurization rate, temperature increase rate and oxidation between 600 and 1200°C: The AEKI and the KI tests were performed under isothermal conditions in inert atmosphere at linear pressure increase with as-received and pre-oxidised specimens of original cladding tubes. Sections of irradiated commercial fuel rods were also involved in the tests of the KI in order to investigate the behaviour of high burnup fuel cladding. The FZK tests were carried out in a steam atmosphere at constant loading pressure and linear temperature increase. The specimens were original VVER cladding tube segments with the lengths of 50 mm, 150 mm and 475 mm in the AEKI, KI and FZK tests, respectively.

The computations were carried out case-by-case for altogether 214 experiments. Figure 7 represents the calculated strain history of a typical isothermal (700°C) ballooning test with pre-oxidised cladding tube (ECR= 5.5%) at linear pressure increase. The marked point indicates the residual tangential deformation of the specimen measured after the test. Unfortunately, the tube ballooning process had not been recorded online during the experiments, and the residual deformations measured after the tests showed relatively large deviations. Therefore, the highly non-linear ballooning process was characterised with the time to burst and the evaluation of the code simulations was based on this parameter. Figure 7 clearly visualizes the effect of cladding oxidation on the calculated strain history, as well. The dashed line represents a case where the oxygen concentration of the cladding was not considered in the strain rate relation ($b(x)$= 0) and consequently both the time of burst and the tangential strain increased as compared to the corresponding data of the oxidised cladding ($b(x)$= 2.52).

Presenting the calculated time to failure versus the measured time to failure for all the simulated tests we could get an overall view of the TRANSURANUS simulations (Fig. 8). The comparison indicated that the extended code predicts the time of burst of the Russian Zr1%Nb cladding reliably for a wide range of situations representing slow as well as fast experiments, with as-received, oxidised or irradiated cladding specimens.

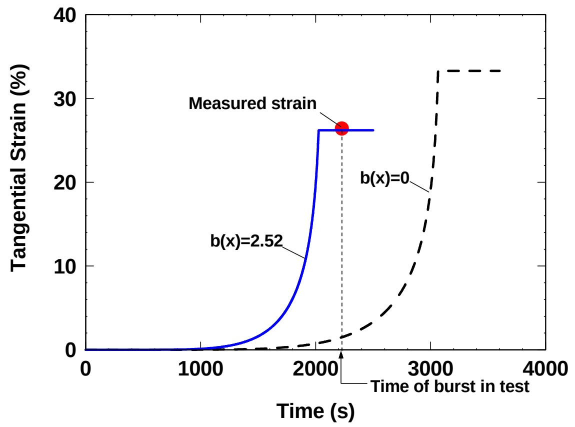

Fig. 7: Calculated tangential strain histories for oxidised and unoxidised Zr1%Nb cladding. Results of TRANSURANUS analyses of a burst test with a pre-oxidised specimen.

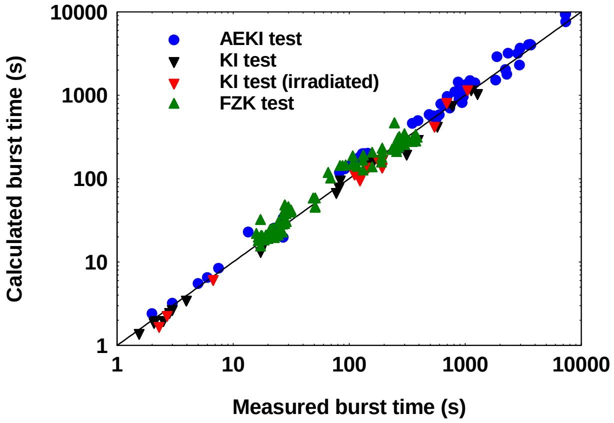

Fig. 8: Calculated versus measured times to cladding burst. Results of TRANSURANUS analyses of 214 Zr1%Nb tube burst tests.

2.4 Application of the extended TRANSURANUS code

The extended TRANSURANUS code is being used for the evaluation of fuel safety in accidents. In design basis accidents (DBA) analyses the TRANSURANUS code is applied to complement the thermohydraulic simulations for a more precise verification of the fuel-related acceptance criteria and for the prediction of the number of failed fuel rods. An analysis of VVER fuel rod performance in large-break LOCA is illustrated below.

The postulated accident is a 200% (2F) guillotine type break in the cold leg of a VVER-440/213 unit at the nominal power. In addition, a single failure of the passive emergency core cooling system was also assumed, e.g., one hydro-accumulator connected to the upper plenum of the reactor pressure vessel could not be activated. The thermohydraulic analysis of this accident was performed by means of the ATHLET system code [16]. The cladding temperature history in five specific elevations of the hot fuel rod is presented in Fig. 9, indicating a relatively long time period of overheating with the maximum temperature of 1013^{o}C at the middle of the active length. The emergency core cooling system provides the total quenching of the core at 330 s after the transient initiation. The histories of the system pressure and the fuel rod internal pressure are represented in Fig. 10. The pressure difference changes its sign after 23 s, resulting in positive tangential stress in the cladding wall.

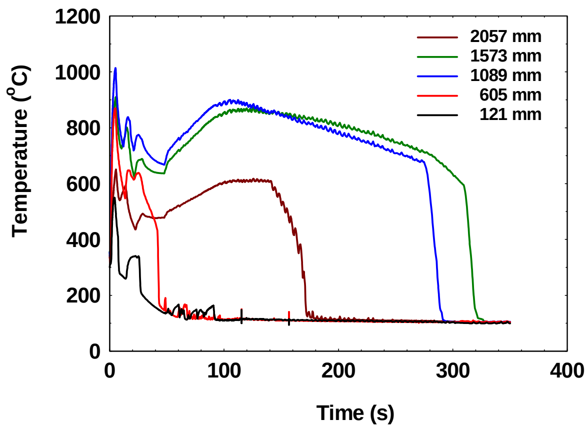

Fig. 9: Cladding temperature of hot fuel rod in a hypothetical 2F-LBLOCA

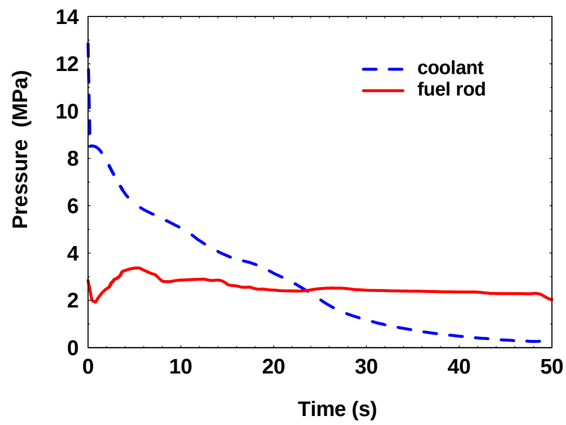

Fig. 10: Fuel rod and coolant pressure histories in a hypothetical2F-LBLOCA

Two TRANSURANUS runs were carried out to study the mechanical performance of the hot fuel rod and the effect of the cladding oxidation. In the first computation the oxygen concentration of the cladding was taken into account in the strain rate equation, whilst in the second analyses this effect was eliminated and so the deformation rate of unoxidised cladding was considered. According to the computations, the maximum of the local ECR due to Zr-steam reaction is approximately 1%. At this low level of cladding oxidation, a positive effect was observed in the mechanical performance of the fuel rod. Namely, the slight oxidation decreased the deformation rate and increased the strength of the cladding, helping to avoid large ballooning and the consequent failure of the fuel rod. This is consistent with the results of the AEKI ballooning tests with pre-oxidised cladding tubes. Figures 11 and 12 illustrate the tangential strain as a function of the time and the elevation for the oxidised and for the unoxidised cladding, respectively. Due to the considerable overheating, the cladding becomes plastic in an approximately 1 m long segment at the middle of the heated length. At the beginning of the transient, the outer pressure exceeds the rod inner pressure and the plastic deformation is negative, i.e., the cladding collapses into the gap. As the pressure difference becomes positive and the temperature exceeds 800^{o}C the cladding starts ballooning. The extent of the deformation highly depends on the level of oxidation. The calculated maximum residual strains are on the order of 5% and 15% for the oxidised and for the unoxidised claddings, respectively.

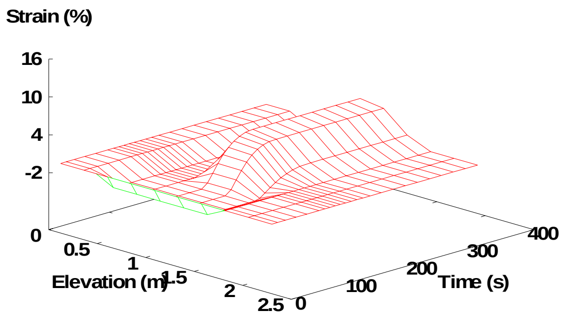

Fig. 11: Tangential strain of an oxidised cladding in 2F-LBLOCA simulation with TRANSURANUS.

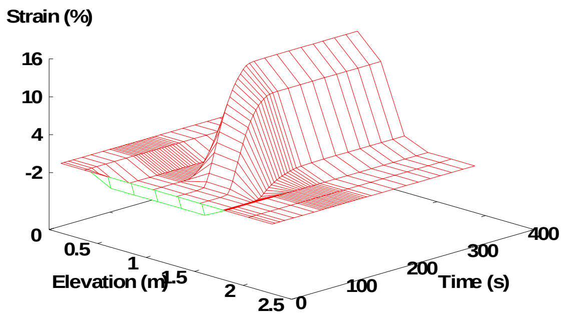

Fig. 12: Tangential strain of an unoxidised claddinng in 2F-LBLOCA simulation with TRANSURANUS.

3. INCLUSION OF THE HYDROGEN UPTAKE BY THE CLADDING UNDER ACCIDENT CONDITIONS

Several investigations have already revealed that the hydrogen uptake under specific LOCA conditions plays a significant role in the mechanical deterioration of the Zr-based cladding materials. The study of the circumstances of the fuel cleaning incident at the Paks NPP has also indicated that the hydrogen absorption of the cladding may have contributed in the embrittlement of the rods. This effect, however, is presently not taken into account neither in the thermo-mechanical analyses of fuel rods nor in the safety criteria for PWR and VVER reactors. Therefore, a new project was initiated between the ITU and the AEKI to extend the modelling capabilities towards hydrided cladding through the extension of the EXTRA database, the implementation of new correlations into the TRANSURANUS code and further code validation.

3.1 Experimental program

The realization of the new project is based on the most recent experimental program of the AEKI to map the effects of hydrogen uptake on the oxidation kinetics, the ductility and the fracture toughness of the Zr1%Nb alloy. Out-of-pile separate effect tests are carried out according to the following program:

- Ring specimens of un-irradiated Zr1%Nb claddings are oxidised and saturated with hydrogen in controlled hydrogen-steam mixture atmosphere. The specimens are exposed at different temperatures (900 – 1200^{o}C) for different time periods. The extent of the oxidation is measured through the weight gain of the specimens.
- The mechanical properties of the oxidised and hydrogen charged cladding specimens are measured through uniaxial, standardized ring compression tests, tensile tests and tube burst tests.

- The amount of hydrogen absorbed in the specimens is measured after the mechanical tests by a hot extraction method. Metallographic investigations are performed to study the oxide layer morphology and the distribution of hydride precipitates.

Figure 13 represents the AEKI best estimate mass gain rate correlation (Eq. 5) as compared to the best fit of mass gain rate constants measured in a steam-hydrogen mixture atmosphere (the hydrogen content was 20 vol%). The practically parallel lines suggest identical activation energies, which could indicate that similar mechanisms are operative.

Data of ring compression tests at room temperature reveal the effect of the hydrogen absorption on the cladding embrittlement. Figure 14 shows the specific energy at failure as a function of the hydrogen concentration in the cladding. The results demonstrate that increasing the hydrogen content causes a drastic decrease of cladding strength. On the basis of earlier studies with oxidised Zr1%Nb rings [17] the ductile-brittle transition was assumed at 50 mJ/mm specific energy. In view of this limit the cladding brittleness is expected at 500 ppm hydrogen concentration.

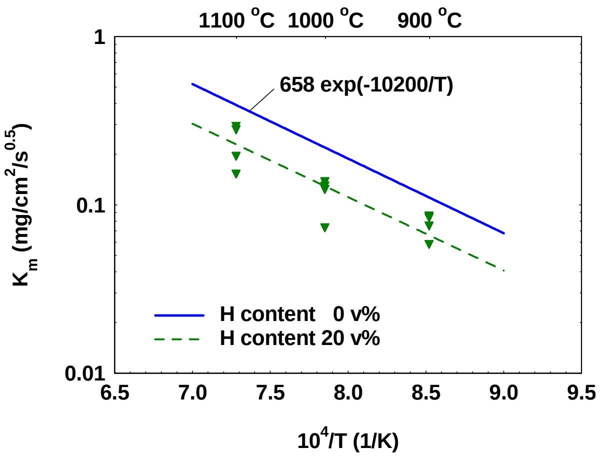

Fig. 13: Oxidation rate as a function of reciprocal temperature in pure steam and in steam-hydrogen mixture (measured points and best-fit curve).

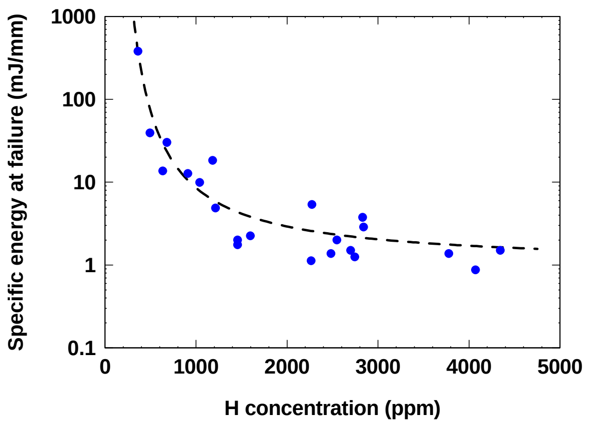

Fig. 14: Specific energy at failure of hydrided Zr1%Nb in ring compression tests as a function of H concentration (measured data and best-fit curve).

The preliminary results of the tests demonstrate that the hydrogen uptake decelerates the cladding oxidation and, at the same time, strongly reduces the cladding ductility. Comparing the oxidation rate constants measured in pure steam and in steam hydrogen mixture atmosphere, the slow-down effect of the hydrogen on cladding oxidation is obvious.

3.2 Model developments

The ongoing model development aims at the elaboration of new correlations for the hydrogen absorption and the improvement of the Zr1%Nb mechanical property functions as well as the cladding failure criteria involved in the TRANSURANUS code. The objectives are to be achieved through the following tasks:

- Evaluation of the AEKI test data in view of the kinetics of the hydrogen absorption, the degradation of the mechanical properties and the ductile-brittle transition.
- Development and implementation of a new empirical correlation of the hydrogen absorption of Zr1%Nb.
- Elaboration of factors for the yield strength, the failure stress and the creep rate as a function of the hydrogen concentration, and their incorporation in the TRANSURANUS code structure.
- Implementation of a new cladding failure criterion based on cladding ductility for LOCA simulations.

The validation of the extended TRANSURANUS code will cover the post test analysis of the recent ballooning experiments with oxidised cladding tubes. Furthermore, the active participation in the OECD LOCA benchmark program was also proposed to compare the TRANSURANUS results with the predictions of different codes and with the experimental data of the Halden Reactor Project.

4. CONCLUSIONS AND PERSPECTIVES

Thanks to a clearly defined mechanical-mathematical framework and a consistent modelling, the TRANSURANUS fuel performance code has been able to cope with normal, off-normal and accidental operating conditions right from the beginning in 1973. Its flexibility also enabled the application to various types of reactors.

Simulation of accident conditions in VVERs by means of the TRANSURANUS code was initiated in the frame of the EXTRA project, which ended in 2003. The project focused on the development of a data-base for Zr1%Nb cladding and on the elaboration of new correlations for plastic deformation, high-temperature oxidation and cladding failure in the temperature range 20^{o}C – 1200^{o}C.

The oxidation tests confirmed the diffusion-controlled oxidation process for both Zr1%Nb and standard Zircaloy-4 in the temperature range 500^{o}C – 1200^{o}C. The oxidation of Zr1%Nb below 1100^{o}C results in a multi-layer ZrO_2 structure due to the periodic break-away phenomenon. On the other hand, a compact oxide layer evolves when the oxidation temperature exceeds 1100^{o}C. This compact layer impedes the hydrogen uptake, like for standard Zircaloy-4.

The mechanical behaviour of PWR and VVER claddings are similar. Nevertheless, the experiments revealed that in the temperature range 800^{o}C-1000^{o}C the mechanical strength of the Zr1%Nb cladding is lower in comparison with that of Zircaloy-4, since the α-β phase transition is shifted to lower temperatures by approximately 100^{o}C. The tests also revealed that an oxidation limited to 2% ECR strengthened the Zr1%Nb material, whereas any oxidation level beyond this level leads to embrittlement, as reflected in the reduced pressures at burst or the tensile strength.

The new models were incorporated into the TRANSURANUS code and validated against burst tests for as-received, oxidised, and irradiated cladding specimens. Furthermore, the upgraded version of the code was applied for assessing the fulfilment of safety acceptance criteria in design basis accidents. An application for the simulation of fuel rod performance in large break LOCA has been presented.

In order to account also for the hydrogen uptake by the cladding under accident conditions, which has detrimental effects on the mechanical properties of the cladding, a new program has been launched. It encompasses experiments concerning oxidation kinetics, mechanical strength and embrittlement of hydrogen saturated cladding, and is carried out at the AEKI in Hungary. The preliminary results confirm the drastic strength reduction of the cladding material due to hydrogen uptake, as well as the inhibiting effect of the hydrogen content in steam (20 vol%) on the oxidation rate of the cladding material. More experimental data regarding the layer morphology and the total hydrogen content are in preparation. The corresponding model developments are also still ongoing.

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