EXTRA Project Final Summary Report

EXTENSION OF TRANSURANUS CODE APPLICABILITY WITH NIOBIUM CONTAINING CLADDING MODELS

CO-ORDINATOR

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CONTRACT N°: FIKS-CT2001-00173

EC Contribution:	ECU 219.500
Partners Contribution:	ECU 219.500
Starting Date:	December 2001
Duration:	24 months

CONTENTS

LIST OF ABBREVIATIONS AND SYMBOLS

AEKI	KFKI Atomic Energy Research Institute
DBA	Design Basis Accident
ECR	Equivalent Cladding Reacted
FZK	ForschungsZentrum Karlsruhe
ITU	EC JRC Institute for Transuranium Elements
JRC	Joint Research Centre
KI	Kurchatov Institute
LBLOCA	Large Break Loss Of Coolant Accident
LOCA	Loss Of Coolant Accident
NPP	Nuclear Power Plant
PWR	Pressurized Water Reactor
RRC	Russian Research Centre
VUJE	VUJE Trnava Inc.
VVER	Water-Water Energetic Reactor
WP	Work Package

EXECUTIVE SUMMARY

The EXTRA Project of the EURATOM 5th Framework Programme focused on the simulation of the behaviour of the nuclear fuel in Russian-design VVER reactors under accident conditions. The analysis of the state of the art showed that the available information and computer tools to predict the performance, especially the off-normal performance of the niobium containing cladding, had been scarce. The main objectives of the project were the systematisation of the knowledge on experimental data of the Zr1%Nb alloy, the incorporation of newly developed correlations into the TRANSURANUS fuel performance code, code validation computations and the improvement of the safety analyses' methodology through the application of the extended TRANSURANUS code. These objectives were achieved in four main work packages.

In the first phase of the project a new database was compiled on the basis of the VVER-specific separate effect tests of the AEKI. The database of nearly 400 tests provides detailed information on the Zr1%Nb cladding behaviour (oxidation ballooning and rupture) under LOCA conditions and gives a solid background for code extension and validation.

The main task of the project was carried out in the second work package. The TRANSURANUS code was improved with new models for the high temperature steam oxidation, plastic deformation and failure of the cladding tube. New VVER-specific empirical correlations for the mass gain rate, the zirconium-dioxide layer growth rate, the deformation rate and the cladding failure were evolved and adapted to the models. An advanced multidimensional minimization procedure was applied to fit the material constants of the correlations on the compiled experimental data. Outstandingly, the recent mechanical model takes into account the oxygen concentration as a parameter of the deformation rate and the failure stress, as well. In this manner, the effect of the oxidation on the cladding mechanical performance can be simulated in an accurate way.

Extensive code validation computations were performed in the third work package of the project. Comparison of the code results with analytic solutions and with the data of numerous high temperature cladding oxidation and ballooning tests provided the core of the analyses. The computations proved the correctness of the approaches applied in the extended TRANSURANUS code and indicated the reliable prediction of the Zr1%Nb claddings' failure under simulated accident conditions.

The EXTRA project has widened the scope of the licensing analyses and helped to improve the safety evaluation of the VVER reactors by promoting the simulation of off-normal fuel rod performance. In order to demonstrate the applicability and the advantage of the improved TRANSURANUS code in safety analyses, fuel rod performance in a hypothetical DBA were simulated in the fourth work package of the project. The code was applied to evaluate the number of failed fuel rods in a LBLOCA assumed in a VVER-440/213 unit of the Bohunice NPP in Slovakia.

The extended models will be included in the next official release of the TRANSURANUS code. Hence, a broad network of users –research institutes, licensing authorities and consultancies throughout Europe– is the potential basis of the utilisation of the project's results.

A. OBJECTIVES AND SCOPE

The safety assessment of commercial reactors operating with improved nuclear fuels for longer cycles requires more and more sophisticated analytical tools that consider the effects of higher burnups and also the applied new materials. Since the extended fuel cycles make augmented utilisation of the nuclear fuel assemblies, the accurate modelling of the fuel rod performance has an increased priority in the evaluation of the safety margins.

Due to its flexibility, the TRANSURANUS fuel performance code [1] (developed by the Modelling Group of the ITU) is widely used in the safety evaluation of different types of nuclear reactors in both West and East Europe. The code has a comprehensive materials data bank for different fuels, claddings and coolant. The scope of the covered phenomena and the numerical solution methods of the equation systems make the code capable to simulate both long fuel cycles and hypothetical accidents. Options for probabilistic analysis are also involved in order to provide the possibility of statistics-based evaluation.

The fuel licensing procedures established recently in the East-European countries entail the intensive utilization of the TRANSURANUS code for VVER reactors, as well. However, the involved VVER-specific material functions were limited to normal operating conditions, and consequently, the code was not applicable in VVER accident analyses. Inadequate information of the high temperature performance of the Zr1%Nb cladding alloy resulted in the above shortcoming, although, due to their improved corrosion resistance, the niobium containing zirconium alloys are perspective materials in Western design PWRs, as well.

Therefore, the EXTRA project focused on the simulation of the Zr1%Nb cladding performance under accident conditions with the aim to diminish the incompleteness in this field. The main objectives of the project were to systematise the knowledge on experimental data of the Russian Zr1%Nb cladding alloy and to extend the TRANSURANUS code applicability for accident analyses. The goals are achieved through two main activities:

- the compilation of a new experimental database containing VVER-specific separate effect tests to provide an appropriate background for model development and validation and
- the improvement of the widely used TRANSURANUS fuel performance code via the incorporation of newly developed correlations for off-normal conditions.

These objectives fully corresponded to the requirements of the TRANSURANUS users interested in nuclear fuel licensing to widen the scope of the TRANSURANUS code and to provide a tool for the consistent simulation of the VVER fuels' performance under normal and accident conditions. Before the EXTRA project, no European fuel performance code with the above capabilities was available.

B. WORK PROGRAMME

The objectives of the project were achieved in four main work packages:

- **WP-1**: Database compilation and verification for model development and validation.
- **WP-2**: Code development to extend the TRANSURANUS with high temperature oxidation, plastic deformation and cladding failure models.
- **WP-3**: Code validation computations.
- **WP-4**: VVER plant applications for DBA cases.

The objected tasks are summarised below.

B.1 Database Compilation (WP-1)

Since the beginning of the 90s several experimental series have been performed at the AEKI with Zr1%Nb and Zircaloy-4 claddings to map and to compare the mechanical properties of the cladding materials in the temperature range of 20-1200 ^{o}C and to investigate the effect of oxidation on the mechanical performance of the claddings [2]. The systematic compilation of the experimental data and the official release of a database to support model development and code validation were the main tasks of WP-1. An overview of integral tests simulating VVER fuel rod performance under accident conditions was also planned.

B.2 Model Development (WP-2)

To extend the applicability of the TRANSURANUS fuel code for accident analyses, the implementation of new models and VVER-specific correlations were projected for this work package. The work covered the elaboration of new correlations, the programming of the algorithms, the verification procedure and the incorporation of the new subroutines into the existing code structure considering conformity and numerical stability.

B.3 Code Validation (WP-3)

In order to evaluate the code improvements and to provide feedback information on model development, the comprehensive validation of the extended TRANSURANUS code was the main task of Work Package 3. The post-test analyses of cladding oxidation tests, mechanical tests and VVER-specific integral tests were intended.

B.4 Plant Application (WP-4)

The 4th work package aimed to demonstrate the applicability and the advantage of the extended TRANSURANUS code in the comprehensive safety analysis of VVER power plants. The simulation of fuel rod performance and the assessment of cladding failure in DBA were projected.

C. WORK PERFORMED AND RESULTS

C.1. Database Compilation (WP-1)

The AEKI experimental programme has covered ballooning experiments, tensile tests and steam oxidation tests with Zr1%Nb and Zircaloy-4 claddings for almost 15 years. Beyond the mechanical properties of as-received claddings special effects of the oxide layer morphology on hydrogen uptake and mechanical performance were also studied. The steam oxidation has a considerable effect on the mechanical strength of the E110 Zr1%Nb cladding. The effect was clearly demonstrated in the experiments (Figure 1).

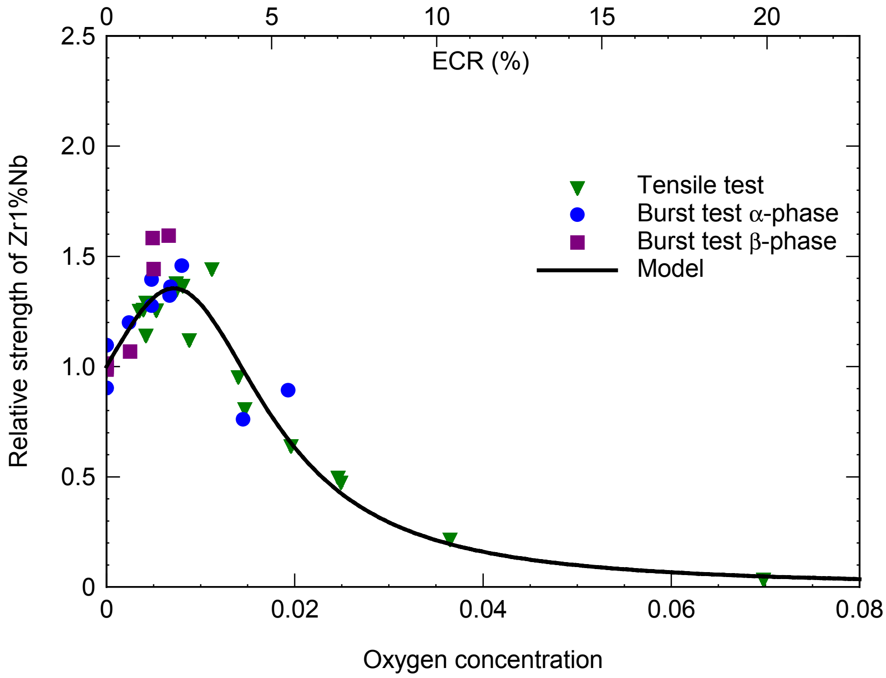

Figure 1. Relative cladding strength as a function of the oxygen concentration. Data measured in tensile an biaxial burst tests and best-fit curve applied in sensitivity study.

Beyond comparative analyses, the data of the tests are applicable for model development and validation purposes, as well. With this end in view, the systematic compilation, verification and the publication of the experimental data were performed in the first phase of the EXTRA project. The experimental database [3] was compiled by considering the aspects of the simulation of fuel rod performance under LOCA conditions. As a main deliverable, the data and all the relevant information of nearly 400 individual tests concerning high temperature oxidation, cladding ballooning and tensile strength were issued on CD-ROM. The experimental data were clustered in three main groups in the database:

Oxidation tests:

- one-side steam oxidation of Zr1%Nb tubes at 900 ^{o}C,
- double-side steam oxidation of Zr1%Nb rings at 500 - 1200 ^{o}C.

Cladding ballooning tests:

- 7-rod bundle tests to investigate coolant flow blockage under LOCA conditions,
- isothermal burst tests with as-received and pre-oxidized Zr1%Nb tube specimens,
- isothermal burst tests with as-received Zircaloy-4 tube specimens,
- isothermal burst tests to investigate the effect of pressurization rate,
- burst tests on pre-pressurized Zr1%Nb rods with linear temperature increase.

Tensile tests:

- tests with Zr1%Nb and Zircaloy-4 sheet specimens,
- tests with Zr1%Nb and Zircaloy-4 tube specimens.

Beyond the test conditions and the measured data the database contains publications, conference papers, photos and figures of the specimens and post-test investigations. In addition, a summary report gives an overview of the comprised experiments and helps the navigation in the database.

C.2. Model Development (WP-2)

The improvement of the TRANSURANUS code were focusing on the best-estimate description of the key phenomena under accident conditions, as the zirconium-steam reaction, the plastic deformation and the rupture of the VVER fuels' cladding tube [4]. Accordingly, the work-package involved three sub-tasks:

- the implementation of a high temperature cladding oxidation model for transients,
- the elaboration of a proper stress-strain relation for the Zr1%Nb claddings and
- the development of appropriate cladding failure criteria.

C.2.1. Compilation of model options for high temperature oxidation

This subtask aimed at the implementation of a metal-steam reaction model adequate for Zr1%Nb and Zircaloy claddings in all respects. The implemented new model is based on parabolic kinetic correlations for both the oxygen mass gain and the ZrO_2 layer thickness growth and is adequate to simulate the cladding oxidation under temperature transients. The incorporated numerical algorithm calculates the mass of oxygen absorbed in the cladding and the ZrO_2 layer on the basis of a simple recursive formula:

$$X_n = \sqrt{X_{n-1}^2 + K_n^2\, dt_n}$$

Where:

X_n	–	extent of the oxidation at the end of time step n (oxide layer thickness δ_{ZrO_2} or mass gain Δm)
X_{n-1}	–	extent of the oxidation at the beginning of time step n
K_n	–	kinetic constant of the reaction in time step n
dt_n	–	length of time step n

In order to characterise the oxidation of the VVER cladding, new best-estimate formulae for oxidation rates were also derived from experimental data. The new AEKI correlations describe the oxidation kinetics of the Zr1%Nb alloy in the temperature (*T)* interval of 800-1500 K according to the following relations:

$$K = \begin{cases} 658\, e^{\frac{-10200}{T}}, & if \;\; X = \Delta m, \quad (mg/cm^2/s^{0.5}) \\ \\ 4\, e^{\frac{-10200}{T}}, & if \;\; X = \delta_{ZrO_2}, \quad (mm/s^{0.5}) \end{cases}$$

Beyond the new AEKI correlations, four optional models, as the *Cathcart-Pawel* model, the *Leistikow* model, the *Baker-Just* model and the Zr1%Nb-specific *Solyany* model are now applicable in the code to define the reaction rate constants.

C.2.2. Mechanical model extension

The mechanical model extension focused on the correct simulation of the Zr1%Nb claddings' plastic deformation at high temperature, as it has primary importance in the forecast of the coolant flow blockage and the number of the failed fuel rods.

The one-dimensional mechanical model of the TRANSURANUS fuel code is based on a semi-analytic solution of the principal mechanical equations (the equilibrium, the compatibility and the constitutive relations) for the radial deformation. The change of the total strain is assumed as a linear superposition of elastic and all non-elastic (creep, plasticity, thermal expansion, cracking, relocation, etc.) strain increments. Due to their complexity the expressions of the non-elastic strains involved in the analytic formula are integrated numerically along the radius. A flexible spatial discretization of the rod is realized through the variable multizone concept. The non-elastic strain components are calculated incrementally in time. The increments of the creep strain or the plastic strain can be defined through an optional non-linear function of the stress. Both explicit and implicit numerical solution methods are involved in the code for the treatment of the problem. The numerical stability is assured by proper time step control mechanisms [5].

The implementation of an appropriate creep rate correlation was essential to simulate the plastic deformation of the Zr1%Nb cladding under accidental conditions. A modified Norton-type equation was considered as the most suitable relation to describe the effective strain rate as a function of the effective stress, the temperature and the crystallographic phase of the cladding. The unknown parameters of the relation were defined by an advanced multidimensional minimization procedure (called the *Levenberg-Marquardt* method) based on statistical methods. Outstandingly, the evolved creep rate correlation takes into account the actual oxygen concentration in the cladding, as well. In this manner, the relevant effect of the oxidation on the strength and deformation of the cladding can be simulated in an accurate way.

$$\dot{\varepsilon} = f_\alpha\, k_\alpha e^{\frac{-Q_\alpha}{RT}+b(x)} \sigma^{n_\alpha} + (1-f_\alpha)\, k_\beta e^{\frac{-Q_\beta}{RT}+b(x)} \sigma^{n_\beta}$$

Where:

f_α	-	weight fraction of the α zirconium (Figure 2)
$\dot{\varepsilon}$	-	effective strain rate (1/s)
σ	-	effective stress (MPa)
R	-	universal gas constant (J/mol/K)
T	-	temperature (K)
k, Q, n	-	Norton parameters in the α and β phases (Table *I*)
$b(x)$	-	oxygen concentration term (Table *II*)

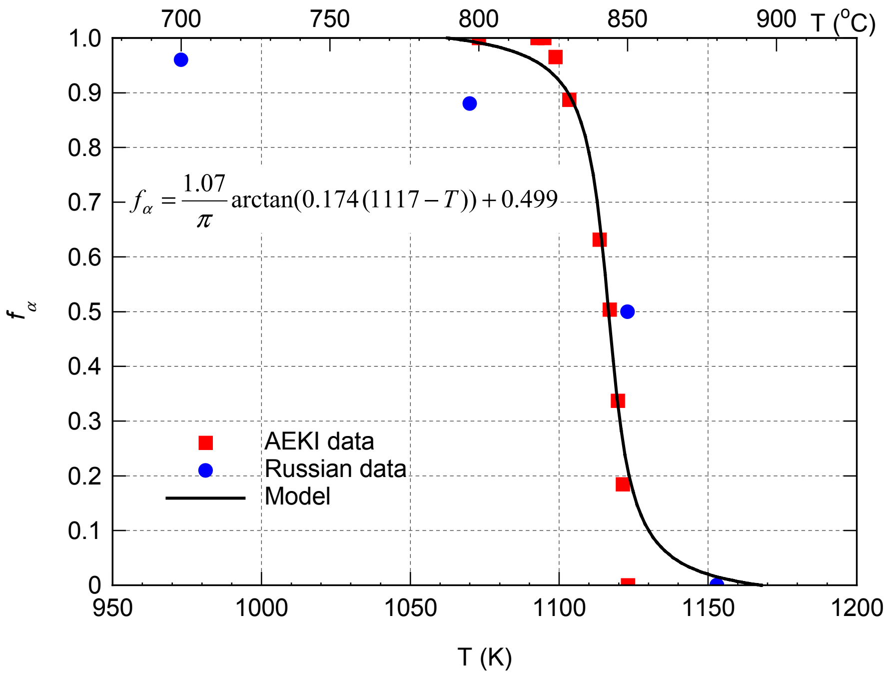

Figure 2. Fraction of the α-zirconium in Zr1%Nb alloy as a function of the temperature. Measured data and best-fit curve.

Table *I*. Norton parameters for un-oxidized Zr1%Nb cladding.

	Norton parameters	
***α*-phase (600 - 800 °C)**	k_0	6.059578E+06
	Q	3.578327E+05
	n	5.182323
***β*-phase (900 - 1200 °C)**	k_0	1.439244
	Q	1.815405E+05
	n	5.820723

Table *II*. Oxygen concentration term in the Norton-type creep rate equation for the α and β crystallographic phases of the Zr1%Nb cladding alloy.

	***b(x)* in *α*-phase**	***b(x)* in *β*-phase**
$x < 0.02$	$-6.71E5\,x^3 + 4.94E4\,x^2 - 5.73E2\,x$	$-7.40E5\,x^3 + 5.45E4\,x^2 - 6.32E2\,x$
$x \geq 0.02$	$2.34E4\,x^3 - 6.411E3\,x^2 + 7.38E2\,x - 9.48$	$2.58E4\,x^3 - 7.076E3\,x^2 + 8.15E2\,x - 10.5$

C.2.3. Modelling of cladding failure

This subtask dealt with the implementation of appropriate criteria to predict the cladding failure and to make the evaluation of the number of burst fuel rods possible this way. Two optional criteria were incorporated into the code.

The first criterion is a typical stress-based evaluation. Cladding failure is indicated when the true tangential stress exceeded the threshold stress defined on the basis of experimental data. (A characteristic failure stress function of the Zr1%Nb alloy is represented in Figure 3.) Since the threshold stress, similarly to other material properties, can be handled in the TRANSURANUS code as a statistical variable with a given distribution, the likelihood of the fuel rod failure can be analysed on a statistical basis, as well.

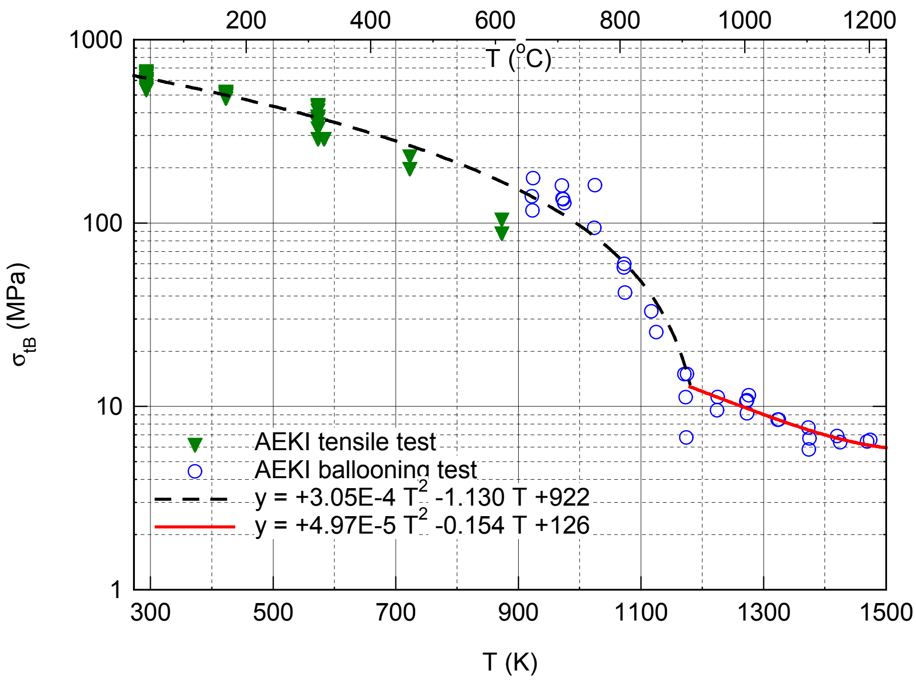

Figure 3. Failure criterion for un-oxidised Zr1%Nb cladding: true tangential stress at burst as a function of the temperature. Data of AEKI tests and best fit curves.

On the other hand, due to the significant uncertainty of the stress computation in the case of large cladding deformation, a plastic instability criterion was also implemented in the code, mainly for LOCA conditions. When both the strain and the strain rate exceed certain threshold values (0.02 and 100 1/h, respectively) the cladding is assumed inhermetic.

C.3. Code Validation Computations (WP-3)

The verification of the newly developed models and the validation of the extended TRANSURANUS code were carried out in WP-3 [6]. Comparison of the code results with analytic solutions proved the correctness of the applied algorithms. Nevertheless, the simulation of VVER-specific separate effect tests was the most important part of the code validation for accident conditions. Altogether 122 cladding oxidation tests and 214 cladding ballooning tests of the AEKI [3], the RRC Kurchatov Institute (KI) [7] and the Forschungszentrum Karlsruhe (FZK) [8] were analysed by the TRANSURANUS code. The comparison of the calculated and measured data indicated that the code predicts correctly the behaviour of the VVER fuel rods' cladding in a wide range of conditions simulating LOCA accidents.

The evaluation of the cladding oxidation simulation was based on the comparison of calculated and measured oxygen mass gain data. Figure 4 presents the mass gains calculated by the TRANSURANUS code using the AEKI oxidation rate correlation versus the measured data of isothermal oxidation tests performed in the temperature range of 500 – 1200 ^{o}C. The figure illustrates very satisfactory agreement.

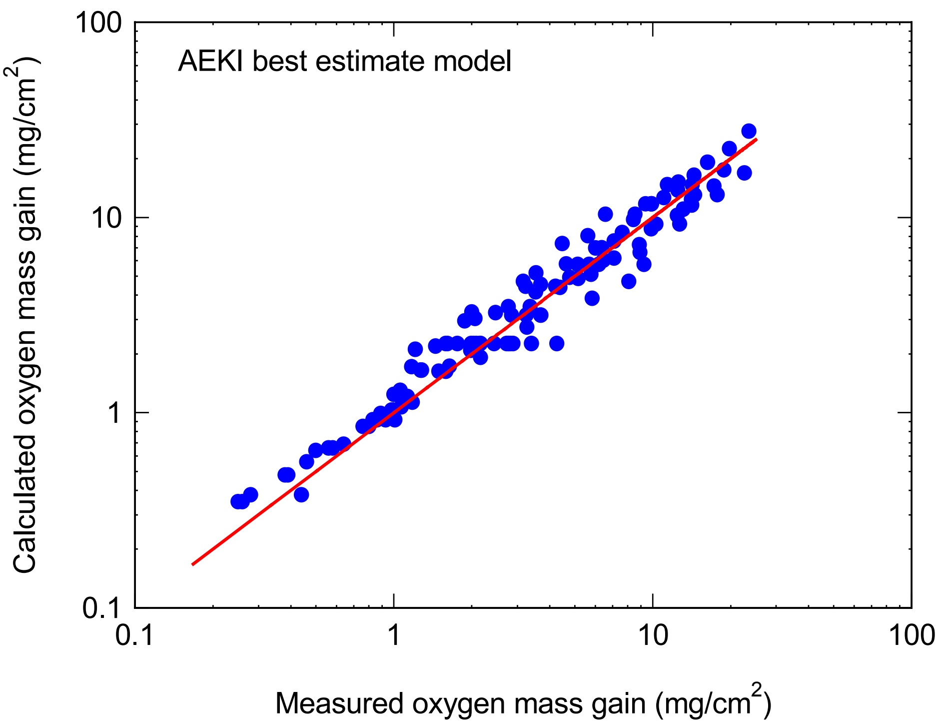

Figure 4. Validation of the TRANSURANUS cladding oxidation model: calculated versus measured oxygen mass gain for Zr1%Nb cladding.

The validation of the cladding mechanical model was focused on the comparison of the measured and calculated times of burst in cladding ballooning tests carried out under different (isothermal or isobaric) experimental conditions between 600 and 1200 °C. Figure 5 presents the history of a typical burst test simulation with pre-oxidised specimen when the rod internal pressure was increased linearly under isothermal conditions. The predicted burst time and residual tangential strain can be compared with the corresponding experimental data. In order to visualize the effect of the cladding oxidation on the predicted time of burst and deformation, the figure illustrates two strain histories calculated with and without considering the oxygen concentration of the specimen.

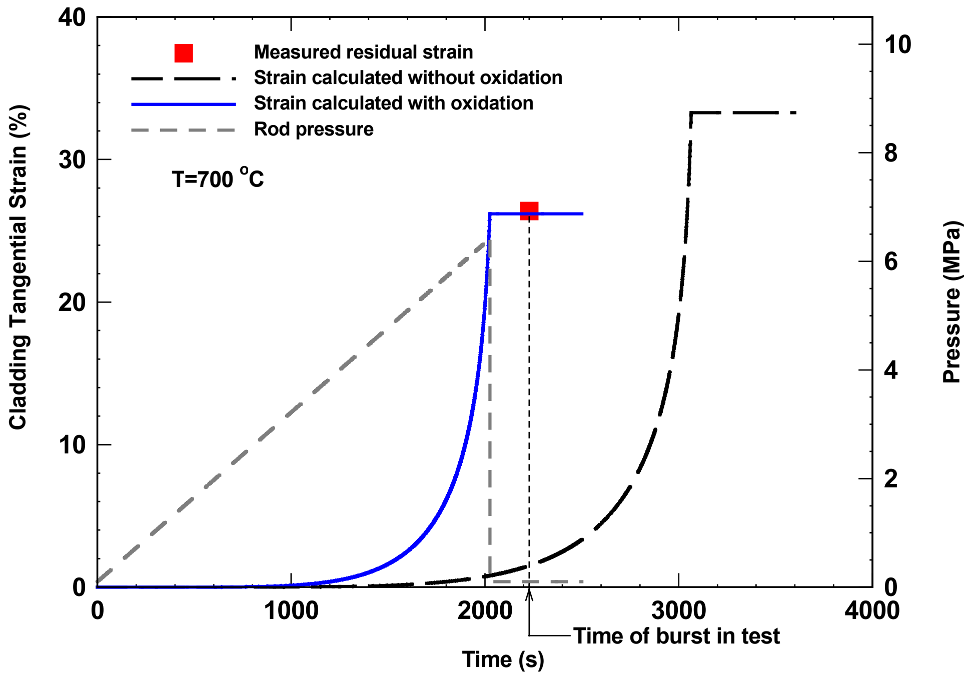

Figure 5. Rod internal pressure and tangential strain calculated by the TRANSURANUS code for an AEKI burst test. (The red square presents the measured strain.)

Figure 6 gives an overall view of the TRANSURANUS predictions. It presents the calculated burst time as a function of the measured burst time for all the simulated tests. This comparison confirms that the TRANSURANUS code reliably predicts the time of burst of the Russian Zr1%Nb cladding for a wide range of situations. The data cover slow as well as fast experiments either with as-received, oxidised or irradiated cladding specimens. The differences between the measured and calculated values are in the same range as the spread of the experimental data.

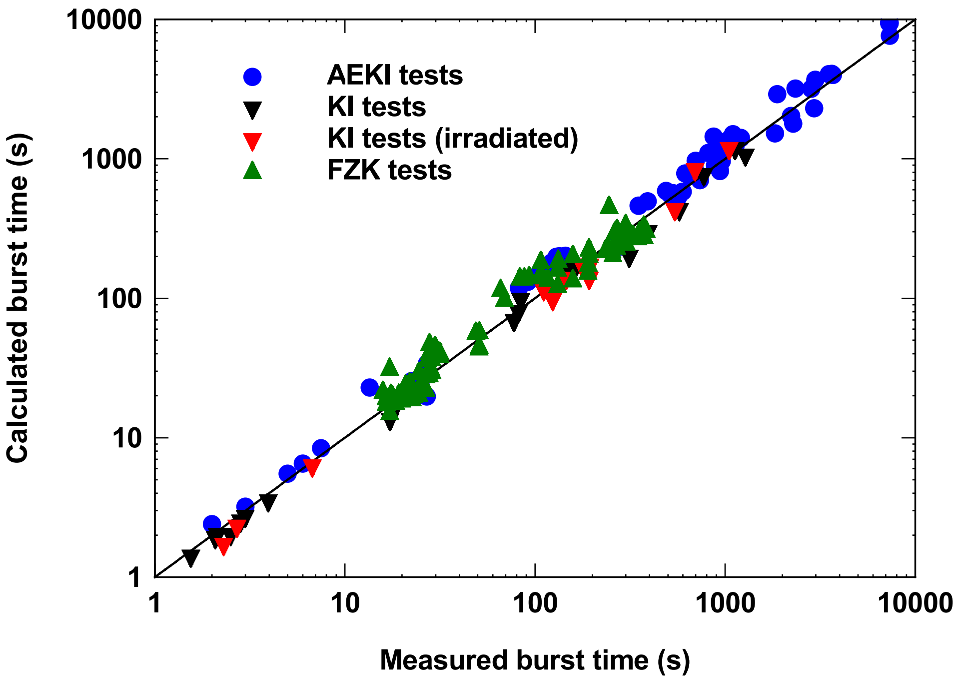

Figure 6. Calculated versus measured burs time for different cladding ballooning tests with as-received, pre-oxidised and irradiated E110 specimens.

C.4. Plant Application of Extended TRANSURANUS Code (WP-4)

The TRANSURANUS code has a special role in the licensing procedures in Hungary, as well as in the Slovak Republic. The nuclear fuels' safety evaluation computations are generally performed by the fuel vendor however, the national atomic energy authorities also demand independent analyses for comparison. Since the cross-check computations are to be performed by the TRANSURANUS code in both countries, the implemented code extensions have special importance for the licensing-related application. In order to demonstrate the applicability and the advantage of the improved TRANSURANUS code in safety analyses, fuel rod simulations for a hypothetical VVER-440 plant accident and for a real incident were performed in the last phase of the project. The code was applied to evaluate the number of failed fuel rods in a hypothetical LBLOCA in Units V2 of the Bohunice NPP in Slovakia and to assess the fuel failure mechanisms in the Paks fuel cleaning tank incident [9].

CONCLUSIONS AND EXPLOITATION OF RESULTS

The compiled experimental data provide useful information about the high temperature mechanical performance and oxidation of the Zr1%Nb cladding alloy and help to expose special interferences of cladding oxidation and mechanical performance. The database was intensively used in model refinement and code validation in the EXTRA project. In order to promote information and know-how exchanges, the database is available not only for the members of the consortium but also for third party research institutions, on a bilateral basis.

The TRANSURANUS code was extended with new correlations for the high temperature oxidation, plastic deformation and failure of the Russian Zr1%Nb cladding. Hence, as the main innovation of the project, the improved TRANSURANUS code provides the unique possibility of the consistent simulation of fuel rod performance under normal as well as accidental conditions and helps to assess the number of failed fuel rods. Thus the EXTRA project has widened the scope of the licensing analyses and helped to improve the safety evaluation of the VVER reactors. As the extended code models will be involved in the next official release of the TRANSURANUS code a broad network of users –research institutes, licensing authorities and consultancies throughout Europe– is the potential basis of the utilisation of the project's results.

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