IAEA FUMAC BENCHMARK OF FUEL PERFORMANCE CODES BASED ON LOCA SEPARATE-EFFECTS CLADDING TESTS

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ABSTRACT
Through the IAEA Coordinated Research Project on Fuel Modeling in Accident Conditions (FUMAC), a benchmark of fuel performance codes for the simulation of selected Loss of Coolant Accident (LOCA) experimental tests was performed. In this paper, we present the FUMAC modeling benchmark for separate effects LOCA tests of Zircaloy-4 cladding tubes subject to inner pressure transients under isothermal conditions. Five organizations and the fuel performance codes BISON, FRAPTRAN and TRANSURANUS were involved in the benchmark. We present comparisons of calculation results to each other and to experimental data. Considered figures of merit are time to cladding burst, cladding inner pressure at burst and maximum engineering hoop strain at burst. Results are critically analyzed and future needs are identified in terms of the improved fuel performance modeling for LOCA accidents.

1. Introduction
To coordinate and support research on nuclear fuel modeling for accident scenarios in member countries following the Fukushima accident, the International Atomic Energy Agency (IAEA) initiated the Coordinated Research Project on Fuel Modeling in Accident Conditions (FUMAC) [1,2], which took place during 2015-2018 and focused on loss-of-coolant accidents (LOCA). In the framework of the FUMAC project, various institutions performed fuel performance simulations for selected LOCA experiments with different fuel performance codes. The outcome of the project included code-to-code benchmark comparisons of results from the institutions involved, as well as comparisons of simulations to experimental data. The result is an overview of the current state of the art of nuclear fuel simulation capabilities for LOCA accidents and an insight into future needs.
Among the experimental cases selected for code simulation and benchmarking within the FUMAC project were the PUZRY separate-effects, cladding-only ballooning and burst tests. These were performed at AEKI (whose successor is the Hungarian Academy of Sciences, Centre for Energy Research – MTA EK), to study the mechanical behavior (ballooning and burst) of Zircaloy-4 cladding subject to inner pressure transients at high temperature that mimic LOCA conditions [3,4,5].
In this paper, we present the FUMAC modeling benchmark for the AEKI separate effects LOCA tests PUZRY. Simulation results for these experiments from FUMAC participants are compared to each other and to experimental data. Results are presented of simulations performed with the fuel performance codes BISON, FRAPTRAN and TRANSURANUS. Benchmark comparisons include results in terms of time to cladding burst, cladding inner pressure at burst and maximum engineering hoop strain at burst.
The paper is organized as follows. A description of the simulated experiments is provided in Section 2. Benchmark calculations from participating modeling groups in FUMAC are presented in Section 3. Conclusions are drawn in Section 4.
2. Experiments

The PUZRY experimental series [3-5] was performed with the objective to study the mechanical behavior (ballooning and burst) of Zircaloy-4 cladding subject to inner pressure transients at high temperature. In particular, the effects of temperature and pressurization rate on the deformation and the failure (burst) pressure were investigated.

The specimens were 50 mm long unirradiated, unoxidized Zircaloy-4 tubes. The specimens' inner/outer diameters of 9.3/10.75 mm corresponded to typical parameters of PWR fuel cladding. The schematic drawing of the tube specimen is reported in Fig. 1. The specimen was placed in a quartz test tube filled with inert argon gas, and heated up in an electrical furnace. The pressure of the inert gas in the quartz tube was kept constant at 0.1 MPa. After an approximately 1000 s heat-up period to temperatures in the range of 700–1200 °C, the tube was pressurized with argon gas at a constant pressurization rate and isothermal conditions until burst failure occurred. Pressurization rates between $7 \times 10^{-4}$ and $2.6 \times 10^{-2}$ MPa/s were tested.

Six of the PUZRY tests were selected for FUMAC, namely, those whose experimental conditions were closest to realistic large-break LOCA scenarios. Table 1 summarizes experimental conditions for the PUZRY cases selected for FUMAC. The results of the tests are summarized in Figs. 2 and 3, which also show visual inspection images of the tested samples.

![Fig 1. Drawing of the tube specimen for the AEKI cladding-only ballooning and burst tests.](image)

<table>
<thead>
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<th>Test number</th>
<th>Temperature (°C)</th>
<th>Pressure ramp rate (MPa/s)</th>
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</tr>
<tr>
<td>12</td>
<td>1200</td>
<td>0.00723</td>
</tr>
</tbody>
</table>

Tab 1. Conditions of the 6 AEKI PUZRY cases included in FUMAC [5].
Fig 2. Experimental results of time to burst vs. test temperature for the six AEKI PUZRY cases selected for FUMAC. Visual inspection images of the tested samples are also shown.

Fig 3. Experimental results of tube inner pressure at burst vs. test temperature for the six AEKI PUZRY cases selected for FUMAC. Visual inspection images of the tested samples are also shown.
2. Benchmark of fuel performance codes

A total of 5 FUMAC participant organizations performed simulations of the AEKI ballooning tests PUZRY. Organizations and respective adopted fuel performance codes are as follows:

- MTA EK (Hungary), FRAPTRAN 2.0 code
- JRC-Karlsruhe (European Commission, Germany), TRANSURANUS v1m2j17 code
- INL (USA), BISON 1.4 code
- CIEMAT (Spain), FRAPTRAN 1.5 code
- SSTC NRS (Ukraine), TRANSURANUS v1m1j11 code

For the FUMAC benchmark, calculation results are compared to each other and to experimental data. Considered figures of merit are time to cladding burst, cladding inner pressure at burst and maximum engineering hoop strain at burst. Benchmark results are presented in the following subsections.

2.1. Results for time to burst failure

Results from participants in terms of time to burst failure for the six AEKI cases are reported in histogram form in Fig. 4. Experimental data are also included. The order of cases as presented in the graph is one of decreasing test temperature. The overall comparison points out a general tendency of the codes to under-predict the time to burst. The TRANSURANUS code (both JRC and SSTC NRS), however, compares very well to the experimental data. The BISON code also compares well, although it tends to moderately under-predict the data. The FRAPTRAN code appears to under-predict the time to cladding burst more pronouncedly than other codes, as emerges from the results from both MTA EK and CIEMAT.

JRC commented that the accuracy of the TRANSURANUS predictions of time to burst is in line with previous simulations of similar ballooning tests (e.g., [6]). Also, JRC tested two different criteria for rod failure (i.e., limiting hoop stress and limiting hoop strain) and noted that the cladding failure criterion has only a small influence on the predicted time to burst, because the ballooning that leads to burst occurs very rapidly in its late stages.

Fig 4. Time to burst for the AEKI separate-effects tests PUZRY considered in FUMAC. Code-to-code comparisons and experimental data are illustrated.
Both JRC and INL analyzed the burst time results obtained with TRANSURANUS and BISON, respectively, as a function of the test temperature. The comparison for BISON in particular is presented in Fig. 5. Both institutions noted that the reduction of the burst time as a function of the temperature was reproduced. Deviations of predictions from the experimental data appeared to increase at the lower test temperatures. The latter circumstance was also confirmed by MTA EK in reference to their calculations with FRAPTRAN. Higher discrepancies between calculations and experiments at the lower temperatures indicate that deviations may be partly due to a lack of properly modeling anisotropic creep behavior, which characterizes alpha-Zr (i.e., in absence of phase transition to beta-Zr at high temperature) [7,8].

It is also worth noticing that high-temperature creep correlations in the codes are generally based on the experimental work of Erbacher, Neitzel, Rosinger et al. [7,8] and differences may exist in composition (consequently, in creep behavior) between the Zry-4 alloy used in the PUZRY experiment and in [7,8]. Small differences in results by different participants using the same codes (user effects) observed for the TRANSURANUS and FRAPTRAN results may be due to differences in the applied code versions. In particular, according to the MTA EK experience in comparing FRAPTRAN code versions from 1.3 onwards, there are significant differences between simulation results of any two FRAPTRAN versions, including 1.5 and 2.0. Furthermore, CIEMAT used a modified version of FRAPTRAN 1.5, with modifications in both thermal and mechanical modeling. Finally, different selections for the modeling options available in the codes may also contribute to user effects.

2.2. Results for pressure at burst failure

Results from participants in terms of cladding inner pressure at the time of burst failure are reported in Fig. 6. Experimental data are also included.

The general tendency is one to under-predict the experimental values for the burst pressure. Because the pressure increase rate is an experimental parameter and input for the code calculations, the burst pressure can be correlated to the time to burst. The observed tendency to under-predict the burst pressure thus corresponds to the tendency to under-predict the time to burst (Section 2.1).
The calculations from both TRANSURANUS users appear to be in good agreement with the data. Predictions with the BISON code are also reasonable. A significant under-prediction is associated with the FRAPTRAN calculations.

2.3. Results for maximum hoop strain at burst failure

Results from participants in terms of engineering hoop strain at axial peak position (burst location) on the cladding outer surface at the time of burst failure are reported in Fig. 7. Experimental data are also included. Large differences are observed between results from different codes and in many cases predictions deviate markedly from the experimental data. Prediction of cladding strains is notoriously difficult for fuel performance codes, which relates to the number, complexity and mutual dependence of the involved phenomena [9,10]. In particular, uncertainties in cladding burst strain calculations are large for LOCA analysis, whereby very high strain rates are reached as cladding burst is approached. This implies that small differences in the time of predicted rod burst correspond to large differences in the calculated maximum strain. In consequence, the maximum strain is sensitive to the specific burst criterion adopted. This has been clearly demonstrated in a previous study by JRC-Karlsruhe where different failure criteria were tested in cladding ballooning and burst simulations with the TRANSURANUS code [6].

The burst failure criteria themselves are affected by significant uncertainties. For example, stress-based failure criteria typically are data fits for the limiting (burst) hoop stress in the cladding as a function of the temperature, with considerable scatter existing in the stress data (calculated from measured pressures) used for the fitting (see, e.g., [7,8,11]). In addition, burst stress criteria are generally derived based on the assumption of uniform strain along the axial direction in the ballooned section [8]. Hence, application of these criteria in detailed fuel rod models is not fully consistent. In order to derive more suitable criteria, measuring the radius of curvature of the balloon along the axial direction in the experiments would be a minimum requirement [12].

INL, JRC and CIEMAT noted the inherent uncertainty in burst strain predictions related to the burst criterion. JRC also noted that the burst strain results from TRANSURANUS should be considered very carefully since they exceed the range of acceptability of most models that rely on the small strain approximation. Finally, JRC mentioned that the strains obtained from
Fig 7. Maximum engineering hoop strain at the cladding outer surface at burst time for the AEKI separate-effects tests PUZRY considered in FUMAC. Code-to-code comparisons and experimental data are illustrated.

Bundle tests (e.g. QUENCH experiments [13]) are typically smaller than those observed in single rod tests, which can be ascribed in part to the azimuthal temperature gradient along the cladding, as indicated by the available experimental evidence [14]. Taking the effects of azimuthal temperature variations into account in calculations requires full 3D modeling\(^1\), while calculations within FUMAC were performed using either 1.5D or 2D-rz geometrical representations.

Besides modeling uncertainties, there is an uncertainty in the measurements that adds to the expected discrepancies between calculations and experimental data. Furthermore, in addition to the uncertainty that is associated with the measurement process and instrumentation, another issue in comparing code predictions to experimental data of cladding burst strain relates to the interpretation of the measurements. Because they are taken post-test, measurements may include the effect of the burst opening (cladding flaps that protrude outwards following burst), which introduces a bias in the measured strain relative to the strain due to ballooning only. This is evident, for example, in the post-test cladding diameter profile measured for the Halden IFA-650.10 experiment\(^2\) [2,15], as well as in the PIE of the QUENCH LOCA L1 experiment [2,13]. Code predictions refer to the strain in the cladding just before burst, i.e., the maximum ballooning strain. For the AEKI tests, the nature of the measurements could not be clarified for certain during FUMAC.

As mentioned in Section 2.1, observed user effects may be due to the different code versions adopted by different users and/or usage of modified versions that differ from the original ones (CIEMAT with FRAPTRAN). Also, different selections of the modeling options available may contribute to user effects. For instance, different choices of the burst failure criterion (for which multiple options are available in TRANSURANUS [6]), may lead to significantly different predictions of the burst strains.

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\(^1\) Strictly speaking, azimuthal variations can also be captured with 2D-rθ representations. However, 3D is needed to include also axial variations.

\(^2\) During the FUMAC Third Research Coordination Meeting it was clarified that the peak observed in the measured cladding diameter profile for IFA-650.10 [2,15] is an effect of the burst opening and should not be considered when comparing to calculations.
5. Conclusions

In this paper, an account was given of the IAEA FUMAC benchmark of fuel performance codes based on LOCA separate-effects cladding tests. In particular, the AEKI ballooning and burst tests PUZRY on Zircaloy-4 claddings subject to inner pressure transients under isothermal conditions were considered. Simulations by FUMAC participating organizations were presented and compared to each other and to experimental data. Participants included users of the fuel performance codes BISON, FRAPTRAN and TRANSURANUS. Results in terms of time to cladding burst and inner pressure at burst were generally satisfactory, although a tendency of the codes to under-predict the burst time and pressure was noted. In particular, a tendency to increasingly under-predict the data with decreasing test temperature was consistently observed for the applied codes. This indicated that deviations may be partly due to a lack of properly modeling anisotropic creep behavior of Zircaloy-4.

Calculated maximum cladding hoop strains at burst pointed out large differences between predictions from different codes, and in many cases predictions deviated markedly from the experimental data. Discrepancies were ascribed to various factors including (i) the inherent uncertainties in burst strain predictions related to the burst criterion, (ii) the small strain approximation in the mechanical analysis for some codes, (iii) the effect of azimuthal temperature variations in the cladding which cannot be captured in 1.5D or 2D analyses, and (iv) measurement uncertainties and interpretation of the measurements. In reference to item (i), uncertainties in cladding burst strain calculations are large for LOCA analysis, whereby very high strain rates are reached as cladding burst is approached. This implies that the maximum strain reached in the calculation is very sensitive to the specific criterion adopted to determine the time to rod burst. Also, burst stress criteria are generally derived based on the assumption of uniform strain along the axial direction in the ballooned section, which makes their application in detailed fuel rod models not fully consistent. In this respect a definition of burst strain consistent with the modeling approach in the codes would be necessary.

The FUMAC benchmark of fuel performance codes presented in this paper leads to recommendations for future work on fuel modeling developments for LOCA analysis. In particular, further investigation and sensitivity analysis of cladding strain calculations during ballooning, including the sensitivity of calculated maximum strains to the specific burst criterion and the relative uncertainties, appears advisable. Also, improvements in predictions of cladding strains as well as cladding burst times may be achieved by considering the anisotropic creep behavior of alpha-Zr under LOCA conditions. Finally, since another potential source of discrepancy is the 1.5D or 2D representation of a behavior that involves inherently 3D effects such as localized cladding ballooning and burst associated with azimuthal temperature variations, exploring full 3D calculations in the future is deemed useful.

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References
