Evaluation of Loss-of-Coolant Accident Simulation Tests with the Fuel Rod Analysis Code FRAPTRAN-1.4

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27 December 2011

Abstract

An integrated computer model for reactor fuel cladding rupture under loss-of-coolant accident (LOCA) conditions has been implemented in the transient fuel rod performance code FRAPTRAN. The model treats the zirconium alloy solid-to-solid phase transformation kinetics, cladding oxidation, cladding deformation, and eventually cladding rupture concurrently. It is for use together with the recently developed finite element based solution module in FRAPTRAN-1.4. The model has been employed to calculate ex-reactor single-rod transient burst tests in which the rod internal pressure and the heating rate were kept constant during the tests. The calculations are compared with experimental data on cladding rupture strain, temperature and pressure. Furthermore this model in FRAPTRAN-1.4 has been used to evaluate a LOCA simulation test within the IFA-650 series performed in the Halden boiling heavy-water reactor. The Halden test was made on a pressurized water reactor fuel rod with Zircaloy-4 cladding. It simulated the blowdown and refill (heattup) phase of a LOCA. The results of the FRAPTRAN-1.4 calculations are compared with experimental data on (i) maximum hoop strain at rupture, (ii) cladding diameter increase versus axial position, (iii) internal rod pressure versus time, (iv) peak cladding temperature at rupture, and (v) post-test cladding outer surface layer thickness. The results are discussed in terms of various uncertainties in the calculations. Nevertheless, the new implementation of the cladding rupture models indicates an overall improvement of the code for fuel rod LOCA analysis.

Presented in HI TEMP 2011 Conference, 20-22 September 2011, Boston, USA.
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1 Introduction

A loss-of-coolant accident (LOCA) is a design basis accident in which a “guillotine” break is postulated to occur in one of the cold legs of a pressurized water reactor (PWR) or in one of the circulation pump intake lines of a boiling water reactor (BWR) [1]. Consequently, the primary system pressure would drop and almost all the reactor coolant (water) would be discharged into the reactor containment. The drop in pressure would activate the reactor protection system and the reactor would trip. The fission chain reaction in the fuel due to the loss of moderator coolant would be terminated. Nevertheless, the heat would continue to be released from the fuel rods by fission product radioactive decay. Subsequently, the emergency core cooling system (ECCS) must provide adequate cooling in time to minimize overheating of fuel cladding, its damage and eventual core meltdown.

The LOCA in a PWR is especially grave since the pressure vessel of a PWR does not have a recirculation system. The events occurring within the first couple of minutes following a design basis LOCA in a PWR are separated roughly into three periods: (1) blowdown, in which the coolant would be expelled from the reactor vessel, (2) refill, when the emergency coolant water would begin to fill the vessel up to the bottom of the core, and (3) reflood, when the water level would rise enough to cool the core. Blowdown would take about 20 seconds during which fuel cladding temperature may rise to \( \approx 1250 \text{ K} \). The refill period (10-15 s) begins when ECCS injects borated water into the vessel, but cladding temperature would continue to rise (heatup phase) to \( \approx 1300 \text{ K} \) due to poor heat transfer from fuel rod to steam-water mixture in the core. The reflood period would start when the water level gets to the bottom of the fuel rods, then after a period of about 60 s the cladding temperature would drop fairly rapidly [1, 2].

Such a sequence of events is addressed in the acceptance criteria for ECCS [3] in light water reactors (LWRs). In regard to fracture of Zircaloy cladding during a LOCA, the criteria include the following items: (i) The calculated peak fuel element cladding temperature shall not exceed 1477 K, (ii) the calculated equivalent cladding reacted (ECR), defined as the ratio of the oxidized metal thickness to initial cladding wall thickness, must not exceed 0.17 times the cladding wall thickness, (iii) a specific model [4] must be used to calculate Zircaloy steam oxidation rates for LOCA conditions. Moreover, other regulatory bodies can impose additional restrictions. For example, the Reactor Safety Commission of Germany RSK [5] demands that the calculated number of fuel rods ruptured during a LOCA in a PWR shall remain below 10% of the total number of fuel rods in the core. Hence, besides cladding temperature and oxidation analysis, cladding creep deformation and rupture also need to be modeled.

In this paper, a unified model for cladding oxidation, creep and rupture in LOCA conditions within the fuel rod transient code FRAPTAN [6] is used...
to evaluate a number of LOCA experiments. The utilized model is based on the description given in our previous article [7] with some extensions and modifications discussed in the ensuing section. A special attribute of the model is that it accounts for the kinetics of the solid-to-solid zirconium phase transformation during both heating and cooling of the alloy and also evaluates the influence of oxygen pickup on the transformation. For example, in Zircaloy-4 fuel cladding tube with a nominal chemical composition: Zr-base,1.5Sn-0.2Fe-0.1Cr-0.12O by wt\%, the alloy undergoes a phase transformation from the low temperature hexagonal closed-packed (hcp) \( \alpha \)-phase to body-centered cubic (bcc) \( \beta \)-phase. In equilibrium conditions, the transformation temperatures are \( \approx 1080 \) K for \( \alpha \Rightarrow (\alpha + \beta) \) and \( \approx 1280 \) K for \( (\alpha + \beta) \Rightarrow \beta \) [7, 8].

The experiments assessed with \textsc{Fraptran} in this paper are the single-rod burst tests conducted at the former Karlsruhe Nuclear Research Center, Germany with well-defined boundary conditions [9] and a test performed in the Halden test reactor in Norway to simulate the blowdown and refill periods of a LOCA. The former tests were especially designed to develop and verify a cladding rupture criterion for LOCA.

The structure of the paper is as follows. Section 2 presents the computer codes and models used in our evaluations. Details of the new implemented model in \textsc{Fraptran-1.4} is banished to Appendix A. In Sec. 3, we briefly review the LOCA experiments considered. In Sec. 4, the results of computations and comparisons with measurements are presented. The input information regarding cladding mechanical model options to \textsc{Fraptran} for the IFA-650.2 test is listed in Appendix B. We conclude with some remarks on the main points in Sec. 5.
2 Computer models

For the analysis of the experiments considered in this note, we have utilized the computer program FRAPTRAN-1.4, and in particular the version FRAPTRAN-QT1.4b comprising an adaptation of the model presented in Ref. [7]. The code FRAPTRAN (Fuel Rod Analysis Program Transient) simulates the LWR fuel thermal-mechanical behaviour when power and/or coolant boundary conditions are rapidly changing [6]. More specifically, the code computes fuel rod attributes, such as fuel and cladding temperatures, cladding elastic and plastic strains, cladding stresses, fuel rod internal gas pressure, etc. as a function of irradiation time. FRAPTRAN affords a best-estimate code for analysis of fuel response to postulated accidents such as LOCA and interpreting experiments simulating such accidents. The FRAPTRAN-1.4 code assessment, that is, comparison between code computations and data from selected integral irradiation experiments and post-irradiation examination programs is documented by Geelhoed and coworkers [10].

The standard models and modelling options available in FRAPTRAN-1.4 are described in Ref. [6]. The models implemented in the version 1.4 of FRAPTRAN can be used with the finite element based solution module of the code developed by Knuutila [11]. In the present note, we delineate the cladding behaviour models of version QT1.4b of the code, which are related to LOCA conditions. The QT1.4b computational method is similar to that described in Ref. [7] with some extensions, modifications and adaption to an integral fuel rod modelling code.

The main quantities calculated by the method are (i) oxygen parameters generically denoted by $\kappa$, which can be either the oxygen concentration picked up by the cladding during the oxidation process, the oxide layer thickness, or the oxygen concentration in the cladding metal layer; (ii) the volume fractions of the $\beta$-Zr $y$ and $\alpha$-Zr (1-$y$) during the phase transformation; (iii) the cladding hoop strain due to creep $\varepsilon_\theta$; (iv) and the cladding burst stress $\sigma_B$. All these quantities are coupled through a set of kinetic equations and a burst criterion. They can be expressed generically in the form

\[
\frac{d\kappa}{dt} = f_1(\kappa, T, \varepsilon_\theta), \quad (1)
\]

\[
\frac{dy}{dt} = f_2(y, \kappa, T), \quad (2)
\]

\[
\frac{d\varepsilon_\theta}{dt} = f_3(T, \sigma_\theta, y, \kappa), \quad (3)
\]

and

\[
\frac{d\sigma_B}{dt} = f_4(\kappa, T), \quad (4)
\]

where $f_i$, $i = \{1, 2, 3\}$ are the respective functions for the evolution of the variables, $f_4$ is purely an empirical function of cladding temperature and oxygen concentration, $\sigma_\theta$ is the cladding hoop stress, $T = T(t)$ is the cladding temperature, which is a function of time $t$ controlled by power and/or coolant
boundary conditions during the transient event. These functions are identified in Appendix A. This set of three first order differential equations (1)-(3) needs to be solved numerically to obtain the time evolution of the respective variables during the transient.

We should point that the main difference between the present method and the one presented in Ref. [7] is that now the $\beta$-phase domain variable $y$ is a function of oxygen concentration and also the oxygen concentration in the metal is distinguished from the oxide layer thickness as detailed in Appendix A.
3 Experiments

In this paper, we consider two types of LOCA experiments for computer analysis of LOCA conditions. The first type is from single-rod transient burst tests, which were conducted at Kernforschungszentrum Karlsruhe (KfK), Germany using fuel rod simulators with indirect electric heating [12]. These tests were analyzed in our previous paper using an integrated fuel cladding model for LOCA conditions [7]. The second type is from a test series (IFA-650.2) conducted at the Halden reactor on a single UO₂ fuel rod [13, 14]. Here, we have used the FRAPTRAN code to simulate both types of experiments.

3.1 Karlsruhe tests

Three test series conducted at KfK are considered here; namely (I) FR2 in-pile tests [15], (II) single-rod REBEKA tests [12], (III) multi-rod REBEKA tests [16]. These tests had well-defined boundary conditions, and the internal rod over-pressure and the heating rate were kept roughly constant during the deformation process. They were designed to validate fuel cladding burst computer models. The tests used fuel rod simulators with indirect electric heating and 325 mm heated length. The cladding tube samples of the Karlsruhe tests (I, II and III) analysed here were made of Zircaloy-4 and had the nominal inner and outer diameters of 9.30 mm and 10.75 mm, respectively. The main characteristics of these tests are summarized in Table 1.

FR2 in-pile tests In the Karb et al. [15, 17] experiments, the intent was to study the effects of nuclear environment on fuel cladding failure mechanisms. In these experiments both unirradiated and pre-irradiated PWR-type test fuel rods were subjected to temperature transients simulating the second heatup phase of a LOCA. Nuclear milieu was distinguished by the heat generated in UO₂ fuel and the presence of fission products (the heat is transferred from the fuel to the cladding outer surface). The tests were conducted in a loop of the FR2 research reactor at Karlsruhe, which provided the LOCA thermal-hydraulic conditions. In addition, 8 reference rods with electrically rod simulators with Al₂O₃ pellets were tested in the in-pile loop under conditions identical with those of the nuclear tests [15].

In these tests, the cladding burst data (temperature at rupture, rupture pressure and rupture strain) of the nuclear fuel rods did not indicate differences from the results obtained from electrically heated fuel rod simulators, and nor did they show the effect of irradiation exposure (up to 35 MWd/kgU). In our analysis, we only consider the unirradiated rods and the electrically heated fuel rod simulators by prescribing temperature histories to the cladding and simulate the burst behaviour with the FRAPTRAN code (section 2). The heating rate of the unirradiated rods varied between 7 to 19 Ks⁻¹, whereas that of the electrically heated rod simulators had heating
3.2 Halden IFA-650 test

Table 1: Karlsruhe test data for the FRAPTRAN code validation. Samples were unirradiated Zircaloy-4 cladding tubes, with an outer diameter of 10.75 mm and a wall thickness of 0.725 mm

<table>
<thead>
<tr>
<th>Data set</th>
<th>Rod internal over-pressure, MPa</th>
<th>Heating rate K/s</th>
<th>Clad burst temperature, K</th>
<th>Clad burst strain, %</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>5-12</td>
<td>7-19</td>
<td>1083-1288</td>
<td>26-64</td>
<td>[15]</td>
</tr>
<tr>
<td>II</td>
<td>1-14</td>
<td>1-35</td>
<td>970-1400</td>
<td>14-116</td>
<td>[12]</td>
</tr>
<tr>
<td>III</td>
<td>6.5</td>
<td>7</td>
<td>1063-1143</td>
<td>28-55</td>
<td>[16]</td>
</tr>
</tbody>
</table>

rates of 12-13 Ks⁻¹.

**Single-rod REBEKA tests** The single-rod burst transient tests within the REBEKA program in steam were conducted at KfK. The rod simulator comprised Al₂O₃ pellets (instead of UO₂ fuel pellets) clad with Zircaloy-4 tubing [18, 12]. The temperature history of the cladding during the test was measured by thermocouples spot-welded on the outer surface of the cladding. The deformation of cladding as a function of time was recorded by X-ray cinematography by using a high-speed camera, which allowed the observation of cladding ballooning process during the test. Data on burst temperature, burst pressure and burst strain are presented in Ref. [12]. The heating rate in these tests ranged from 0.8 to 35 Ks⁻¹. The test parameters, rod over-pressure and heating rate, were in the range of 1 to 14 MPa and 1 to 30 Ks⁻¹, respectively.

**Multi-rod REBEKA tests** Erbacher and Leistikow [16] have presented Zircaloy-4 burst data obtained from multi-rod burst tests performed within the REBEKA program. The data represent tests that had the potential for maximum ballooning, i.e. burst taking place in the α-phase of Zircaloy around 1070 K. The heating rate during heatup in the tests was 7 Ks⁻¹. The burst pressures in the test were between 5 and 7 MPa and the measured hoop strains ranged from 0.28 to 0.55. Moreover, the circumferential temperature variation in the tests varied between 20 and 70 K.

3.2 Halden IFA-650 test

The Halden IFA-650 test series were performed in the Halden boiling heavy-water reactor (HBWR) under simulated loss-of-coolant accident (LOCA) conditions. In the second experiment of this series, IFA-650.2 [13, 14], considered here, an unirradiated PWR UO₂ fuel rod was tested. The data for the rod used in the IFA-650.2 experiment are summarized in Table 2. The IFA-650.2 test rig design and instrumentation is described in [13].
Table 2: IFA-650.2 test rod data.

<table>
<thead>
<tr>
<th>Pellet</th>
<th>Material</th>
<th>UO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter</td>
<td>mm</td>
<td>8.29</td>
</tr>
<tr>
<td>Length</td>
<td>mm</td>
<td>8</td>
</tr>
<tr>
<td>Dishing</td>
<td></td>
<td>dished in both ends</td>
</tr>
<tr>
<td>Dish depth</td>
<td>mm</td>
<td>0.20</td>
</tr>
<tr>
<td>Land width</td>
<td>mm</td>
<td>1.15</td>
</tr>
<tr>
<td>Density (UO₂)</td>
<td>% of TD</td>
<td>95</td>
</tr>
<tr>
<td>U-235 enrichment in UO₂</td>
<td>wt.%</td>
<td>2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cladding</th>
<th>Material</th>
<th>Low-tin† Zircaloy-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer diameter</td>
<td>mm</td>
<td>9.5</td>
</tr>
<tr>
<td>Wall thickness</td>
<td>mm</td>
<td>0.57</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fuel rod</th>
<th>Burnup</th>
<th>MWd/kgU</th>
<th>0 (fresh fuel)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active length</td>
<td>mm</td>
<td>500</td>
<td></td>
</tr>
<tr>
<td>Radial pellet-clad gap</td>
<td>mm</td>
<td>0.035</td>
<td></td>
</tr>
<tr>
<td>Plenum volume</td>
<td>cm³</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>Fill gas</td>
<td></td>
<td>helium</td>
<td></td>
</tr>
<tr>
<td>Fill pressure at fabrication</td>
<td>MPa</td>
<td>4.0</td>
<td></td>
</tr>
<tr>
<td>Fabrication temperature</td>
<td>°C</td>
<td>25</td>
<td></td>
</tr>
</tbody>
</table>

† “Low-tin” refers to Sn content in the lower part of the range specified for Zircaloy-4 (1.2-1.7 wt.% Sn) according to ASTM R60804 specification.

In the IFA-650.2 test, the LOCA simulation was initiated by a blowdown phase, during which the pressure in the coolant channel decreased from 7.0 to 0.4 MPa in about 35 seconds. After the blowdown, the heatup (refill) period of the LOCA was simulated. The temperature of the cladding was provided by an annular-shaped electrical heater surrounding the fuel rod. Furthermore, during the test, the rod was kept at a small constant average nuclear power of 2.3 kW/m to provide suitable conditions for cladding deformation (ballooning) and oxidation. The axial rod power distribution produced by nuclear heating was roughly sinusoidal (0 to 2π) with a peaking factor of about 1.06 at the half-height position of fuel stack.

During the heatup phase the cladding was subjected to a temperature rise from 488 to 1323 K in about 200 seconds. Cladding rupture was detected inter alia by the cladding thermocouple and elongation (rod length change) signals at about 1070 K, i.e. at about 100 s after initiation of the blowdown. The average cladding heating rate up to the instant of rupture was about 8 Ks⁻¹. A retardation of the heating rate (to around 5 Ks⁻¹) was observed in the cladding thermocouple temperature recordings just before the occurrence of rupture (rod failure).

Post-test visual examination of the rod revealed that the fuel cladding
had ruptured by an axial crack at the fuel rod peak power position. The average hoop strain prior to burst, obtained by measuring the diameter increase close to the burst opening was in the range of 35-40%. Over an axial distance of about 300 mm, including the burst area, the rod showed an acicular diameter increase [13]. The test results from the IFA-650.2 test are summarized in Table 3.

Table 3: Summary of measured results from IFA-650.2 test [13, 14].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time to rupture after start of blowdown</td>
<td>99 s</td>
</tr>
<tr>
<td>Axial location of rupture</td>
<td>195-230 mm$^a$</td>
</tr>
<tr>
<td>Axial length of rupture (crack)</td>
<td>35 mm</td>
</tr>
<tr>
<td>Maximum lateral width of crack opening</td>
<td>$\approx$20 mm</td>
</tr>
<tr>
<td>Average rod pressure during LOCA (prior to rupture)</td>
<td>6.7 MPa$^b$</td>
</tr>
<tr>
<td>Rod pressure at rupture</td>
<td>5.6 MPa$^b$</td>
</tr>
<tr>
<td>Cladding diameter increase close to rupture area</td>
<td>35-40%$^c$</td>
</tr>
<tr>
<td>Maximum cladding diameter increase in rupture area</td>
<td>$\approx$90%$^d$</td>
</tr>
<tr>
<td>Cladding temperature at time of rupture</td>
<td>$\approx$1073 K (800°C)</td>
</tr>
<tr>
<td>Average cladding heating rate up to instant of rupture</td>
<td>$\approx$8 Ks$^{-1}$</td>
</tr>
<tr>
<td>Typical cladding azimuthal temperature variation during heatup phase prior to rupture</td>
<td>$\approx$5 Ks$^{-1}$f</td>
</tr>
<tr>
<td>Maximum temperature measured at cladding lower and upper thermocouple positions, respectively</td>
<td>1364, 1309 K</td>
</tr>
<tr>
<td>Post-test inner and outer surface oxide layer thickness (below and above crack opening)</td>
<td>40-50 µm</td>
</tr>
</tbody>
</table>

$^a$ From bottom end of the 300 mm long fuel stack. $^b$ To obtain the differential pressure across the cladding wall, the rod pressure value shall be subtracted by the coolant channel pressure (0.4 MPa) after blowdown. $^c$ Estimated from measured diameter increase $\Delta D$ with respect to initial cladding outer diameter $D_0$ by $\Delta D/D_0 \times 100\%$. $^d$ Estimated from measurements of circumferential length $L$ of fractured cladding. The diameter increase is obtained by relating $L$ with initial cladding circumference $L_0$ by $L/L_0 \times 100\%$. $^f$ Estimated from upper thermocouple measurements (TCC 2-3 and -4).
4 FRAPTRAN computations

In this section the results of the analyses of the KfK and Halden IFA-650.2 tests, described in the foregoing section, using the FRAPTRAN code are presented. For the KfK tests FRAPTRAN-QT1.4b, described in Appendix A, is used, whereas for the IFA-650.2 test, three versions of FRAPTRAN including the aforementioned version was utilized for comparison.

4.1 Comparison with KfK tests

Cladding burst computations with FRAPTRAN-QT1.4b, for comparison with experimental results, are carried out by varying the constant rod internal over-pressure in the range from 0.1 to 14 MPa (in steps of 0.1 MPa) at two different constant heating rates, 1 and 35 Ks

Similar model assumptions as in our previous paper [7] are made (see Appendix A). The resulting cladding burst curves, calculated in this way, i.e. (i) burst temperature versus internal over-pressure and (ii) cladding hoop burst strain versus burst temperature, together with burst test data referred in Sec. 3 are plotted in Figs. 1a and 1b, respectively.

Comparing the results depicted in Figs. 1a and 1b, with those obtained by the stand-alone model (figure 7 of Ref. [7]), it is seen that they are quite close despite some differences between the modelling assumptions as pointed out in Appendix A and that FRAPTRAN-QT1.4b is a large thermal-mechanical code with many submodels, which affect the results. Moreover, due to a large scatter in experimental data the results of two sets of calculations are practically equivalent.

4.2 Comparison with IFA-650.2 test

The results from the calculations are compared with measured data for the following parameters: (i) Maximum hoop strain at rupture; (ii) Cladding diameter increase at rupture versus axial position of rod; (iii) Fuel rod pressure as a function of time; (iv) Maximum cladding temperature at rupture; and (v) post-test cladding outer surface layer thickness. The computations of the IFA-650.2 test involve the use of three different versions of the FRAPTRAN code, namely, versions FRAPTRAN-1.4 [6], FRAPTRAN-QT1.4b (cf. Appendix A), and FRAPTRAN/GENFL0 [19].

The FRAPTRAN-1.4/FRAPTRAN-QT1.4b computations of the IFA-650.2 test, presented here, utilize thermal-hydraulic boundary conditions calculated by Miettinen et al. [19] using the GENFL0 code. More specifically, we employ the computed time variations of coolant pressure and cladding outer surface temperatures [20], see Figs. 2a and 2b, respectively, as prescribed boundary conditions for the cladding in our computations with FRAPTRAN-1.4 and FRAPTRAN-QT1.4b.
4.2 Comparison with IFA-650.2 test

Figure 1: FRAPTRAN-QT1.4b computed burst curves for Zircaloy-4 cladding generated by varying constant internal over-pressure in the range from 0.1 to 14 MPa at two different constant heating rates, 1 and 35 Ks⁻¹. Three sets of measured burst data, namely Karb et al. [15] (FR2 in-pile tests), Erbacher et al. [12] (single-rod REBEKA tests), and Erbacher-Leistikow [16] (multi-rod REBEKA tests) are included for comparison; cf. Sec. 3.3.1.
Figure 2: Time-dependent boundary conditions used in FRAPTRAN-1.4 and FRAPTRAN-0T1.4b for the IFA-650.2 test: (a) Coolant pressure versus time; (b) cladding outer surface temperatures at thermocouple positions calculated by FRAPTRAN compared with measured values in the IFA-650.2 test. TCC1: lower thermocouple, TCC2: higher thermocouple; 100 mm and 400 mm from bottom end of the rod, respectively.
The computations in our work are performed by using either the traditional cladding model FRACAS-I in FRApTRAN-1.4 [6] or the finite element based cladding model FEA in FRApTRAN-1.4 [6]. In the computation with the FEA module, the cladding rupture criterion option irupt=2 [6] is selected. This option selects the burst hoop strain versus burst temperature correlation for cladding heating rates \( \leq 10 \text{ Ks}^{-1} \) (slow-ramp) tabulated in the NUREG-0630 document [21] as a rupture criterion. A similar burst correlation for heating rates \( \geq 25 \text{ Ks}^{-1} \) (fast-ramp) is also tabulated in [21], which can be selected in FRApTRAN-1.4 by setting irupt=1. However, since the average heating rate during the heatup phase in the IFA-650.2 test is about 8 Ks\(^{-1}\) (Table 3) we apply the former of these two burst options.

The active length of the fuel rod (0.5 m) is divided into 10 axial segments, each of equal length. The cladding is structurally treated as a thin-walled tube, both in the FRACAS-I and the FEA models. In FEA, the cladding is represented by a single finite element across its thickness. The input options defining the cladding models applied in the FRApTRAN calculations are summarized in Table B.1 of Appendix B. The cladding model options are set in the $\$model$ block of the FRApTRAN input files. The time equal to zero \( t=0 \) in the analyses refers to the start of the blowdown phase. A constant time step length of 5 ms is applied in the heatup phase of the LOCA transient.

Output of FRApTRAN computations regarding cladding permanent hoop strain as a function of time for the IFA-650.2 test is presented in Ref. [22]. The maximum value of the permanent cladding hoop strain (rupture strain) from the FRACAS-I model amounts to 81\%, whereas the corresponding values from the FEA package of FRApTRAN-1.4 and FRApTRAN-QT1.4b amount to 35\% and 111\%, respectively. These rupture strain values are obtained in axial segment (node) number 5 (burst node).

Calculated cladding outer diameter over the fuel stack region of the ruptured test rod, using the FRApTRAN-1.4 and FRApTRAN-QT1.4b programs, is compared with measured values in Fig. 3. The measured data in Fig. 3 have been obtained as the average of three diametral trace measurements, at 0, 45 and 135 degrees orientation [14], along the rod. The burst region in the rod diameter measurement is indicated by a gap in the data (dot line), since no relevant data were reported in this region by this measurement method.

We note that the cladding deformation, particularly outside the burst region, is generally underestimated by computations compared with measurements. We also observe that the calculated cladding deformation below the burst region is smaller than above that region, which is clearly the opposite of what is indicated by the measurement (Fig. 3). The underestimation of cladding deformation is also seen in the calculated rod pressure, which is overestimated until the occurrence of cladding rupture; see the sudden drops in rod pressure shown in Fig. 4.

The best agreement between measured and calculated variation of final cladding outer diameter along the test rod is obtained with the FEA cladding.
module of the FRAPTRAN-QT1.4b code. The FRAPTRAN-QT1.4b-calculated diameter shown in Fig. 3 matches roughly the measured diameter profile above the burst region, but is about 1.0-1.3 mm smaller than measurement in the lower half of test rod, i.e. below the cladding breach. We should also note that, cf. Fig. 2, during the heatup phase, the lower thermocouple temperature is roughly 30-40°C higher than that for the upper thermocouples. The measured cladding deformation shown in Fig. 3 is thus consistent with the cladding temperature recordings, i.e. a higher temperature leads to more creep deformation than a lower temperature. The computed values for the time to cladding rupture and cladding temperature, the maximum cladding hoop strain and rod pressure at rupture and cladding outer surface oxide thickness, are compared with measured results in Table 4.

![Graph](image)

Figure 3: Calculated cladding outer diameter at burst for the IFA-650.2 test using FRAPTRAN code versions. The corresponding measured diameter along the rod is shown by the dash-dot line.
Figure 4: Rod gas pressure (plenum pressure) vs. time for the IFA-650.2 test calculated with the FRAPTRAN codes. Cladding rupture is calculated to occur after 70-80 s. The measured evolution of the rod pressure is shown by the dash-dot curve. In reality, the measured rod pressure reaches the rig pressure soon after the instant of cladding rupture after 99 s (asterisk symbol).
Table 4: Comparison of calculated and measured results for IFA-650.2 test.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Computation</th>
<th>Measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time to cladding rupture, s</td>
<td>75.8</td>
<td>99</td>
</tr>
<tr>
<td>Rupture temperature, °C</td>
<td>708</td>
<td>≈800</td>
</tr>
<tr>
<td>Max. rupture hoop strain, %</td>
<td>81</td>
<td>≈90</td>
</tr>
<tr>
<td>Rod pressure at rupture, MPa</td>
<td>8.9</td>
<td>≈5.6</td>
</tr>
<tr>
<td>Max. post-test outer surface oxide layer thickness, μm</td>
<td>35</td>
<td>40-50</td>
</tr>
</tbody>
</table>

(1) FRApTRAN-1.4 with FRACAS-I.
(2) FRApTRAN-1.4 with FEA.
(3) FRApTRAN-QT1.4b with FEA.

A point worth commenting is that a principal difference between the FRApTRAN computations using either the FRACAS-I or the FEA module is that by using the latter, the cladding deformation is calculated for all cladding segments until rupture occurs. In computations using FRACAS-I, at the instant at which the cladding strain, at a certain axial node, reaches the strain instability criterion, additional permanent deformation (until rupture) is calculated only for that particular node [23]. In the IFA-650.2 test, in which the cladding experienced relatively large diameter increases over a significant length of the rod, the local ballooning approach used in FRACAS-I leads to a gross underestimation of the cladding deformation until the instant of rupture, cf. Fig. 3.

Finally, we observe that cladding burst occurred at ≈ 1073 K (800 °C), well below the PCT acceptance limit of 1477 K. Similarly, the measured oxide layer (below and above the cladding split opening) was between 40-50 μm at both sides of the cladding [14]. This corresponds to an ECR of about 10%, which is well below the 17% limit.
5 Conclusions

In this paper, we have presented results of computations made on LOCA simulation experiments conducted in Karlsruhe and a test performed in the Halden reactor, the LOCA test IFA-650.2. For the latter experiment, we have used both the conventional FRAPTRAN-1.4 code and a modified/extended version of that code, FRAPTRAN-QT1.4b, whereas for the latter tests we have only employed FRAPTRAN-QT1.4b. The models unique to FRAPTRAN-QT1.4b are also described in our paper. The extended capability of the FRAPTRAN-QT1.4b code includes cladding material models for high-temperature oxidation, phase transformation, creep deformation and rupture, in tandem, combined with the finite element (FE) based cladding model for mechanical calculations.

The results of our computations of the Karlsruhe tests, displayed in terms of cladding burst temperature versus rod pressure and cladding burst strain versus temperature, are in conformity with the data; and also they benchmark with our previous computations [7], which employed a stand-alone program comprising similar material models as in FRAPTRAN-QT1.4b. The fuel rod behaviour in our simulations of the IFA-650.2 test was carried out, for the sake of comparison, by both the FRACAS-I and the FEA modules of FRAPTRAN. Furthermore, the thermal-hydraulic boundary conditions input to our analysis were taken from the output of the FRAPTRAN/GENFLO code.

Our results show sufficient differences between calculation and measurement regarding the cladding diameter increase (axially along the rod), rod pressure and time to cladding rupture. In general, the calculated cladding diameter increase is rather small compared with measurement. We believe that this underestimation arise partly because the prescribed temperatures at the cladding outer surface are rather low. The measurement recordings by the cladding thermocouples indicate that the cladding temperature should be about 30–40 K higher than the calculated values (FRAPTRAN/GENFLO). The calculated cladding deformations affect, in turn, directly the magnitude of the calculated rod pressure. Nevertheless, our evaluation of the IFA-650.2 test shows that the introduction of the new material models in FRAPTRAN-QT1.4b improves the cladding deformation calculation at rupture (relative to measurement) compared to results obtained by conventional FRAPTRAN-1.4.

Acknowledgement

We express our gratitude to Jan-Olof Stengård of the Technical Research Centre of Finland (VTT) for providing precalculated thermo-hydraulic boundary conditions by the FRAPTRAN/GENFLO code for our FRAPTRAN calculations. The work was supported by the Swedish Radiation Safety Authority (SSM) under the contract number SSM2011-2200/2030048-12.
References


A Models for FRAPTRAN-QT1.4b

In this section, we briefly describe the models for cladding high temperature oxidation, phase transformation, creep and failure introduced in the FRAPTRAN-1.4 code [6]. The models are intended for usage with the finite element based solver module of the code [11]. A more detailed description is provided in Ref. [24]. As noted in section 2 the principal difference between the present method and that described and used in Ref. [7] is that now the phase transformation kinetics is oxygen concentration dependent and also the oxygen concentration in the metal is distinguished from the oxide layer thickness.

A.1 Cladding oxidation

The cladding oxidation model is based on the work of Cathcart et al. [25]. The basic expression for the rate of oxidation reaction of cladding is the parabolic law in the form

$$\frac{d\kappa}{dt} = \frac{1}{\kappa} \frac{\delta^2 \kappa}{2},$$

(A.1)

where $\kappa$ stands for a kinetic variable, e.g., the total oxygen concentration (kgm$^{-2}$) consumed by the cladding surface $\kappa \Rightarrow \rho$ or the oxide layer thickness (m) at the surface of the cladding $\kappa \Rightarrow \xi$. The parameter $\delta_\kappa$ is the parabolic rate coefficient expressed by the Arrhenius relation

$$\frac{\delta^2 \kappa}{2} = A_\kappa e^{-Q_\kappa/RT},$$

(A.2)

where $RT$ has its usual meaning and the numerical values for $A_\kappa$ and $Q_\kappa$ are: $A_\rho = 36.22$ (kgm$^{-2}$)$^2$s$^{-1}$, $Q_\rho / R = 20112$ K, $A_\xi = 2.252 \times 10^{-6}$ m$^2$kgm$^{-1}$, and $Q_\xi / R = 18073$ K. The integrated form of Eq. (A.1) is $\kappa = \sqrt{\kappa_0 + \delta_\kappa^2 t}$.

The oxygen concentration rate in the cladding metal layer $x_M$, assuming one-sided oxidation of cladding tube’s outer surface, is

$$\frac{dx_M}{dt} = \frac{2R_o}{\rho_{Zr}(R_o^2(\xi) - R_{ci}^2)} \left( \frac{d\rho}{dt} - M \frac{d\xi}{dt} \right),$$

(A.3)

where $\rho_{Zr} = 6560$ kgm$^{-3}$ is the density of cladding metal, $M = 1475.1$ is the ratio of the atomic mass of O$_2$ to that of ZrO$_2$, $R_o(\xi) = R_{co} - \xi / R_{PB}$, $R_{co}$ and $R_{ci}$ are the as-fabricated cladding outer and inner radii, respectively, and $R_{PB} = 1.56$ is the Pilling-Bedworth ratio for Zr.

A.2 Zircaloy phase transformation

The phase transformation model has been detailed in our preceding articles [26, 27]. It expresses the rate of the transformed volume fraction of the $\beta$
A.2 Zircaloy phase transformation

Phase, $y$, according to

$$\frac{dy}{dt} = \frac{y_s(T, x_M) - y}{\tau_c(T)},$$

(A.4)

where $y_s(T, x_M)$ is the equilibrium value $y$ at temperature $T$ and $\tau_c(T)$ is the characteristic time of phase transformation. The expressions for $y_s$ is given as

$$y_s(T, x_M) = \frac{1}{2} \left[ 1 + \tanh \left( \frac{T - T_m(x_M)}{T_s(x_M)} \right) \right],$$

(A.5)

where $T_m$ and $T_s$ are oxygen concentration ($x_M$) dependent parameters related to the mid and the span of the mixed-phase temperature region, respectively. They are calculated according to

$$T_m(x_M) = \frac{T_\alpha(x_M) + T_\beta(x_M)}{2},$$

(A.6)

$$T_m(x_M) = \frac{T_\alpha(x_M) - T_\beta(x_M)}{2.3}.$$

(A.7)

For Zircaloy-4 cladding, the phase boundary temperatures $T_\alpha$ and $T_\beta$ can be written as

$$T_{\alpha(\beta)}(x_M) = T_\alpha + A_p x_M^m,$$

(A.8)

where $A_p$ and $m$ are constants, presented in Table A.1. The phase boundary temperatures versus excess oxygen concentration, calculated through Eq. (A.8), are matched with experimental data for Zircaloy-4 in Ref. [28]. It should be remarked that $T_\beta$, calculated through Eq. (A.8), may exceed the Zircaloy-4 melting temperature for high oxygen concentrations. The melting (solidus) temperature of Zircaloy-4 increases from about 2025 K at zero oxygen concentration to about 2320 K for $x_M \geq 0.04$ [29]. The characteristic time for the phase transformation, i.e. $\tau_c$ in Eq. (A.4), is calculated from an empirical correlation, formulated on the basis of experimental data produced by Forgeron and co-workers [8]. Under heating, the phase transformation is diffusion controlled and its rate depends strongly on temperature. Accordingly, $\tau_c$ (s) is calculated through

$$\tau_c(T) = \tau_d(T) = 4.0 \times 10^{-6} e^{16650/T}.$$

(A.9)
A.3 Cladding creep

Under cooling, the phase transformation is partly martensitic, and $\tau_c$ is calculated through

$$\tau_c(T) = \frac{1}{\tau_d(T)} + \frac{1}{\tau_m}, \quad (A.10)$$

where $\tau_d$ is given by Eq. (A.9) and $\tau_m = 5.0$ s is a constant. Equation (A.10) implies that martensitic transformation becomes important for the $\beta \rightarrow \alpha$ phase transformation at low temperatures, since $\tau_c \rightarrow \tau_m$ as temperature decreases.

### A.3 Cladding creep

In the single phase domains, i.e. when the cladding material is in pure $\alpha$- or $\beta$-phase, the steady-state effective creep strain rate, $\dot{\varepsilon}_{\text{eff}}$ (s$^{-1}$) is correlated to temperature $T$ (K), the von Mises effective stress $\sigma_{\text{eff}}$ (Pa), and the excess oxygen weight fraction in the cladding metal layer $x_M$ (–) through

$$\frac{d\varepsilon_{\text{eff}}}{dt} = A_c e^{-B_c x_M} e^{-Q_c/RT} \sigma_{\text{eff}}^n, \quad (A.11)$$

where $A_c$, $B_c$, $Q_c$ and $n$ are constants, defined in Table A.2. We should note that Eq. (A.11) is used within a model for isotropic creep deformation in FRAPTRAN-GT1.4b, but that the strength coefficient $A_c$ is determined from uniaxial creep tests by use of Hill’s theory for anisotropic plasticity [30].

<table>
<thead>
<tr>
<th>Phase domain</th>
<th>$A_c$</th>
<th>$B_c$</th>
<th>$Q_c/R$</th>
<th>$n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure $\alpha$</td>
<td>$4.00 \times 10^{-32}$</td>
<td>$342$</td>
<td>$38487$</td>
<td>$5.89$</td>
</tr>
<tr>
<td>Pure $\beta$</td>
<td>$1.65 \times 10^{-22}$</td>
<td>$0.0$</td>
<td>$17079$</td>
<td>$3.78$</td>
</tr>
</tbody>
</table>

The strain rate in the two-phase coexistence ($\alpha + \beta$) region follows a separate mechanism than in the single phase region [32, 33]. For computational convenience in the coexistent two-phase region of zirconium alloy, we have considered creep rate homogenisation according to the rule

$$\frac{d\varepsilon_{\text{eff}(\alpha+\beta)}}{dt} = \frac{d\varepsilon_{\text{eff}(\alpha)}}{dt}(1 - y) + \frac{d\varepsilon_{\text{eff}(\beta)}}{dt}y \quad (A.12)$$

where subscripts $\alpha$ and $\beta$ denote the respective phases, and $y$ the volume fraction of the $\beta$-phase calculated from Eq. (A.4).
A.4 Cladding burst criterion

Cladding failure is assumed to occur, when the cladding hoop stress exceeds the burst stress \( \sigma_B \), given by the empirical correlation [12]

\[
\sigma_B = A_b e^{-B_b T} \exp \left[ - \left( \frac{x_T}{0.00095} \right)^2 \right],
\]

where \( T \) (K) is temperature, \( x_T \) (-) is the total weight fraction of oxygen picked up in high temperature metal-water reactions, and \( A_b \) and \( B_b \) are constants. Three different sets of constants are available in FRAPTRAN-QT1.4b, and any of these can be selected by an option from the input file. The values used in the present work are given in Table A.3. The burst stress defined by Eq. (A.13) is applicable to Zircaloy cladding.

Table A.3: Constants used for Eq. (A.13) [12]. In the mixed-phase temperature region, \( T_\alpha < T < T_\beta \), \( A_b \) and \( B_b \) are calculated by linear interpolation of \( \ln A_b \) and \( B_b \) between \( T_\alpha \), \( T_\alpha\beta \) and \( T_\beta \).

<table>
<thead>
<tr>
<th>Temperature</th>
<th>( A_b )</th>
<th>( B_b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>K</td>
<td>Pa</td>
<td>K(^{-1})</td>
</tr>
<tr>
<td>( &lt; T_\alpha = 1085 )</td>
<td>8.3\times10^8</td>
<td>1.0\times10^{-3}</td>
</tr>
<tr>
<td>( T_\alpha\beta = 1166 )</td>
<td>3.0\times10^9</td>
<td>3.0\times10^{-3}</td>
</tr>
<tr>
<td>( &gt; T_\beta = 1248 )</td>
<td>2.3\times10^9</td>
<td>3.0\times10^{-3}</td>
</tr>
</tbody>
</table>

In the \((\alpha + \beta)\) domain it is assumed that a fixed temperature span exists from 1104 or 1085 to 1260 or 1248 K; see Table A.3. An alternative method to calculate \( \sigma_B \) in this domain is to use

\[
\sigma_{B(\alpha+\beta)} = (1 - y) \sigma_{B(\alpha)} + y \sigma_{B(\beta)},
\]

where \( \sigma_{B\alpha} \) and \( \sigma_{B\beta} \) are the single-phase burst stresses, as defined through Eq. (A.13) and Table A.3.

B Input to FRAPTRAN for the IFA-650.2 test

The input parameters defining the cladding models and options applied in the FRAPTRAN calculations in section 4 for the IFA-650.2 test is given in Table B.1, below. The default values are used for those options for which no values are given explicitly. The cladding model options are set in the $model$ block of the FRAPTRAN input files. Further details on the input instructions are given in Refs. [6, 24].
Table B.1: **FRA**PTRAN cladding models and options used in the calculations of the IFA-650.2 test.

<table>
<thead>
<tr>
<th>Program</th>
<th>Cladding model</th>
<th>Description of selections</th>
</tr>
</thead>
<tbody>
<tr>
<td>FRA<strong>P</strong>TRAN-1.4</td>
<td>mechan=2</td>
<td>FRACAS-I cladding model</td>
</tr>
<tr>
<td></td>
<td>mechan=1/</td>
<td>FEA cladding model</td>
</tr>
<tr>
<td></td>
<td>irupt=2</td>
<td>Strain criterion for heating rates ≤10°C/s.</td>
</tr>
<tr>
<td></td>
<td>ruptstrain</td>
<td>from NUREG-0630 [21] for cladding failure.</td>
</tr>
<tr>
<td></td>
<td>frcoef</td>
<td>Max. effective plastic+creep strain value (default=1.0).</td>
</tr>
<tr>
<td></td>
<td>irefine=2</td>
<td>Coulomb coefficient of friction in pellet/cladding interface (default=0.015).</td>
</tr>
<tr>
<td></td>
<td></td>
<td>No mesh refinement in case of ballooning.</td>
</tr>
<tr>
<td>FRA<strong>P</strong>TRAN-Q<strong>T</strong>1.4b</td>
<td>mechan=1/</td>
<td>FEA cladding model</td>
</tr>
<tr>
<td></td>
<td>icplcr=2</td>
<td>Calculate only high-temperature creep deformation in cladding.</td>
</tr>
<tr>
<td></td>
<td>iccrp=1</td>
<td>Calculate mixed-phase creep rate by interpolation between single-phase creep rates.</td>
</tr>
<tr>
<td></td>
<td>irupt=6</td>
<td>Stress criterion by Erbacher et al. [12] for cladding failure.</td>
</tr>
<tr>
<td></td>
<td>icrup=2</td>
<td>Use temperature + phase composition for calculating cladding mixed-phase burst stress.</td>
</tr>
<tr>
<td></td>
<td>plendef=0</td>
<td>No creep deformation of gas plenum walls.</td>
</tr>
<tr>
<td></td>
<td>ruptstrain=3.0</td>
<td>Maximum effective plastic+creep strain value</td>
</tr>
<tr>
<td></td>
<td>frcoef</td>
<td>Coulomb coefficient of friction in pellet/cladding interface (default=0.015).</td>
</tr>
<tr>
<td></td>
<td>irefine=2</td>
<td>No mesh refinement in case of ballooning.</td>
</tr>
</tbody>
</table>