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EVALUATION AND ADAPTATION OF THE RIA CODE
SCANAIR FOR MODELLING BWR FUEL AND CONDITIONS

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ABSTRACT

The SCANAIR code, developed by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN), is designed for modelling the behaviour of a single fuel rod in fast transient and accident conditions during a reactivity initiated accident (RIA) in pressurized water reactor (PWR). In SCANAIR, the available fuel material properties and the thermal-hydraulics (TH) model are for PWR fuel and coolant conditions, respectively, but the code does not have similar models for boiling water reactor (BWR) to be applied in BWR RIA, the rod drop accident (RDA). Thus, the code lacks material properties of Zircaloy-2 (Zry-2) which is the cladding material in BWR fuel rod. Up until now, the only Zry-2 models implemented into the code are the laws for yield stress (YS) and ultimate tensile stress (UTS) of irradiated cladding from a bibliographic study, and the laws have not been validated with SCANAIR. New YS and UTS laws are now fitted based on PROMETRA mechanical tests and implemented into SCANAIR.

1. Introduction

The main issues to be considered in order to be able to model BWR RDA with SCANAIR are firstly the Zry-2 cladding material properties and behaviour (elastic, plastic and viscoplastic models), and secondly the BWR thermal hydraulics modelling in RIA conditions.

In this paper, the needs for the adaptation of the material properties and the TH model in SCANAIR to be sufficient for BWR fuel and conditions are discussed. The ring tensile tests for fresh and irradiated Zry-2 cladding made as part of the French PROMETRA [1] programme are utilized in fitting new YS and UTS correlations in order to more accurately model the cladding plastic behaviour. After implementing these laws into the V_7_2 version of the code, comparative SCANAIR simulations are performed by applying the old and new correlations to BWR fuel tests LS-1 and FK-1 performed in the NSRR facility in Japan at room temperature and atmospheric pressure conditions. The effect of the new models on cladding strain energy density (SED) and failure propensity is investigated. In this context, the adequacies of the code’s cladding failure models regarding Zry-2 are also evaluated.

2. Zircaloy-2 material properties

As the cladding strain rates in an RIA can be around 1 s⁻¹, the cladding mechanical properties tests have to be specifically designed for reaching high strain rates. The French PROMETRA (TRAnsient MEchanical PROperties) programme is internationally the most extensive series of mechanical tests on cladding materials of PWR fuel rod under RIA loading conditions but there have not been tests on Zry-2 cladding until the recent tests utilized here. Other mechanical tests
on Zry-2 reported in open literature are GNF mechanical test on Zry-2 under RIA conditions at room temperature [2], NFD and Studsvik tests on irradiated and un-irradiated Zry-2 [3].

The integral effect test data on BWR fuel mainly comes from the NSRR facility. The test series made in NSRR on irradiated fuel consist of TS series (5 tests), FK series (11) and two LS tests, all in stagnant water. The LS-2 test was conducted in the newish high temperature, high pressure (HTHP) capsule of NSRR, and all the other tests were performed at room temperature and atmospheric pressure (RTAP). Tests on BWR fuel have also been made in SPERT facility (in USA, 10 tests during 1969-1970 on low burn-up fuel, RTAP). The rodlets tested in SPERT were of different design than the current BWR fuel rods.

Zry-2 cladding elastic behaviour, enthalpy, conductivity and thermal expansion are reported to be similar to those of Zircaloy-4 (Zry-4) [4]. Also the transition between alpha and beta phase is similar to Zry-4. There is no viscoplastic model available in open literature specifically for Zry-2 in RIA conditions but it is expected that the high temperature viscoplastic behaviour of Zry-2 is similar to Zry-4 as the differences in the heat treatment during the manufacturing process no longer play any role at high temperatures.

In contrast to the stress relieved annealing (SRA) typical for Zry-4 cladding, the heat treatment of Zry-2 is typically recrystallization annealing (RXA). This difference affects the ductility of the cladding: in RXA cladding, there are more radially oriented grains, and as the hydrides preferably precipitate along the grain boundaries, the RXA cladding has more radial hydrides [5]. It is especially the radial hydrides that make the cladding vulnerable to a pellet-cladding mechanical interaction (PCMI) induced rupture when there is a strong tensile stress in the circumferential direction.

3. Coolant modelling in BWR RDA

The thermal-hydraulics model in SCANAIR is one dimensional, single-phase model with mass and energy balance equations, and therefore the bulk boiling in BWRs cannot be taken into account. The clad-to-coolant heat exchange modelling is based on a boiling curve approach with correlations describing different boiling regimes. The model has been developed using the data from the separate effect programme PATRICIA studying the PWR conditions (280 °C inlet, 15.5 MPa, 5 m/s). In addition, the TH model has been accommodated to model stagnant water in RTAP conditions using the test results from the NSRR facility. Then again, the coefficients of the TH model have not been fitted for any other (intermediate) combination of temperature and pressure than RTAP and PWR conditions. The pressure and the temperature in BWR hot zero power (HZP) conditions (240 °C, 7 MPa) are close to the NSRR HTHP capsule (280 °C, 7 MPa) with the difference in the coolant velocity (2 m/s in BWR HZP [5]). The coefficients of the TH model may be tuned for these conditions using the test results from NSRR HTHP capsule but more instrumented tests are needed in order to do so.

On the other hand, the cold zero power (CZP; ~20-30 °C, 0.1 MPa) is considered to be the worst initial state of an RIA in BWR’s because of the highest reactivity addition and the high content of undissolved radial hydrides in the cladding [5]. The coolant conditions in RTAP capsule of NSRR resemble the coolant state at BWR CZP conditions. Still, there is some difference in the coolant flow velocity as there is flow in BWR CZP conditions (0.7 m/s [5]) whereas in NSRR capsule the coolant is stagnant. However, if the flow rate is less than 1 m/s it should not have an effect to the maximum cladding surface temperature (though it has a significant effect on the film boiling duration). Then again, the initial cladding temperature in CZP conditions in BWR RDA is reported to be closer to 80 °C than to room temperature [6]. This may require some fine adjustment to be done for the TH model parameters, but more importantly the elevated
temperature affects the ductility of the cladding: the brittle to ductile transition is possible already at temperatures close to 80 °C [6].

4. New yield stress and UTS correlations
The PROMETRA data on Zry-2 originates from 12 tensile tests on ring specimens of irradiated cladding, and from 9 tests on fresh cladding specimens. The irradiated cladding material (LK3 with inner liner) has been base-irradiated 7 cycles up to the discharge burn-up of ~58 MWd/kgu during the years 1998-2005.

The corresponding PROMETRA test matrix is presented in Tab 1. The strain rate in the tests has been 1.0 s\(^{-1}\) but one test with both fresh and irradiated specimen has been done with a strain rate of 0.001 s\(^{-1}\). Not a significant strain rate effect can be seen with the irradiated specimens.

With the fresh fuel samples, it should be noted that when including the measurement point of deviant (0.001 s\(^{-1}\)) strain rate, the best-fit curve may be significantly different compared to if this point would be excluded. Thus more measurements at the temperature range 200-300 °C are needed in order to verify the corresponding values of YS and UTS. Here the point is excluded from the fits. With the irradiated samples, the transition from furnace heating to induction heating may induce too low values with two measurements prior to the transition. The same samples also showed macroscopic deformation. These measurements are excluded from the fits.

As there are no measurement points above 800 °C for Zry-2, points from Zry-4 mechanical tests are added to the high temperature region when fitting the correlations. In SCANAIR, the values of YS and UTS are limited to stay at or above 50.0 MPa in order to ease the convergence so in practice this inclusion has no effect as regards the simulation results.

4.1 Fitting the new correlations
Different forms of correlations are tested in order to find the best fit with the measured points. First, the same formulation is tried as with the irradiated Zry-4, M5 and Zirlo claddings [1], presented in Eq. (1). This is also the correlation for Zry-2 YS and UTS already in SCANAIR:

\[
\sigma_{[\text{MPa}]} = \frac{a - b \cdot T}{1 + e^{c(T - 14)}},
\]  

(1)

The other correlations that were tested are a second-order polynomial for the fresh fuel points, and a linear fit for the irradiated case. The most suitable correlations (in terms of the higher coefficient of determination, R\(^2\)) are: Eq. (1) for the irradiated Zry-2 YS and UTS, and the polynomial fit for the fresh Zry-2 YS and UTS. However, to be consistent, Eq. (1) is used also with fresh Zry-2 as the differences in R\(^2\) values between the polynomial fit and Eq. (1) are not
significant (polynomial: $R^2=0.9642$ (UTS), $=0.9740$ (YS); Eq. (1): $R^2=0.9486$ (UTS), $=0.9681$ (YS)). With irradiated samples, linear fit is found to be almost as good as the formulation in Eq. (1). The fitted curves and the trial fits as well as the previous correlations are presented in Fig 1.

**4.2 Testing the changes by simulating NSRR tests LS-1 and FK-1 with SCANAIR**

The NSRR test LS-1 [8] (reactivity insertion 4.6 $\%$; pulse full width at half maximum 4.4 ms; targeted fuel enthalpy 126 cal/g; enthalpy at failure 53 cal/g; time of failure 240.6 ms) and FK-1 [9] (4.6 $\%$; 4.4 ms; 130 cal/g; survived) have been conducted on irradiated BWR fuel (69 and 45 MWd/kg\(\text{U}\), respectively). With the LS-1 test, according to the base-irradiation calculation with VTT-ENIGMA (amended version of v5.9b), the gap is closed prior to the transient, while with the new correlations in SCANAIR.

With both cases, there is not a significant impact on cladding outer temperatures whether one uses the old or the new correlations. If the gap is open (FK-1), the maximum mechanical SED remains unchanged. With both cases, there is not a significant impact on cladding outer temperatures whether one uses the old or the new correlations.

**Fig 2.** Cladding mechanical SED in FK-1 and LS-1 tests with the old and the new YS and UTS correlations in SCANAIR.
5. Cladding failure criteria for Zry-2 cladding

There are three different approaches in SCANAIR for predicting cladding failure: fracture mechanical model CLARIS for the PCMI type failure, strain limit based model for post burn-out ballooning failure, and a model based on calculating the strain energy density (SED) which is then compared to the critical SED (CSED) given as an input to the code. The ballooning type of failure is more relevant with fresh fuel but the problem is that there are no up-to-date tests on fresh BWR fuel in open literature for the development and validation of a ballooning type RIA failure criterion in SCANAIR.

5.1 Fracture mechanical model CLARIS

As the CLARIS model is developed for the failure predictions of PWR fuel, several additions and changes would be needed in order to apply it to BWR fuel. The J-integral database needs to be re-calculated with the CAST3M code using BWR fuel geometry (the J-integral values in CLARIS database are evaluated using three different values for the cladding thickness: 470, 520 and 570 μm, but the BWR cladding is thicker than this). The material properties of Zry-2 need to be implemented into CLARIS. The general approach in CLARIS is based on the assumption that the cladding outer brittle (hydrided) zone depth can be evaluated, but the hydride morphology is different in Zry-2 cladding than in Zry-4 (less hydrides in total, but more radial hydrides which are more detrimental). Also the fracture toughness values used in CLARIS differ between Zry-2 and -4 claddings. Because all of these factors would cause inaccuracy to the results, it is better for the moment to apply the CSED criterion for the PCMI failure predictions of BWR fuel instead of CLARIS.

5.2 Strain Energy Density

The new CSED criterion for Zry-2 by EPRI is presented in Eq. (2) [6, 7]. It is based on two open-end burst test series at room temperature [2], and thus the correlation is valid only for the PCMI phase.

\[
CSED[\text{MJ/m}^3] = 35.89 e^{0.0146[H[ppm]]} + 2.09. \tag{2}
\]

In Eq. (2), \(H\) designates the total hydrogen content absorbed into the cladding. When the hydrogen content is not known, it can be estimated from the cladding outer oxide layer thickness with a correlation. For the FK-1 and LS-1 tests, the calculated CSEDs according to Eq. (2) are 17.9 (max. hydrogen content 72 ppm [10]) and 3.3 MJ/m³ (hydrogen content 300 ppm [8]), respectively, which means that FK-1 is correctly predicted to survive the transient, and LS-1 to fail (cf. Fig 3). Eq. (2) is applicable to be used with these tests as the cladding temperatures remain near the room temperature during the early phase of the PCMI. With LS-1, the calculated enthalpy at failure is 50 cal/g and the time of failure is 240.1 ms; thus those are in good agreement with the measurements.
6. Summary and Conclusions

New yield stress and UTS correlations are fitted based on the PROMETRA mechanical tests, and implemented into SCANAIR. The failure predictions with SED are found to be very sensitive to the gap size calculated by the irradiation code. Compared to the source of uncertainty resulting from that, the new YS and UTS correlations have only a minor significance to the failure predictions.

7. References