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#### COMPUTATIONAL ASSESSMENT OF LOCA SIMULATION TESTS ON HIGH BURNUP FUEL RODS IN HALDEN AND STUDSVIK USING CYRANO3 CODE

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#### ABSTRACT

CYRANO3 is the thermal mechanical industrial code developed and used by EDF to simulate in-pile nuclear fuel rod performance under normal and transient conditions (power ramp tests) within Pressure Water Reactors (PWR) and during transport and storage periods as well. This code has already been successfully used by EDF for the last thirty years to justify normal operations and category 2 transients, covering various types of fuels: UO2, UO2 + gadolinium, MOX and various claddings as well proposed by the nuclear fuel suppliers: Zircaloy-4, Zirlo<sup>™</sup>, Optimized Zirlo<sup>™</sup>.

The CYRANO3 code was recently extended from normal and incident operating sequences to accidental scenarios. In this paper, a global overview of CYRANO3 ability to simulate thermal mechanical behavior of fuel rods under loss-of-coolant accident (LOCA) conditions is presented with a focus on recent developments carried out to assess fuel rod behavior under these conditions. CYRANO3 is demonstrated to be a powerful tool to provide reliable values of fission gas release, fuel fragmentation / relocation and cladding strains under LOCA conditions.

As part of validation of these development works, computer calculations have been used to assess two LOCA simulation experiments (for example computed fuel fragment sizes and axial relocation zones are compared to the related measures), carried out in an experimental core in Halden, Norway (IFA-650.15 test), and in Studsvik laboratory hot cells, Sweden (Counter-part test). The experiments were done on short test rodlets that had been sampled from high burnup fuel rods after unloading from commercial light water reactors. The main objectives of the work are to expand knowledge of the thermal mechanical behavior of high burnup fuel under LOCA by making interpretations of test simulations and to validate newly developed computational models for high burnup fuel fragmentation and axial relocation that have been implemented in an extended version of the CYRANO3 fuel code.

The father rod (36U-N05) chosen for the counter-part LOCA tests in Halden and Studsvik has been characterized by fuel performance modelling. The steady-state irradiation power history was input and modelling was performed. For the IFA-650.15 and the Counter-part test, key results of the experiments, such as cladding tube temperatures and power history, are reproduced with fair accuracy by means of the computer simulations.

Results demonstrate the good ability of CYRANO3 to simulate these tests. The times and conditions of failure and ballooning are in particular well predicted. Calculated clad diameters when failure is detected are in good agreement with experimental measurements. Nevertheless, the modelling of fuel fragmentation and axial relocation needs to be improved.

#### 1. Introduction

The CYRANO3 code [1] computes thermal mechanical performance of LWR fuel rods under both steady-state and transient conditions. The active stack length region of the fuel rod is represented by a series of axial zones, each of it being able to afford for different fuel pellet design or materials. In each axial zone, the fuel is divided into radial meshes of equal volume. The fuel code is based on a  $1\frac{1}{2}D$  representation.

In 2020, CYRANO3 code was enhanced to simulate nuclear fuel rod performance under LOCA transients. Material properties, constitutive laws and models (fission gas behavior, fuel fragmentation and relocation) were extended to accidental conditions. A constitutive model describing clad ballooning and phase transformation process under dynamic conditions was implemented in the CYRANO3 code. In addition, CYRANO3 was coupled to CARACAS V3.3 [2], an advanced mechanical physical-chemical model developed in the framework of a CEA-EDF-Framatome project, which enabled a fission gas release calculation and a fuel relocation modelling. CYRANO3 becomes relatively complete compared to other codes which only simulate the fuel rod behavior under normal or accidental conditions.

To confirm the validity of the advanced version of CYRANO3, the father rod (36UN05) behavior was simulated using the power history provided in [3]. Results have been compared to experimental measurements provided in the SCIP works.

Then, computer calculations have been used to assess two LOCA simulation experiments, carried out in Halden, (IFA-650.15), and Studsvik (Counter-part test). Numerical results have been compared to experimental measurements.

#### 2. Steady-state irradiation modelling

#### 2.1 Rod characteristics

The father rod chosen for LOCA tests in Halden and Studsvik was manufactured by Framatome and irradiated in the Ringhals-4 PWR for 5 cycles from September 1999 to September 2004 [3]. The rod called 36U-N05 was taken at lattice position N05 from a 17x17 assembly. Table 1 summarizes the characteristics of this rod.

Rod	36U-N05	
Reactor	Ringhals 4 (PWR)	
Number of cycles of irradiation	5	
Mechanical design	17x17	
Cladding type	M5™	
Pellet type	UO <sub>2</sub>	
Clad diameter [mm]	9.5	
Pellet diameter [mm]	8.19	
Pellet height [mm]	13.46	
Clad thickness [mm]	0.57	
Initial pellet-clad gap [mm]	0.17	
Chamfer	yes	
Pellet average grain size [µm]	10	
Total rod length [mm]	3886	
Plenum length [mm]	180.9	
Gas composition	100 % He	
He Pressure at 25°C [MPa]	2.1	
Mean rod burnup [MWd/kgU]	60.763	
Maximum rod burnup [MWd/kgU]	64.729	

Table 1 Rod characteristics [3] [4] [5]
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#### 2.2 Irradiation results

The steady-state irradiation history of the fuel rod used in Halden and SCIP III LOCA tests was obtained from [3] and [6]. The power history was then used as an input for the fuel performance code CYRANO3. The fuel performance analysis gives detailed information on the fuel thermal mechanical behavior during irradiation and provides results for the key parameters after irradiation.

Figure 1 shows the average rod power evolution during the five cycles and the burnup axial profile at the end of irradiation. The burnup profile obtained is flat between ~500 and 3000 mm, thus reflecting a homogeneity of the burnup over the rodlets positions.

Average (60.92 MWd/KgU) and maximum (64.85 MWd/KgU) burnups calculated using CYRANO3 exhibit a good agreement with the experimental measurements carried out at Studsvik [5] whatever the physical-chemical model used (CYRANO3 native model or CARACAS V3.3 model). In general, the calculated burnup profile is in very good agreement with these measurements which were evaluated from measured axial Cs-137 activity profiles.



Figure 1 Average rod power as a function of accumulated operating time (a) and calculated axial burnup profile (b)

The results of the simulation of the steady-state irradiation behavior are presented in Figure 2. The results are compared to post-irradiation measurements. The values calculated by CYRANO3 were associated with the allowed deviation<sup>1</sup> provided in [7] determined for the 3.7 version of CYRANO3. The advanced model CARACAS was calibrated and validated by EDF during steady state irradiation in 2020. Under normal conditions, the simulations of the father rod show a good capacity of CYRANO3 V3.7.3 to reproduce the measurements carried out on this rod after irradiation whatever the physical-chemical model used to simulate the behavior of the gas and of the fission products.

<sup>1</sup> The validation of a calculation code is based on the appreciation of the differences between the measurement and the "best-estimate" calculation results. This assessment of the differences between experiments and predictions must take into account a number of uncertainties related to the measurement technique or to the experiment.



Figure 2 Fission Gas Release (FGR) (a), rod inner pressure (b) and rod free volume (c) evolutions as a function of accumulated operating time

Table 2 summarizes simulations results obtained with or without coupling CYRANO3 to CARACAS V3.3.

Rod 36U-N05	C3 + CARACAS	C3	Experimental measures
Inner pressure at 25 C (MPa)	4.22	3.75	3.5 ±0.577
Total free volume (cm <sup>3</sup> )	13.96	13.77	12.85 ±2.5
FGR (%)	3.68	1.68	2.4 ±0.96
Rod elongation (%)	0.566	0.528	0.486 ±0.15
Rod elongation (mm)	22.01	20.50	18.9 ±5.829

Table 2 Steady-state irradiation modelling results

The power history modelling during steady-state irradiation was also performed as part of the SCIP III program using ALCYONE, ENIGMA and FRAPCON codes [8]. The results obtained with CYRANO3 are especially in good agreement with these calculations considering differences between available models.

#### 3. LOCA modelling

The father rod was cut into segments to carry out the LOCA tests. The length of the segments is detailed in [5]. The 725-1185 mm segment of the 36U-N05 rod was sent to Halden for the LOCA IFA-650.15 test. The 1285 -1685 mm segment of the same rod was dedicated to perform the LOCA "counterpart-test" at Studsvik.

Figure 3 shows the burnup profile [9] on the segments from the 36U-N05 rod which are selected for the manufacture of IFA 650.15 and its counterpart-test. Table 3 summarizes the

characteristics of these tests. In the LOCA modelling, some fuel characteristics (clad diameter, oxide thickness...) coming from the irradiation calculation are used as initial conditions in LOCA simulations. The rodlet inner pressure and the plenum size are updated for each LOCA calculation.



Distance from rod bottom end (mm)



LOCA Test	IFA-650.15	Counterpart-test	
Heating	External and nuclear	External	
Sample length (mm)	442.5	296	
Thermocouples	1 at 100 mm and 2 at 366 mm	1 at 198 mm	
Conditioning	Few days	Stabilization at 300°C in steam atmosphere during ≈15 min	
Plenum temperature (°C)	160-260	30-100	
Plenum volume (cm <sup>3</sup> )	17	9.6 (top) + 3.6 (bottom)	
Maximum temperature (°C)	897	895.98	
Failure temperature (°C)	800	747.98	
Maximum pressure (bar)	73	73	
Failure time (s)	245 (after blow-down)	227 (after blow-down)	
Failure pressure (bar)	56.34	70.84 (top) 68.09 (bottom)	
Maximum diameter (mm)	22.97 (predicted)	15.91 (at 0°) and 15.32 (at 90°)	

Table 3	LOCA tests	characteristics

#### 2.1 The Halden LOCA test IFA-650.15

The rod was inserted into a pressure flask in the IFA-650 test rig [10] [11] which was connected to a high pressure heavy water loop and a blow-down system. Test details are presented in [10] [12]. To simulate the IFA-650.15 LOCA test, the axial temperature profile was calculated from measured axial power profile [10] and adjusted to thermocouples measurements. The conditioning step was reproduced by numerical modelling.

The fuel rodlet was meshed in 28 axial slices and the temperature axial profile was imposed as a boundary condition, which was sufficient to comply with the axial position of the thermocouple measures. That allowed us to compare measured and calculated temperatures in Figure 4.



Figure 4 Comparison between measured and calculated temperatures

The ballooning predicted by CYRANO3 is dependent on the temperature axial profile. For the IFA-650.15 test, the predicted balloon location corresponds to the axial position at which a maximum temperature was imposed (rod center).

The failure was predicted by CYRANO3 using a strain energy density (SED) criterion [13] coupled to a thermal mechanical behavior model describing clad ballooning during LOCA conditions. The measured and predicted failure times are compared in Table 4. A difference of 40 seconds is obtained between calculated and predicted failure times.

	Experiment	C3 + CARACAS	C3
Failure time (s)	545	585	586
Elapsed time after the blow-down (s)	245	285	286
Pressure (bar)	56.35	48.39	47.68
Strain (%)	141.89 (calculated from estimated diameter)	46.85	46.4
Temperature (°C) at 100 mm	804.56 (TCC1)	852.54 (Seg 7)	853.53 (Seg 7)
Temperature (°C) at 366 mm	800.83 (TCC2) & 788.92 (TCC3)	843.72 (Seg 24)	844.71 (Seg 24)
Maximum temperature (°C) at 221.5 mm	810.56 (predicted)	864.74 (Seg 14)	865.74 (Seg 14)

Table 4 Measured Vs predicted properties at failure

The measured burst pressure is slightly higher than that predicted by the code. The measured circumferential strain of the rod was calculated from the maximum estimated diameter [12]. The calculated strain at failure is underestimated compared to the experimental estimation. Possibilities of improvements have been identified and development works expected in 2021 will enhance the code predictions.

The post-irradiation measurements [14] [15] carried out following the IFA650.15 test were compared to the CYRANO3 simulations. In particular, a comparison between the measured diameter and the calculated one is illustrated in Figure 5. It should be noted that the calculated diameter takes into account the thickness of the oxide layer.



Figure 5 Measured Vs calculated diameter – IFA-650.15 LOCA test

In the central zone of the rod, a significant difference is observed between the estimated diameter and the calculated one. However, a good agreement is obtained outside the central zone regardless of the physical-chemical model used.

Coupling CYRANO3 with the advanced model CARACAS enabled us to activate the feature of fuel relocation. In fact CARACAS V3.3 is able to predict, as a function of the pellet-clad gap, if the fuel relocation is possible at the segment level.

Following the IFA-650.15 LOCA test, the relocation of the fuel was studied by gamma scan [10] [16] [17] [12]. Figure 6 illustrates a comparison between the relocation [18] [19] [20] predicted by CYRANO3, in particular by the CARACAS V3.3 component, and the gamma scan measurements performed after the test. If the CARACAS V3.3 component predicts a possible axial fuel relocation for one axial slice, the value is different from zero. Therefore, slices values equal to one refer to axial fuel relocation (red curve). The simulated relocation is determined at the time of rupture predicted by the SED criterion.

The fuel relocation simulated by the CARACAS V3.3 component is in good agreement with the experimental measurements. Without taking into account lost fragments, the measurements carried out at Halden showed that the mass fraction of fine particles (<1mm) varies between 2.42 and 3.81% [12] depending on the weighing method used. Considering the lost fragments, the measurements indicated a mass fraction varying from 9.59 to 10.98%. At the instant of simulated rupture, the volume fraction of small fragments calculated with CYRANO3 V3.7.3 coupled with CARACAS V3.3 is 4.8%. The simulated value stands for a volume fraction while the measured values refer to a mass fraction.



Figure 6 Gamma scan measures Vs simulated fuel relocation

#### 2.2 The Studsvik LOCA counterpart-test

The counterpart-test (or 36U-N05-LOCA) performed at Studsvik aims at providing a similar test to the IFA-650.15 LOCA test. The objective is to determine the potential impact of test conditions: in-pile and out-of-pile. The two tests carried out at Halden and Studsvik were carried out by applying, as much as possible, the same test conditions (temperature and inner pressure). The heat-up sequence was employed to simulate the temperature curve typically obtained in Halden in-pile LOCA test. Experimental device and test conditions are presented in [21] [22] [23] [24].

The fuel rodlet was meshed in 18 axial slices, which was sufficient to comply with the axial position of the thermocouple measures. A comparison between measured and calculated temperatures is presented in Figure 7. The temperature was increased by 5.7 °C/s to approximately 700 °C, and then by 1.4 °C/s to 880 °C and finally by 0.2 °C/s to 900 °C, the furnace was turned off afterwards. To simulate the counterpart-test, the axial temperature profile was calculated using Studsvik's recommendation [10]. Temperature axial profile was then adjusted to thermocouple measurements.



Figure 7 Comparison between measured and calculated temperatures

The ballooning predicted by CYRANO3 is dependent on the temperature axial profile. For the counterpart-test, the predicted balloon location corresponds to the axial position at which a maximum temperature was imposed (rod center).

The measured and predicted failure times are compared in Table 5. A difference of 30.5 seconds is obtained between measured and predicted failure times.

	Experiment	C3 + CARACAS	С3
Failure time (s)	894.5	925	927
Elapsed time after the blow-down (s)	259.5	290	292
Pressure (bar)	70.84 (top) / 68.09 (bottom)	64.21	63.39
Strain (%)	67.53 (at 0°) and 61.22 (at 90°)	53.9	53.47
Temperature (°C) at 198 mm	747.98	801.59 (Seg 12)	804.10 (Seg 12)
Maximum temperature (°C) at Z=150 mm	781.18 (predicted via calculated temperature profile)	822.88 (Seg 10)	825.39 (Seg 10)

Table 5 Measured Vs predicted properties at failure

The measured burst pressure is slightly higher than that predicted by the code. The measured circumferential strain of the rod was calculated from the maximum measured diameter [23] [24]. The calculated strain at failure is underestimated compared to the experimental measurements. Also here the development works expected in 2021 will enhance the code predictions. A comparison between measured and calculated diameters is illustrated in Figure 8.



erence is observed between the estimated diameter in the central zone of the rod and

A difference is observed between the estimated diameter in the central zone of the rod and the calculated diameter regardless of the physical-chemical model used.

A comparison between the cladding permanent hoop strain along the test rodlet was calculated using several fuel codes in [4]. Results obtained in [4] are shown in Figure 9 and compared to CYRANO3 results. Most codes show a quite good agreement with the measurement in spite of an underestimated strain. Measured strains are calculated from measured diameters at 0 and 90° of the balloon.



Figure 9 Axial distribution of cladding permanent hoop strain

One of the objectives of the SCIP III program was to investigate the behavior of fuel rods under LOCA conditions, in particular fuel fine fragmentation. In general, tests carried out at Studsvik and Halden have shown a trend: fine fragmentation of fuel increases with burnup. In particular, the quantity of small fragments (<1mm) increases [21]. For the counterpart-test, the advanced model CARACAS was also activated to predict fuel relocation and fragmentation.

Figure 10 illustrates a comparison between the relocation predicted by CYRANO3, in particular by the CARACAS V3.3 component [18], and the gamma scan measurements [25] [23] performed after the test. The relocation studied in Studsvik showed that the central area is characterized by a strong relocation. In the central part of the rodlet, it seems that some of the fuel has relocated in the lower part of the balloon. At the ends of the rod, fuel seems intact. The results of the calculations are in good agreement with this observation. The calculations show a possible relocation at the same rod axial positions. In total, the mass fraction of fine fragmentation ( $\leq 1$  mm) measured at Studsvik is less than 32% [21]. With CARACAS model, about 19.6% of volume fraction was obtained for the small fragments at calculated failure time.



Figure 10 Gamma scan measures Vs simulation fuel relocation – Counterpart-test

#### 4. Summary and perspectives

The presented paper shows several applications of the CYRANO3 fuel code extension to accidental conditions. The father fuel rod 36U-N05 behavior was reproduced under steady-state irradiation using numerical calculation. The extension development works have been

validated by detailed thermal mechanical modelling of fuel LOCA-tests carried out in Halden and SCIP III programs.

This publication deals with a global overview of the CYRANO3 code performance under steady-state irradiation and focuses on recent innovative evolutions regarding fission gas and fuel relocation modelling, thanks to the model named CARACAS, developed in the framework of a CEA/EDF/Framatome co-development project, and recently implemented and validated in the CYRANO3 code.

Calculation results showed a good agreement between code predictions and experimental measures at failure time. The axial temperature profile was well reproduced by numerical calculations. This enabled a good prediction of failure positions. Calculated diameters are underestimated but future code developments will enhance code predictions. The use of the CARACAS V3.3 physical-chemical component enhanced test calculation by providing additional data on fuel relocation and fission gas release fraction during LOCA transients. Fuel fine fragmentation and relocation are well predicted for both experiments.

The CYRANO3 code coupled to CARACAS component was successfully validated under LOCA conditions. In 2021, the LOCA code database will be extended by integrating new experiments carried out in SCIP or CEA/EDF/Framatome co-development project programs.

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