MODELLING REACTIVITY-INITIATED-ACCIDENT EXPERIMENTS WITH FALCON AND SCANAIR: A COMPARISON EXERCISE

A. Romano, H. Wallin, M.A. Zimmermann

A critical assessment is made of the state-of-the-art fuel performance code FALCON in the context of selected Reactivity Initiated Accident (RIA) experiments from the CABRI REP Na series, and contrasts its predictions against those of the extensively benchmarked SCANAIR (Version 3.2) code. The thermal fields in the fuel and cladding, the clad mechanical deformation, and the Fission Gas Release (FGR) are adopted as "Figures of Merit" by which to judge code performance. Particular attention is paid to the importance of fission-gas-induced clad deformation (which is modelled in SCANAIR, but not in FALCON), relative to that driven by the fuel thermal expansion (which is modelled by both codes). The thermal fields calculated by the codes are in good agreement with each other, especially during the initial stages of the transients — the adiabatic phase. Larger discrepancies are observed at later times, and are due to the different models applied to calculate the gap conductance. FALCON predicts clad permanent deformations at the end of the transients with a maximum deviation from the experimental measurements of about 20%. Generally, the code always tends to underpredict the measurements. SCANAIR performs similarly, but grossly overpredicts the permanent clad strain for the case involving a very energetic pulse. The fission-gas-driven clad deformation is only relevant for very fast pulse energy injection cases, which are not prototypical of the RIA transients expected in PWRs. The FGR models in FALCON do not capture the mechanism of "burst-release" in the RIA transients, having been developed for steady-state irradiation conditions. This also explains why they performed poorly when applied to the fast-transient cases analyzed here. In contrast, the FGR results from SCANAIR are in satisfactory agreement with the experimental results.

1 INTRODUCTION

In order to assess the behaviour of nuclear fuel under normal or abnormal operating conditions, it is necessary to have available reliable computational instruments capable of modelling the thermal and mechanical behaviour of the fuel pins under the various irradiation conditions which occur in the reactor.

The build-up of fission gases, and their evolution and interaction with the fuel microstructures that continuously form in the fuel, the radiation damage, the presence of strong thermal and stress gradients in the fuel pin, and the oxidation and hydriding of the clad, all combine to yield complex deformation mechanisms in fuel rods, and which may result in failure of the rod well before its projected lifetime, or after low energy injection during transients [1,2]. The premature failure issue is particularly important for cases in which the rod needs to withstand fast energy pulses, typical of Reactivity-Initiated-Accidents (RIAs), or for high-burnup rods.

The ability to model the irradiation processes in the nuclear fuel, and the interaction of the fuel stack with the cladding, both under steady-state and transient conditions, can have important consequences for the safe operation of the plant. Numerical prognosis, validated against available experimental data, has been written to this purpose, and may ultimately be used to determine criteria for safe operation of the fuel.

For RIAs, it is customary to consider the limits on the maximum values for enthalpy, clad oxidation and burnup achievable during the projected accident [3]. Estimates for these limits are obtained from separate-effect and integral-test results, analyzed with the help of modelling fuel-behaviour, and used in the methodology to rationalize the conditions for clad failure.

The FALCON fuel-performance code [4] has recently been integrated into the suite of tools that constitute the computational framework of the STARS project, and aims to provide a capability to model the thermal-mechanical behaviour of fuel pins under transient conditions. We report here a benchmark analysis of the capability of FALCON MOD01 to model RIA transients, by comparing code predictions against those of SCANAIR3.2, which was developed specifically for application to fast transients. Five experimental tests from the CABRI REP-Na series [5] have been selected for this analysis: REP Na-2, REP Na-4, REP Na-5, REP Na-8 and REP Na-10. The test series includes both slow and rapid power pulses, and cases with extensive clad oxidation, spallation, and clad failure. One objective of the benchmark is the evaluation of the mechanical stress and strain state of the cladding. In particular, in FALCON, the clad deformation is dominated by the thermal expansion of the fuel, while the modules in SCANAIR focus on gas-induced fuel swelling for explaining the additional straining to the clad, especially for fast and energetic power pulses.

The paper is organized as follows: the next Section contains a brief description of the five experimental tests selected for the benchmark exercise; next, the FALCON and SCANAIR results are compared against experimental measurements, and the final section summarizes the main findings of the study.

2 EXPERIMENTAL TESTS

The five experiments used for the benchmark are listed in Table 1, and details are given of selected characteristics of the fuel pins and of the mode of transient energy injection.

Table 1: List of Properties of the RIA Tests Selected for the Benchmark.

Property	Experiment Series				
	NA2	*NA4*	*NA5*	*NA8*	*NA10*
Fuel Type	UO_2	UO_2	UO_2	UO_2	UO_2
Initial Enrichment [%]	6.85	4.5	4.5	4.5	4.5
Burnup [GWd/t]	33.0	62.3	64.3	60.0	63.5
Oxide Thickness [μm]	4	80	25	110	80
Pulse Width [ms]	9.5	64.0	9.0	75.0	31.0
Injected Energy [cal/g](+)	211.0 (882)	97.0 (405)	105.0 (439)	102.9 (430)	108.3 (453)
Spalling	No	No	No	Yes	Yes
Clad Failure	No	No	No	Yes	Yes

(+)Values in parenthesis are expressed in kJ/kg, though the cal/g unit is more traditional in RIA transient analyses.

The CABRI-REP Tests feature sodium as the primary coolant. The tests are operated at a pressure of about 0.5 MPa, and at a temperature of 280°C.
Instrumentation is installed capable of measuring on-line flow rates, pressure, coolant voiding and coolant temperatures at selected locations, as well as clad axial and radial deformations. Microphones are used to detect acoustic events signifying the time and location of the onset of clad failure [5].

The major parameters considered in the suite of CABRI–REP experiments are listed below.

Burnup
Typically, high-burnup fuel pins are considered. Hence, most fuel rods subjected to the RIA power pulses have burnups up to about 65 GWd/t (see Table 1), with extensive fuel-rim restructuring (as large as 200 μm). This burnup level is expected for standard UO_2 fuel during five cycles of operation in LWRs. However, both low and intermediate burnup cases have also been tested (the REP Na-2 and REP Na-3 cases, respectively). The present benchmark considers one low-burnup and four high-burnup cases, as indicated in Table 1.

Clad Corrosion
The suite of tests includes both a negligible clad-oxidation case (REP Na-2), a small clad-corrosion case (REP Na-5), and both medium and extensive oxidized-clad cases, with initial and transient spallation (REP Na-4, REP Na-8 and REP Na-10).

Fuel Type
The CABRI tests were designed to investigate both UO_2 and MOX fuels under RIA operating conditions. The present FALCON benchmark considers only those test cases with standard UO_2 fuel, at different enrichments (see Table 1). Future investigations will assess the performance of the FALCON code against MOX fuel cases, as and when the corresponding data become available.

Energy Deposition
Typical values of the energy deposition for the CABRI tests are around 100 cal/g. Only the REP Na-2 Test features a higher energy injection: more than 200 cal/g.

Pulse Width
Both short and broad pulse widths have been considered in the test series; specifically, 9 to 10 ms pulses in the REP Na-2 and REP Na-5 Tests, about 64 ms for REP Na-4, and 75 ms and 31 ms, respectively, for the REP Na-8 and REP Na-10 Tests.

3 RESULTS

The results of the code calculations, and their comparison with experimental measurements, are discussed in the context of the ability of the code to reproduce the thermal fields in both the fuel and the clad (Section 3.1), the clad deformations at yield, together with the fission-gas-induced effects, such as fuel swelling and release (Sections 3.2-3.4).

3.1 Thermal Fields

Figure 1 shows the evolution of the fuel centreline temperature for the REP Na-2 Test at three different axial locations. As can be seen, the codes yield comparable temperature profiles, with a relative deviation below 20%. The agreement is best (~7%) during the initial stages of the RIA, when heat conduction out of the pellet does not play an important role (i.e. corresponding approximately to adiabatic behaviour). In the present case, the SCANAIR gap conductance has been artificially increased to improve the agreement with the experiments [6]. The increase is based on the following physical arguments:

- the assumption of perfect thermal contact between fuel and clad, as a consequence of the high contact pressure, the high temperature, and zirconia-fuel bonding for high burn-up fuel; that the present fuel-clad solid contact law is semi-empirical, and based on irradiations conditions; and
- the good agreement between the calculated coolant temperatures and those measured in the REP-Na Tests.

Overall, centreline temperatures are lower than those predicted by FALCON, though the opposite has been noted in other studies [7]. This is because the gap conductance calculated by FALCON is generally larger than that of SCANAIR. The agreement between the centreline temperatures for the two codes seen for REP Na-2 Test is representative of all the other tests investigated.

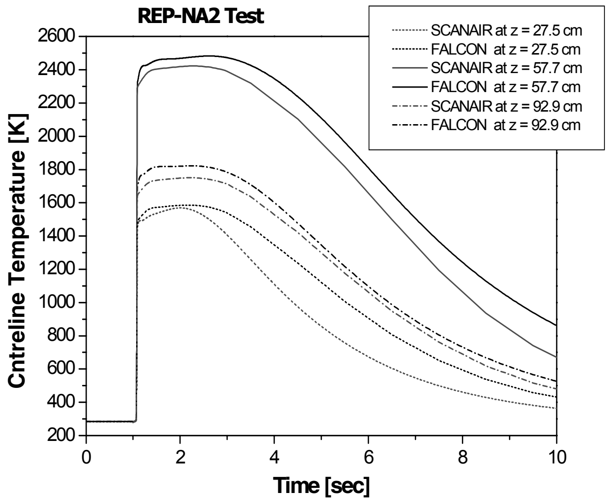

Fig. 1: Fuel centreline temperatures predicted by the codes at three axial locations for REP Na-2.

The time evolution of the fuel radial temperature profile at the peak power node for the REP Na-5 Test, as predicted by FALCON and SCANAIR, respectively, is shown in Figs. 2a and 2b. It is seen that in both cases the temperature profile is peaked towards the fuel rim during the initial adiabatic phase; the maximum temperatures calculated by SCANAIR and FALCON are ~2200^{o}C and ~2000^{o}C, respectively.

At later times, during the tail of the power pulse, the temperature profile becomes parabolic, as the heat transfer to the coolant becomes quasi-steady-state. Note that at later times in the transient the fuel temperatures predicted by FALCON are lower than those of SCANAIR, because the heat transfer through the gap is then more effective.

Note also that SCANAIR allows activation of an option that assumes perfect thermal contact between the fuel and the clad upon contact. This results in larger gap conductance than that calculated by FALCON during gap closure. However, in this comparison, this option has not been utilized.

Overall, there is good agreement between the codes, with maximum relative errors within about 20%, though the long-time relative error is higher: up to 50%.

The clad inner-surface temperatures for the REP Na-4 Test, at three different axial locations, are plotted in Fig. 3 for both the FALCON and SCANAIR calculations. It is seen that, in general, temperature trends are similar for both codes, with maxima predicted to occur about 2 s after the start of the simulation. (Note that the simulation assumes that during the first second of the transient. Subsequently, the power profile is correctly reproduced.)

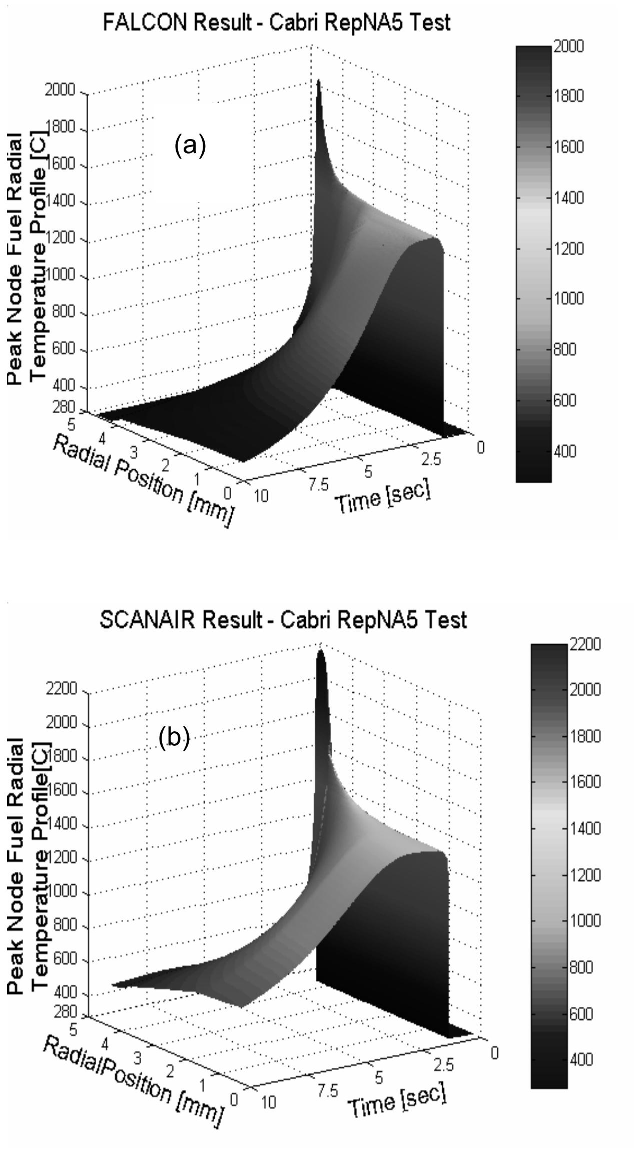

Fig. 2: Peak power node fuel radial temperature profiles for REP Na-5: (a) FALCON; and (b) SCANAIR.

Because the gap conductance calculated by FALCON is larger than that of SCANAIR for the REP Na-4 Test, the clad inner surface temperatures predicted by FALCON are lower than those of SCANAIR (the maximum relative error is about 30% for this case). In general, SCANAIR predicts more prolonged gap closures. Since the gap conductance depends on both the gap thickness and the conductivity of the gas in the gap, this explains the increase of the gap conductance compared with the FALCON results. On the other hand, the large gas release into the gap predicted by SCANAIR leads to a decrease in the conductivity of the gas mixture. FALCON calculates very low fission gas release into the gap for all the tests, except for REP Na-2 (see the discussion on fission-gas release in Section 3.4). Thus, the gap conductance in FALCON is generally higher than that of SCANAIR. Further work on the transient fission gas release model in the code is therefore indicated.

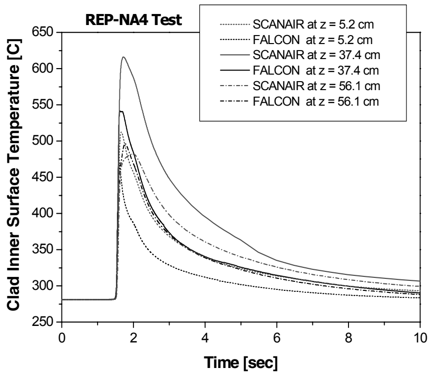

Fig. 3: Clad inner surface temperature predictions at three axial locations for REP Na-4.

3.2 Clad Mechanical Deformation

This section is devoted to analyzing the performance of the codes with respect to predicting the final deformation of the clad, specifically the clad outer diameter and elongation.

3.2.1 Clad Diameter

The maximum average clad hoop strains calculated by the two codes are compared against experimental measurements in Table 2.

Table 2: Maximum Average Clad Hoop Strains.

Test	SCANAIR	FALCON	Measurement
REP Na-2	7.20/ 4.31[+]	2.03	3.50
REP Na-4	0.56/0.46	0.43	0.40
REP Na-5	0.90/1.01	0.77	1.11
REP Na-8	1.05[++]	0.75[++]	Failure
REP Na-10	0.99[++]	0.56[++]	Failure

[+] With modified yield stress law [8]
[++] Calculated at the time of peak power

Both codes are able to reproduce the experimental results with reasonable accuracy. In fact, apart from the REP Na-2 case, clad outer diameters for the other two tests are predicted with relative errors of 7% (Na-4) and 18% (Na-5) using FALCON, and 15% (Na-4) and 9% (Na-5) using SCANAIR. The REP Na-8 and Na-10 Tests did not perform according to specifications, so that no reliable measurements are available. For the REP Na-2 Test, SCANAIR grossly overpredicts the clad diameter (105% error), while FALCON underpredicts by 42%.

The poor SCANAIR prediction for the high-energy pulse test (energy injected about 200 cal/g) can be improved if a modified correlation for the clad yield stress is adopted [8]. About 70% of the total fuel deformation is due to swelling of the intragranular bubbles. In fact, the vacancy diffusion, enhanced by the high temperatures reached during the transient, together with the over-pressurization of the bubble gas, combine to increase the bubbles sizes and thereby extenuate the fuel swelling onto the clad. The large energy injected over a relatively short time exaggerates gas swelling, leading to an overestimation for fuel yielding. Improved code predictions may be expected if the creep fuel behaviour is properly modelled, and if there is correct accounting for the filling of the dish volume [8].

FALCON generally underpredicts the final clad deformation, which may be attributed to the lack of adequate gas-induced clad straining models in the code. Nevertheless, the results indicate that the effect of the fuel thermal expansion onto the clad can account for a large fraction of the total clad deformation. Note that the effect of the gas-induced swelling (discussed later) is more important for short and highly energetic power pulses; for REP Na-4, the gas effect is negligible.

Final clad outer-diameter profiles predicted by the codes are compared with experimental measurement in Figs. 4,5 for, respectively, the REP Na-2 and REP Na-5 test cases. Note the consistent under-prediction of the REP Na-2 Test clad outer diameter by FALCON, and the large overprediction by SCANAIR.

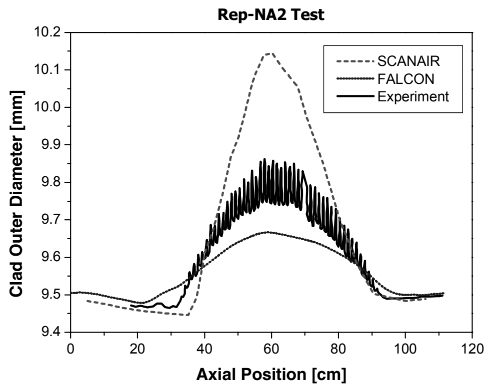

Fig. 4: Clad outer-diameter profile in REP Na-2 Test.

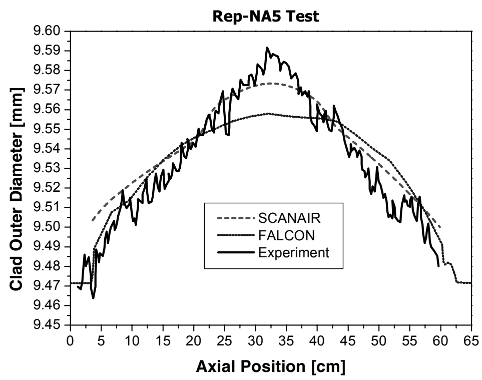

Fig. 5: Clad outer-diameter profile in REP Na-5 Test.

3.2.2 Clad Elongation

The FALCON and SCANAIR predictions of clad elongation are compared against experimental measurements for the five REP-Na cases investigated in Table 3.

Table 3: Maximum clad elongation (mm) 10 s into the transient.

Test	SCANAIR	FALCON	Measurement
REP Na-2	13.32	10.98	11.04
REP Na-4	5.00	4.44	4.08
REP Na-5	5.67	6.10	6.31
REP Na-8	1.46	2.2	~2
REP Na-10	2.8	2.8	< 2

The FALCON predictions are in excellent agreement with experimental measurement, with relative errors under 10%. Best predictions (error less than 5%) are for the narrow pulse cases, while the error is closer to 10% for the broader pulse tests. The SCANAIR predictions are also good, with maximum relative errors around 25%. And, as with FALCON, best results are obtained for the short-pulse case.

These results confirm that both codes have reliable models for axial interaction and friction between the fuel pellet and the clad, once contact between the surfaces has been established because of gap closure.

3.3 Thermal Expansion and Gas-Induced Swelling

In this Section, we discuss the relative importance of the fuel thermal expansion and the gas-induced fuel swelling, and their effect on the state of deformation of the fuel cladding. This analysis refers exclusively to the code SCANAIR, which models fuel thermal expansion and gas swelling due to both intragranular bubbles and pores. As illustration, we plot in Fig. 6 both the ratio of the total gas-induced fuel swelling and the fuel thermal expansion as functions of time for the REP Na-2 Test, for which a large clad deformation was measured (see Fig. 4).

The REP Na-2 Test is characterized by the very large contribution of the gas expansion to the fuel swelling, and, consequently, to the deformation of the clad. The gas expansion is driven primarily by the intergranular bubble expansion resulting from the vacancy diffusion mechanisms, accelerated by the high temperatures reached by the fuel in this test. Additional mechanisms leading to gas-induced fuel swelling are also modelled in SCANAIR, through the equations describing intergranular bubble swelling and fuel expansion, driven by gas-fabricated porosity. However, we have verified that the intragranular bubble expansion was the main contributor to gas-induced swelling of the fuel in the REP Na-2 Test.

It can be seen from Fig. 6 that, at the centre of the pin, where the temperature is high, the thermal expansion dominates till about 2.5 s, after which the bubble expansion produces irreversible fuel deformation. Moreover, gas-induced swelling is seen to be initially more important at the fuel periphery ($r/r_0 = 0.95$), given that the power is larger at the fuel rim during the early stages of the transient. Furthermore, while the time evolution of the fuel thermal expansion follows that of the fuel temperature, decreasing at later times due to fuel cooldown, the changes driven by gas release are irreversible (analogous to plastic deformation), and stabilize only at the time at which the pores and gas bubbles have reached equilibrium. This indicates that the gas expansion results in prolonged fuel-clad contact, extending into the cooling phase of the transient, i.e. even for large clad deformation.

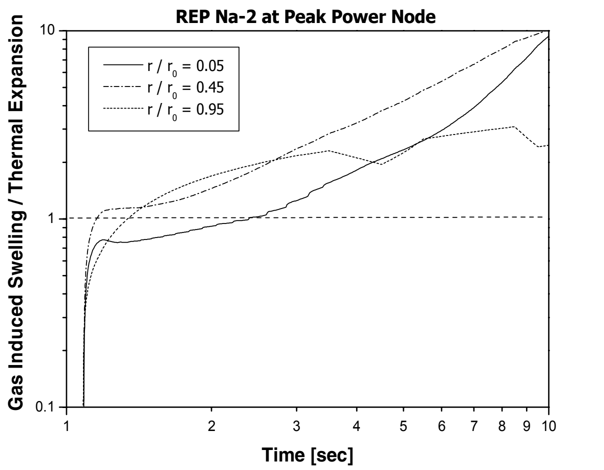

Fig. 6: Ratio of gas-induced to thermal fuel swelling at three different radial positions of the peak power node as calculated by SCANAIR for the REP Na-2 Test.

It is interesting to note that, in the rim region, at the time the steep temperature rise results in large gas over-pressurization, the gas-induced swelling occurs abruptly, in a manner which signifies the triggering of a gas-bubble instability.

A similar analysis to that described above has been conducted for the other tests in the series, from which we conclude that, the relative importance of gas-induced swelling increases with pulse energy, and decreases with pulse width. Thus, for the other tests analyzed, the effect of the gas on fuel swelling was almost always negligible, and only marginally important for the REP Na-5 Test (see Fig. 5).

3.4 Fission Gas Release

The FALCON code features physical models for fission gas release (FGR) that are validated and applicable only to steady-state irradiation conditions. Specifically, transient fission-gas release mechanisms, such as burst release after fuel fragmentation, are not included. Therefore, the code cannot predict the FGR of the three tests for which FGR measurements are available (REP Na-2, REP Na-4 and REP Na-5). In contrast, SCANAIR has transient FGR correlations. Hence, it is expected that this code can capture the amount of gas flowing from the fuel into the gap and the plena during the transient.

Table 4 gives the FGR predictions of the two codes together with the corresponding experimental measurements.

Table 4: Fission Gas Release [%] (Calculated 10 sec after Transient Onset).

Test	SCANAIR	FALCON	Measurement
REP Na-2	4.72	23	5.54
REP Na-4	15.4	1.8	8.4
REP Na-5	16.5	1.42	15.1

SCANAIR accurately reproduces the FGR for the narrow pulse cases, while largely overpredicting the measurement for the REP Na-4 case. For this test, SCANAIR predicts considerable fuel fragmentation (and a subsequently large FGR), even though the energy pulse is broad. In fact, a broader pulse is expected to be less effective in cracking the fuel grains during a fast transient, and only partial fragmentation, and hence a lower FGR, would have been expected [8].

As might have been anticipated, the FALCON FGR results differ from the experimental measurements. For example, if the Massih FGR model is selected in the code, the FGR predicted for the REP Na-2 Test is four times larger than the measured value. In contrast, there is a large underprediction for the other cases. These poor comparisons are to be expected, since the Massih model has only been validated against steady-state irradiation data, and is not applicable to fast transients. Note that the large release for the REP Na-2 Test is due to the large energy associated with the pin. Incorrect prediction of the FGR feeds back into the gap conductance calculations, affecting the final predictions of the temperature fields in the fuel.

These results indicate that FALCON requires the implementation of specific models for transient FGR able to capture the phenomenology of fast transients, such as RIAs. The amount of gas release into the open volumes affects the thermal-mechanical response of the fuel-clad system through the coupling effect of the gap. Therefore, the thermal performance of the code is also expected to change if transient FGR models were to be included.

4 CONCLUSIONS

A comparative assessment of two fuel behaviour codes, FALCON and SCANAIR3.2, has been performed in regard to their capability to reproduce the experimental results of selected RIA experiments from the CABRI REP-Na series for UO_2 fuel (REP Na-2, REP Na-4, REP Na-5, REP Na-8 and REP Na-10). The FALCON code has recently been added to the suite of computational tools used in the STARS project. Hence, the present study has been aimed primarily at evaluating the capability of the code to realistically model fast transients, in view of its planned application to the determination of fuel acceptance limits during RIA-type reactor transients. The SCANAIR code was selected as a comparison tool in the analysis. The assessment considers, as Figures of Merit, the thermal fields in the fuel and clad, and the mechanical state of deformation of the cladding. The main conclusions are listed below.

The temperature field in the fuel (such as the centre-line temperature and radial profile at the peak power node) calculated by the codes are in reasonable agreement with each other, especially during the early phases of the transients, which are almost adiabatic. However, there are large differences in the values predicted by the codes for both the gap thickness and the thermal conductance. Consequently, there are significant discrepancies in the predictions of the thermal coupling between fuel and cladding/coolant, and thus in the values of the fuel and clad temperatures at later times. Specifically, FALCON generally yields larger values than SCANAIR for the gap conductance during pellet-clad mechanical interaction (the opposite occurs if perfect thermal contact is chosen in SCANAIR). This results at late times in (a) lower fuel centreline temperatures, and (b) higher clad outer surface temperatures.

Examination of the clad deformation calculated by the codes compared with experimental measurements indicates that the final, permanent clad strains and axial elongations are reproduced with comparable accuracy. Nevertheless, for the very energetic and fast-pulse case (REP Na-2), SCANAIR grossly overpredicts the extent of the permanent clad diameter deformation at the end of the transient. The effect of gas swelling accounts for about 70% of the total fuel deformation, and is due primarily to the intragranular bubble swelling, activated by both vacancy diffusion and relaxation mechanisms, themselves due to the large over-pressurization at high temperature. Note that if a modified yield stress correlation is used for the clad, the overprediction is reduced.

FALCON is shown to generally underpredict the strain fields generated in the clad, especially at the peak power axial locations. However, for the broad-pulse cases, the codes are in good agreement with the experiments. This is explained by noting that SCANAIR models the fuel swelling induced by the over-pressurized fission gas pores, as well as by intra- and inter-granular bubbles. The gas swelling produces clad deformations in addition to those caused by the thermal expansion of the fuel. This contribution, primarily coming from intragranular bubble swelling activated by accelerated vacancy diffusion effects, has been shown to be important for the very energetic pulse REP Na-2 case, but only marginal for the REP Na-5 Test. FALCON models the fuel-clad interaction as driven solely by the fuel thermal swelling. Therefore, for the fast-pulse tests, at the axial locations where the power is greatest, the clad deformation is underpredicted. As expected, this underprediction is important only for the REP Na-2 Test, for which a large amount of energy was injected during the transient (about 200 cal/g).

For the other tests, the overall agreement between the FALCON results and the experimental measurements for the permanent hoop strain and clad outer diameter profilometry is good, suggesting that the thermal expansion of the fuel is the main driving force leading to clad deformation, especially for broad (half width ≥ 20 ms) and moderately energetic (injected energy ~ 100 cal/g) pulses.

It should also be noted that the final clad elongations predicted by FALCON are in very good agreement with the experimental measurements, indicating that the mechanisms of axial fuel-clad interactions and friction are modelled correctly by the code. The SCANAIR results are also in good agreement with the experimental measurements, though there is a slight overprediction of the final clad elongation for the REP Na-2 Test.

A comprehensive comparison of the capability of the codes to predict transient fission-gas release during the RIA Tests is not possible, since FALCON lacks the appropriate models. In contrast, SCANAIR incorporates specific burst-release models applicable exclusively to RIA transients. It is shown that SCANAIR is able to predict the gas release of the fast pulse tests (REP Na-2 and REP Na-5), and the agreement with the experimental measurements is good. However, for the REP Na-4 Test, the gas release is grossly overpredicted. This result has already been discussed [8], and is due to a partial opening of the porosity, which was observed during the REP Na-4 Test, but was not captured by the SCANAIR code version used in this benchmark.

Taken overall, the present study suggests that the FALCON code is able to model the main thermal-mechanical characteristics of fuel undergoing an RIA power pulse. The lack of specific models for transient fission-gas swelling and release is expected to affect the performance of the code in the form of (a) an underprediction of the state of clad deformation, and (b) a possible incorrect determination of the onset of fuel failure, especially for fast and energetic pulse tests. However, for typical LWR-postulated RIA events, the injected power pulse widths are expected to be about 20-30 ms in duration. Thus, for medium-energy injections, it can be assumed that the code will be able to reproduce the main thermal-mechanical behaviour of the fuel adequately. Nonetheless, further benchmarking is required to fully justify the choice of FALCON as an appropriate computational tool for assessing fuel safety limits, and for the characterization of the thermal and mechanical performance of the fuel. In this respect, the future availability of additional experimental data from the OECD CABRI-WL project, as well as from the Japanese ALPS programme, will be particularly useful.

ACKNOWLEDGEMENTS

The authors would like to thank Dr. J. Papin and Mr. F. Lamare of IRSN, France for providing input files for the SCANAIR code, as well as for their coaching in the implementation of the SCANAIR models needed for these tests. We also acknowledge the valuable insight they have contributed to the analysis of the code results.

The financial support given to this study by the Federal Office of Energy, represented by the Swiss Federal Nuclear Safety Inspectorate, is gratefully acknowledged.

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