Extending the validation database of OFFBEAT fuel performance code for LOCA scenarios

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EXTENDING THE VALIDATION DATABASE OF OFFBEAT FUEL PERFORMANCE CODE FOR LOCA SCENARIOS

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ABSTRACT

The OpenFoam Fuel BEhaviour Analysis Tool (OFFBEAT) is rapidly emerging as a comprehensive fuel performance code for multi-dimensional fuel behaviour analysis. Thanks to its advanced modelling capabilities, OFFBEAT has been selected as the fuel performance code to be further developed under the OperaHPC Project funded by the European Union. OFFBEAT was recently extended to finite-strains mechanical framework to overcome the validity limits of the small-strain approximation for large rod deformations. This enables OFFBEAT to simulate fuel rod behaviour under accidental conditions like the loss-of-coolant accident (LOCA), where large deformations become more prominent, leading to multi-dimensional macroscopic phenomena such as cladding ballooning and burst.
In this paper, the validation campaign of OFFBEAT is extended for LOCA scenarios using the REBEKA tests performed to establish data of cladding ballooning and burst under LOCA conditions. The tests were performed on single PWR-type Zircaloy-4 cladding tube samples subjected to temperature transients in steam at different internal pressures and heating rates. In order to validate the experiments, a 2D axisymmetric analysis has been carried out using OFFBEAT for internal rod pressures in the range of 1-14 MPa and a heating rate of 1 K/s. The burst temperatures obtained using OFFBEAT calculations are compared with available experimental data as well as with analyses available in open literature using the BISON fuel performance code. The expected trend of increasing burst temperature with decreasing internal overpressure is observed and is in good agreement with the experiments and the BISON results. A 3D analysis of the validation for the case with internal rod pressure of 10 MPa and heating rate of 1 K/s has also been done and the results are found to be in good agreement with the 2D case. This validation study strengthens the confidence in the capabilities of OFFBEAT in simulating multi-dimensional macroscopic fuel behaviour encountered during accidental scenarios.

1. Introduction

During normal reactor operations, the nuclear fuel experiences a variety of multi-physics, multi-dimensional phenomena, which impact the thermophysical, mechanical, and chemical properties of the fuel. The fuel undergoes even more complex phenomena in the event of an accident. Understanding fuel behaviour for macroscopic phenomena occurring in the nuclear fuel is essential for maintaining fuel rod integrity and for safe operations of nuclear reactors. Although experimental studies provide detailed analysis of fuel behaviour, they are sometimes limited by the increasing complexity, extreme environments in the nuclear systems, and by time and economic constraints. With improved computational tools and high-performance computing, multi-dimensional fuel performance codes are being developed to analyze the fuel behaviour in normal operating conditions as well as in extreme accidental conditions. In order to test the capabilities of these multi-dimensional fuel behaviour tools, verification and validation studies need to be carried out. Specially as new models developed to simulate physical phenomena are implemented in a code, it becomes imperative to carry out verification and validation studies to test the proper implementation of the numerical methodology and the results obtained.

For a Design-Basis Accident (DBA), the plant design must ensure that a coolable core configuration is maintained. One of the most important DBAs in the context of light water reactors is the Loss-Of-Coolant Accident (LOCA), in which a spectrum of break sizes of the coolant primary system can lead to consequent loss of core cooling capacity. In the event of a LOCA, coolant depressurization can take place in a few seconds, depending on the break size. This rapid depressurization along with the deteriorating heat transfer caused by the loss of coolant causes an increase in biaxial stress and temperature in the cladding. At some point the cladding begins to increase in diameter and then to deform locally. This local plastic deformation is known as cladding ballooning and can cause the cladding to burst.

In this paper, the fuel performance code OFFBEAT has been used to simulate the cladding ballooning and burst effects during a LOCA scenario in the REBEKA tests performed to establish data of cladding ballooning and burst under such conditions.

2. OFFBEAT Fuel Performance Code

The OpenFOAM Fuel BEhavior Analysis Tool (OFFBEAT) [1] is a multidimensional thermo-mechanical fuel performance code, co-developed by EPFL and PSI in Switzerland. OFFBEAT is based on OpenFOAM, an open-source C++ numerical library and uses the Finite-Volume Method (FVM) for the solution of the partial differential equations. Two important components of OFFBEAT are the thermal and the mechanical sub-solver to calculate the temperature distribution and the deformation of the fuel rod, respectively. The material properties based on open literature correlations are provided mostly from MATPRO [2]. OFFBEAT is equipped with fuel behavioral models such as relocation, densification and swelling and with cladding irradiation growth along with plasticity and creep laws to capture the non-elastic deformations of the fuel rod. The fuel-cladding gap is modelled and its characteristics such as gap volume and composition are evaluated using a gap plenum model derived from FRAPCON [3]. The fission gas behaviour is modelled using the open-source 0-D code SCIANTIX [4] which is embedded in OFFBEAT. Further details about the OFFBEAT code can be found in the works of Scolaro et al. [1][5].

The mechanical solver in OFFBEAT deals with solving the linear momentum conservation equation. The initial version of OFFBEAT [1] incorporated only a small-strain mechanics solver, which entails that one can neglect the geometric non-linearity and assume that the integration domain remains undeformed, simplifying the treatment of the governing equation. The strain tensor obtained using the small strain approximation is accurate for standard base-irradiation conditions, but it represents only an approximate metric of strain and gives inaccurate estimates when large body rotations or deformations are involved. A finite-strain approach is then needed to investigate scenarios where the fuel rod undergoes considerable deformation. This becomes imperative for accident transients like a loss-of-coolant-accident (LOCA), which are often associated with the occurrence of large deformations, leading to multi-dimensional macroscopic phenomena such as cladding ballooning and burst. In order to simulate accidental transients, the mechanical framework of OFFBEAT was extended to include the large or finite strain approach [6]. Furthermore, in order to simulate LOCA scenarios, additional models for high temperature conditions were incorporated into OFFBEAT, mostly derived from the BISON fuel performance code. These models include a dedicated cladding thermal creep model for the high-temperature regime, a Zirconium β-phase transition model, and a burst failure criterion. Further details about the implementation of finite-strain approach and the high temperature models can be found in [6].

3. Validation Study for REBEKA Tests

3.1. Experiment Description

The REBEKA (REactor typical Bundle Experiment KArlsruhe) separate effects tests [7][8] are temperature transient tests in steam performed on single PWR-size Zircaloy-4 tubes, electrically heated internally, at a variety of internal pressures and heating rates. The experiments were carried out in the REBEKA single rod test equipment of Kernforschungszentrum Karlsruhe (KfK) in the IRB institute in Karlsruhe. The purpose of the tests was to establish data on cladding ballooning and burst under typical LOCA conditions.
The cladding tubes had a heated length of 325 mm with inner and outer diameters of 9.30 and 10.75 mm, respectively. The tubes were heated from the inside by an electrically insulated heater rod. In order to replicate the fuel, a stack of Al_2O_3 annular pellets surrounding the heater was used. The internal rod pressure was varied in a range of 1 to 14 MPa for heating rates of 1 to 35 K/s. The surrounding test atmosphere was stagnant steam at atmospheric pressure and at a temperature of 473 K. A uniform temperature at the cladding circumference was maintained by heating the rod with a shroud heater tube. Thermocouples spot-welded on the outer surface of the cladding were used to measure the cladding temperatures. The information about the properties of the cladding tube and further test conditions can be found in [7][8]. The burst temperature variation with internal overpressure at different heating rates was plotted and it was noted that with the same heating rate, a higher internal overpressure results in a lower burst temperature and a higher heating rate leads to higher burst temperatures.

3.2. OFFBEAT Simulation Setup

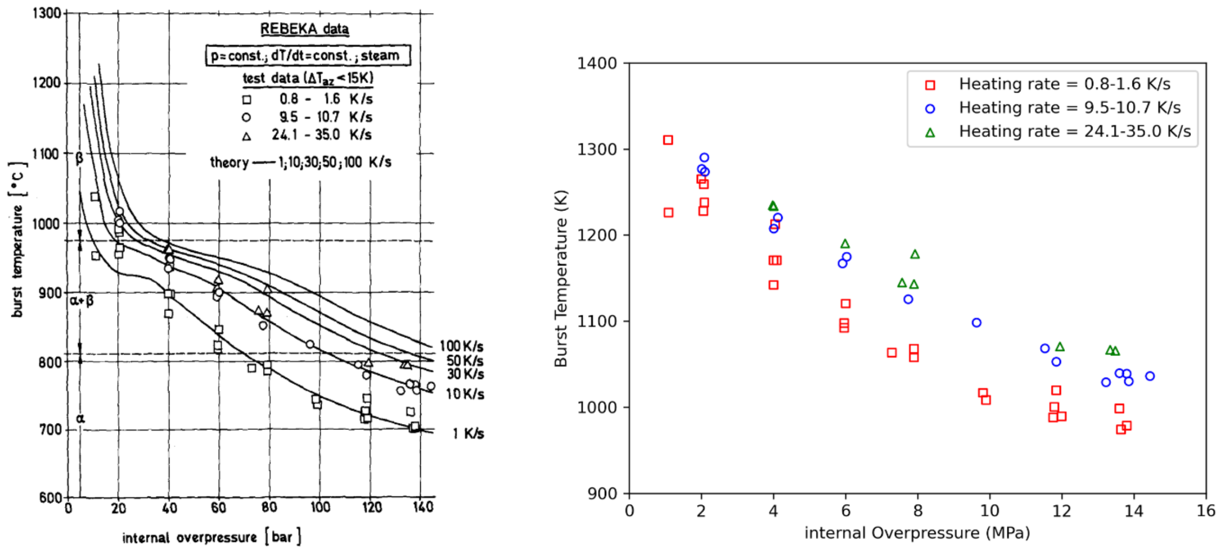
In order to carry out the validation of the REBEKA test for LOCA conditions, the OFFBEAT geometry consisted only of the cladding tube. For the 2D analyses, only the lower half of the heating rod was simulated, considering symmetric boundary conditions on the clad top surface and a zero-displacement boundary condition on the clad bottom surface. The presence of the internal heater was simulated by assuming a time-dependent temperature boundary condition on the clad inner surface with a linear axial temperature variation of 18 K from the bottom to the top of the heating rod, initially at room temperature and peaking at the tube mid-plane. Different cases with case-specific pressure values were provided as a pressure boundary condition on the clad inner surface, while the clad outer surface was provided with a fixed pressure of 1 atm and a bulk temperature of 473 K.

An incremental large strain solver with mesh update at the end of each time-step was used for the simulations. The creep model used is based on Limbäck and Anderson model [9] for the standard temperature region and the Erbacher model [7] for the high temperature region. The overstrain criterion was adopted as the failure criterion with the hoop strain limit set at 33.6% true strain, which is equivalent to 40% engineering strain.

Most of the simulation setup was consistent with a previous validation study of the REBEKA test done using BISON fuel performance code by Pastore et al. [10]. Doing so provides an opportunity for the validation case to be compared with an existing validation study by BISON and to test how close or different the results obtained from the two codes are.

4. Analysis and Results

Firstly, in order to compare the experimental data with the results obtained from OFFBEAT, the experimental data on burst temperature versus internal pressure [7] were digitized using WebPlotDigitizer [11]. The experimental data and the resulting digitized data are presented in Fig. 1 (a) and (b), respectively.



(a) **(b)**

Fig 1. (a) Experimental data from the REBEKA tests [7] and (b) the experimental data digitized for the validation study.

4.1. 2D Analysis

A 2D axisymmetric model of the cladding was created in OFFBEAT with 10 and 80 cells in the radial and axial directions, respectively. A simulation time of 1000 s was set with the simulation set to stop at as soon as the failure criterion was met. A total of 8 cases with internal pressures, P = (1, 2, 4, 6, 8, 10, 12, 14) MPa were carried out. For the present study, only one heating rate of 1 K/s was considered. Each of the 8 cases led to failure of the cladding and the respective burst temperatures and time of burst were obtained. In all the cases, failure occurred due to the overstrain criterion. Fig. 2 shows the plot for burst temperatures at different internal rod pressures obtained using OFFBEAT.

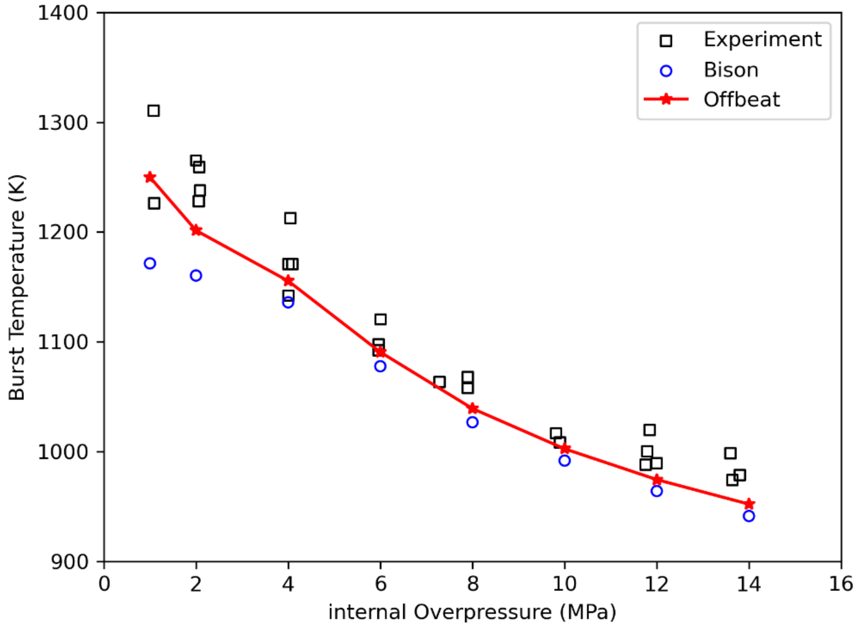


Fig 2. Comparison between OFFBEAT results against experimental data and BISON results for burst temperature vs internal rod pressure for pressure in the range of 1-14 MPa and heating rate of 1 K/s.

The expected trend of decreasing burst temperatures with increasing internal rod pressures is evident from the results. The results obtained by OFFBEAT are found to be in good agreement with the experimental data with a slight underprediction for most of the cases. The results from BISON in the study of Pastore et al. [10] are also plotted in the figure. The OFFBEAT results are in great agreement with those obtained by BISON. For the lower internal pressure values (1, 2 and 4 MPa), OFFBEAT results are in better agreement with experimental data than BISON results. According to Pastore et al. [10], the discrepancies in their results could be due to the uncertainties inherent in the cladding creep, oxidation and phase transformation models, and 3D effects which cannot be captured in the 2D representation. The difference in the OFFBEAT and BISON results could be due to the difference in the axial temperature profile provided at the cladding inner surface. The time of burst for each of these cases is presented in Fig. 3. As is evident, with higher internal rod pressures, the failure occurs earlier and thus the temperatures reached at burst are lower. The burst temperature at different pressure values as calculated from OFFBEAT and the same from BISON and experimental data is presented in Tab. 1. The time of burst, as calculated in OFFBEAT, is also presented in the table.

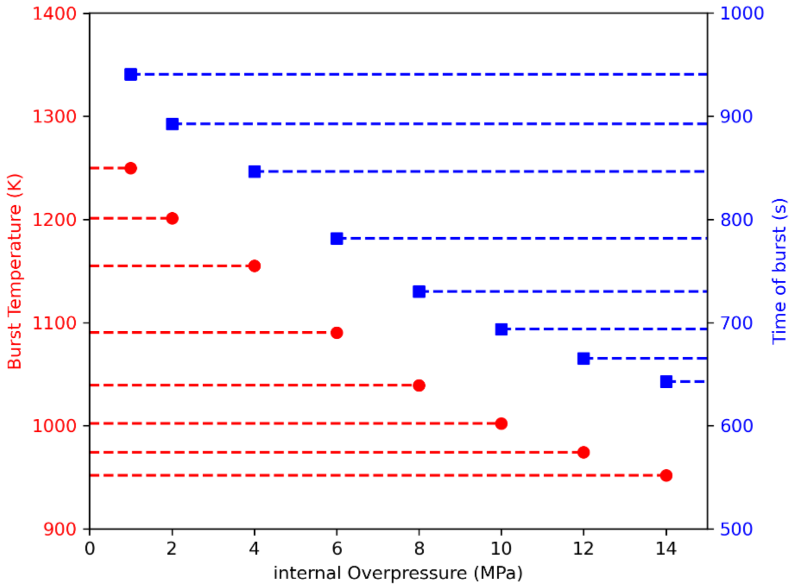


Fig 3. Time of burst at each internal pressure value from 1-14 MPa as predicted by OFFBEAT.

Pressure (MPa)	Burst Temperature (K)			Time of burst (s)
	OFFBEAT	BISON	Experiment	OFFBEAT
1	1249.9	1171.3	1310.5, 1226.2	940.9
2	1201.3	1160.2	1265.1, 1227.9, 1258.9, 1237.9	892.4
4	1155.3	1135.9	1212.4, 1170.8, 1141.9	846.4
6	1090.5	1077.6	1120.3, 1097.6, 1092.1	781.6
8	1039.1	1026.6	1067.6, 1057.7	730.2
10	1002.4	991.7	1016.6, 1008.3	693.5
12	974.4	963.9	1019.4, 999.9, 987.8, 989.5	665.5
14	952.0	941.2	998.3, 978.4, 973.9	643.1

Tab 1. Burst temperatures at different pressures for OFFBEAT, BISON and experimental data.

For the particular case with internal pressure 10 MPa, the contours for temperature and hoop creep strain at the time of burst (failure criterion reached) are shown in Fig. 4. The visualizations were created using ParaView 5.9.1 [12]. The cladding ballooning is evident at the tube mid-plane where the creep strain is maximum and where the burst occurs. The temperature at burst is found to be 1002.4 K with the hoop creep strain reaching the failure limit of 33.6% for the true strain.

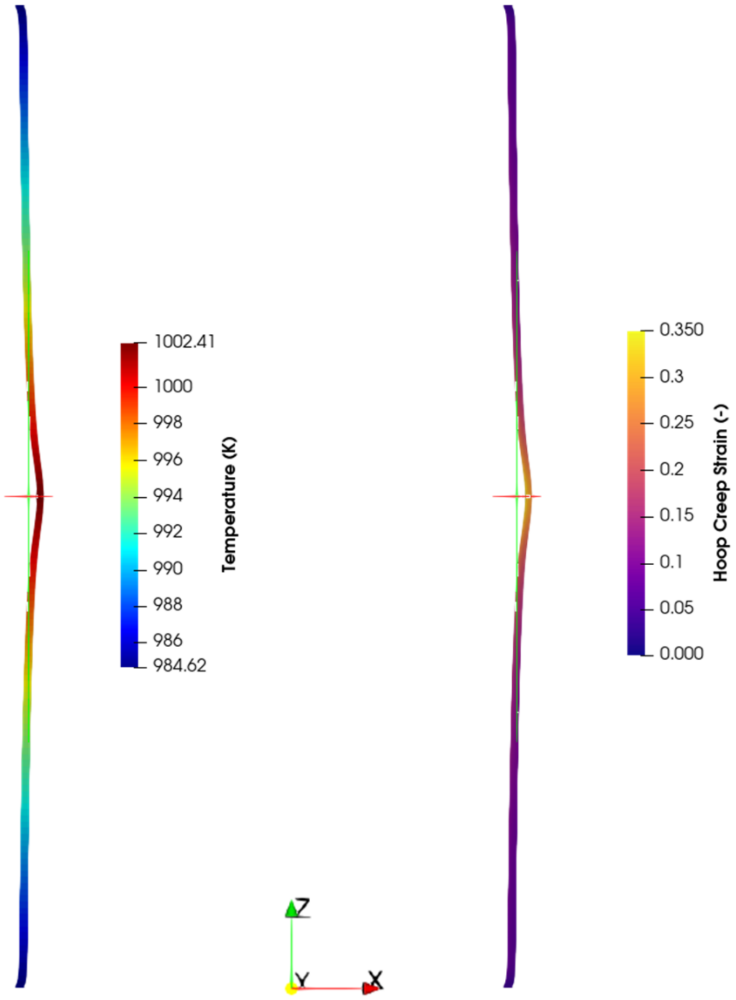


Fig 4. Contours of cladding tube burst temperature and hoop creep strain (true) for the case with P=10 MPa and heating rate=1K/s. The lower half of the tube is reflected on the z-axis to get the full view and the displacement is scaled by a factor of 4 in the radial (x-axis) direction for better visualization.

The time evolution of hoop creep strain for this case is presented in Fig. 5(a). It can be noticed that the burst (hoop creep strain = 33.6%) occurred at 693.5 s, with strain increasing from 20% to the point of burst within ~4 s (as seen from the faded region in the figure). The effect of the different creep models can be observed from Fig. 5(b), which plots the same hoop creep strain curve as a function of temperature. As mentioned earlier, OFFBEAT uses the Limbäck and Anderson creep model for temperatures T < 700 K, the Erbacher creep model for T > 900 K and an interpolation from the two in the range 700 < T < 900 K. No significant hoop creep strain is observed in the standard temperature region up to 700 K, at which point the creep model switches from the Limbäck and Andersson model to the interpolation regime. At 900 K, the Erbacher creep model is activated, and the hoop creep strain values start to increase rapidly, reaching the hoop creep strain limit of 33.6% within the next 100 s, with the temperature at burst reaching 1002.4 K.

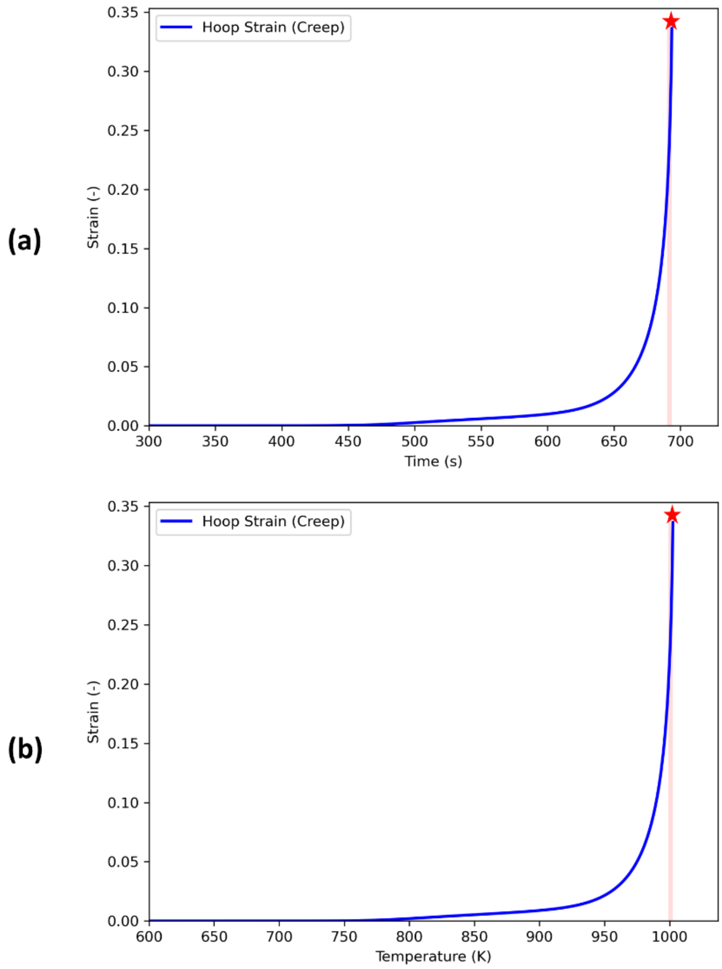


Fig 5. (a) Time evolution of hoop creep strain and (b) hoop creep strain vs temperature.

4.2. 3D Analysis

With the multi-dimensional capabilities of OFFBEAT, further 3D analysis of the cladding ballooning and burst can be done using the data from the REBEKA tests. The case with internal rod pressure of 10 MPa and heating rate of 1 K/s is considered for the 3D analysis. The geometry creation and meshing were done using Coreform Cubit v2022.11 [13]. The upper half of the cladding tube has been modelled and meshed. The meshed geometry has a total of 82'800 cells with (15 x 92 x 60) radial, axial and azimuthal cells, respectively. The same boundary conditions as in the 2D case are applied with an axial temperature profile and fixed pressure of 10 MPa on the cladding inner surface and a fixed pressure of 1 atm on the cladding outer surface, symmetric boundary conditions on the cladding bottom surface and a zero-displacement boundary condition on the cladding top surface. Considering the results from the 2D analysis, the limit for the hoop creep strain was set at 40% and the 3D simulation was allowed to run even after the failure criterion was met.

The parallelization capabilities of OpenFOAM and OFFBEAT were used and the simulation was run using 16 processors. The failure criterion was met at t = 692.8 s and the simulation crashed within the next few time steps. The total time taken for the simulation was ~2.5 hours. The contours for the temperature and the hoop creep strain at the time of burst are presented in Fig 6. In the figure, the simulated upper half of the tube is reflected on the z-axis to show the complete view. The cladding ballooning in the tube mid-plane region is clearly visible. The temperature at burst was found to be 1001.7 K. Fig. 7 shows the contours of temperature and hoop creep strain with the cladding tube sliced along the y-z plane and zoomed in near the tube mid-plane. A uniform cladding deformation with ballooning near the tube mid-plane is observed, where the highest temperature coincident with the maximum hoop creep strain is reached.

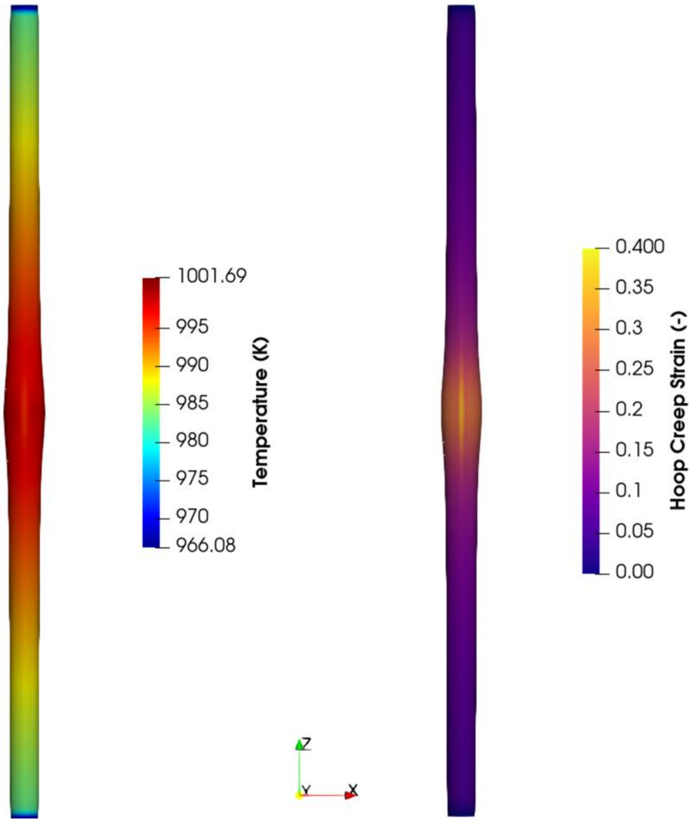


Fig 6. Contours of cladding tube burst temperature and hoop creep strain (true) for the case with P=10MPa and heating rate=1K/s. The upper half of the tube is reflected on the z-axis to get the full view.

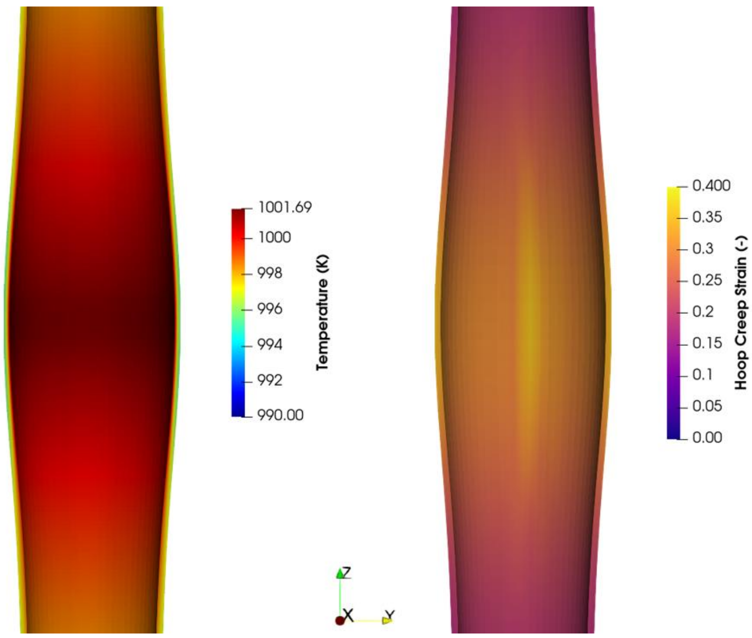


Fig 7. The contours for temperature and hoop creep strain in the inner cladding surface at the time of burst. The view has been sliced in the y-z plane to visualize the effects at the inner surface and zoomed in near the tube mid-plane.

The time and temperature evolution of the hoop creep strain (maximum) was plotted (Fig. 8) just as in the case of the 2D analysis. As can be seen from the figures, the curve shows similar trend to the 2D analysis with very low hoop creep strain values in the normal temperature region (T < 700K), and an exponential rise in the high temperature region (T > 900K), with the hoop creep strain reaching high values (up to burst) in a short span of time. As mentioned earlier, the time of burst was found to be 692.8 s and the temperature at burst was 1001.7 K. These values are in very good agreement to the 2D analysis (Tab. 2).

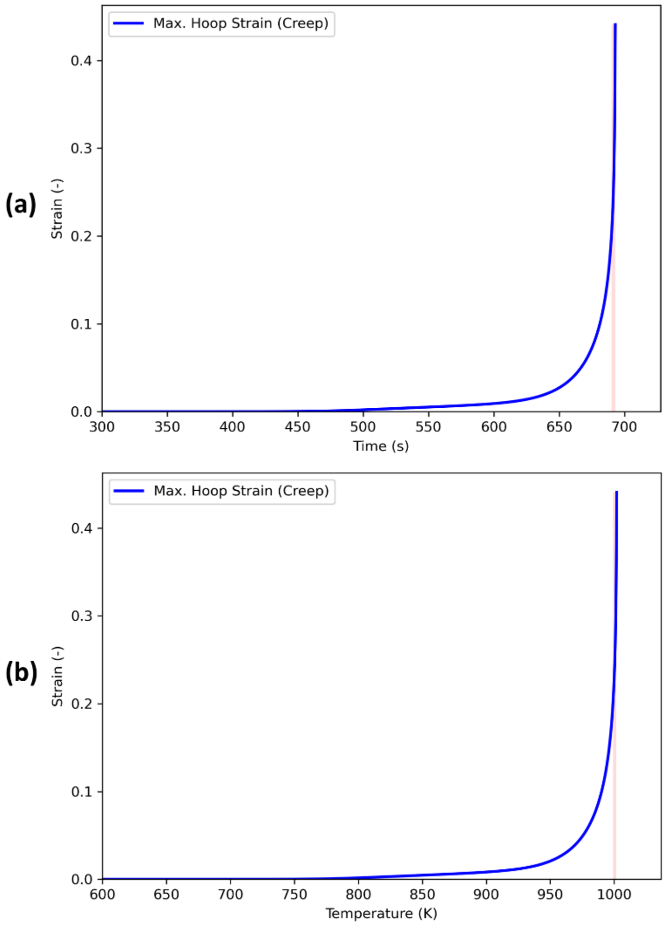


Fig 8. (a) Time evolution of hoop creep strain (b) Hoop creep strain vs Temperature for the 3D analysis.

Burst Temperature (K)		Time of burst (s)	
2D	**3D**	**2D**	**3D**
1002.4	1001.7	693.5	692.8

Tab 2. 2D vs 3D results for burst temperature and time of burst.

As in the 2D analysis, the hoop creep strain values increased from 20% to the burst limit within ~3 s with a rise in temperature of only 3 K. With the 3D results being in close agreement with the 2D results, this analysis demonstrated the multi-dimensional modelling capabilities of OFFBEAT.

5. Conclusions

The REBEKA separate-effects tests performed on single PWR-size Zircaloy-4 tubes at a variety of internal pressures and heating rates to establish data of cladding ballooning and burst with reference to LOCA conditions were simulated using OFFBEAT. Both 2D and 3D analysis were done to predict the burst temperature as a function of the rod internal pressure.

The expected trend of decreasing burst temperatures with increasing internal rod pressures was replicated in the results from OFFBEAT. The obtained results were compared with experimental data and were found to be in good agreement. The results were also compared to a similar study done using the BISON fuel performance code and the results were found to agree well, with even better results at lower values of internal rod pressures. The 3D analysis provided further details into the characteristics of cladding ballooning and burst. The obtained 3D results faired very well against the results of the 2D analysis demonstrating the multi-dimensional modelling capabilities of OFFBEAT for LOCA scenarios. With the current OFFBEAT validation for separate-effects test, further validation for integral rod tests on LOCA conditions would be pursued in the future.

6. References

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