Quantitative Assessment of Zircaloy-4 Pre-Rupture Deformation and Rupture Timing Predicted by MERCURY Using Published DIMAT Strain Histories

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1. Introduction

High-temperature ballooning and rupture of zirconium-alloy cladding are important fuel-safety phenomena because pressure-driven creep can substantially change cladding geometry before failure. MERCURY is a multidimensional finite-element fuel-performance code for transient thermomechanical analysis of fuel-rod behavior, including cladding ballooning and rupture [1]. The DIMAT experiments provide time-resolved circumferential deformation data for Zircaloy-4 tubes under controlled internal pressure and transient heating [2, 3]. A recent KNS study applied MERCURY to the nine DIMAT conditions and reported reasonable reproduction of the experimental deformation, and burst trends with limited mesh dependence [4].

The present work extends that assessment by focusing on the pre-rupture strain response. Strain histories for two selected DIMAT conditions, P40HR28 and P80HR14, were reconstructed from published figures and compared with MERCURY using rupture time, time to 5% engineering hoop strain, and strain-history root-mean-square error (RMSE). The objective is to determine whether reasonable prediction of rupture time is accompanied by agreement in the deformation leading to rupture.

2. Analysis Method

2.1 MERCURY model and boundary conditions

The supplied MERCURY benchmark inputs were used with their prescribed pressure and surface-temperature histories. Internal pressure is held at 4 MPa for P40HR28 and 8 MPa for P80HR14. Central cladding-surface temperature ramps are approximately 28.112 and 14.056 K/s, respectively, with an axial profile peaking near the specimen center. The model uses the coupled thermal-structural solver, the Zircaloy-4 creep option, and the NUREG-0630 strain-based rupture criterion [5]. The 200-mm tube has a 4.18-mm inner radius and 0.57-mm wall thickness. A 4x50 mesh was used for the reference solution and a 4x20 mesh for sensitivity checking.

2.2 Experimental data and comparison method

The original pointwise DIMAT strain dataset was not available, so the published strain histories in Ref. [3] were digitized for comparison. The reconstructed rupture temperatures were checked against independently reported burst data in the same source, giving an RMS difference of 4.7 K and an estimated strain uncertainty of approximately +/-0.003. The digitized curves are treated as approximate experimental references.

DIMAT reports engineering circumferential strain, whereas MERCURY reports logarithmic true hoop strain. MERCURY values were converted to engineering strain before comparison. The principal comparison parameters were rupture time, time to 5% hoop strain, and RMSE of engineering hoop strain over the developed-deformation region, defined here as digitized DIMAT strain >= 0.02. RMSE is reported as an absolute strain difference rather than a relative percentage error. Because the strain histories become steep near rupture, the RMSE is interpreted together with the timing metrics.

3. Results and Discussion

3.1 Numerical sensitivity

The 4x20 and 4x50 meshes predict identical rupture times for both cases. Rupture hoop-strain differences remain below 0.7% and maximum outer-radius differences below 2.3%; therefore, the 4x50 mesh is used for the quantitative comparison.

3.2 Pre-rupture deformation and rupture timing

For P40HR28, the digitized in-situ history ends at 22.13 s and MERCURY predicts rupture at 23.97 s, an 8.3% later prediction. For P80HR14, the corresponding times are 34.91 and 36.11 s, a 3.4% difference. The prescribed surface-temperature histories are interpreted as mechanical-response comparisons rather than independent thermal-validation results.

The pre-rupture trajectories also show delayed strain accumulation in MERCURY. P40HR28 reaches 5% engineering hoop strain at 21.71 s in the digitized history and 22.39 s in MERCURY, giving a delay of 0.68 s. For P80HR14, the corresponding times are 32.97 and 34.25 s, giving a delay of 1.28 s. The engineering-strain RMSE values over the developed-deformation region are 0.019

and 0.075, respectively. For P80HR14, the RMSE is 0.075 in engineering strain. The experimental strain increased rapidly near rupture making the RMSE sensitive to the timing difference between the calculated and measured trajectories; RSME is therefore interpreted as a measure of overall strain-history agreement rather than as a rupture-strain error. Overall, MERCURY reproduces the nonlinear increase in deformation approaching rupture, while significant deformation develops later than in the published DIMAT histories.

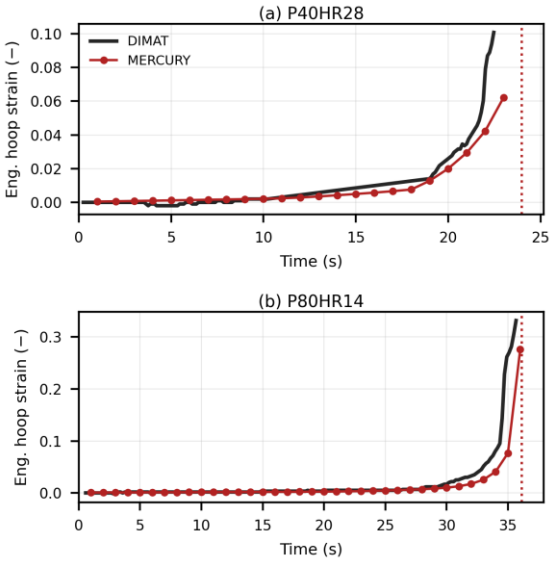


Fig. 1. Digitized DIMAT strain histories and MERCURY predictions for (a) P40HR28 and (b) P80HR14.

Table I: Comparison of DIMAT and MERCURY results

Metric	P40HR28	P80HR14
Rupture time: DIMAT / MERCURY (s)	22.13 / 23.97	34.91 / 36.11
Rupture-time difference (%)	+8.3	+3.4
5% strain time: DIMAT / MERCURY (s)	21.71 / 22.39	32.97 / 34.25
5% strain delay (s)	+0.68	+1.28
Eng.-strain RMSE (DIMAT strain >= 0.02)	0.019	0.075

Late-stage deformation in both MERCURY calculations is largely creep controlled. The 5% strain delay is larger for P80HR14 (+1.28 s) than for P40HR28 (+0.68 s), which may indicate sensitivity to the stress dependence of the Zircaloy-4 creep correlation. However, the two cases differ in both internal pressure and heating rate, so a pressure effect cannot be isolated from this comparison. Temperature-dependent treatment of creep is also a possible contributor. A dedicated sensitivity study varying pressure, heating rate, and relevant creep-model parameters independently is therefore required before attributing the timing difference to a specific mechanism.

4. Conclusions

MERCURY was assessed against published DIMAT strain histories for P40HR28 and P80HR14. The calculated rupture times were 8.3% and 3.4% later than the corresponding endpoints of the digitized experimental histories. Mesh refinement from 4x20 to 4x50 did not change rupture time and produced only small changes in rupture strain and maximum radius.

MERCURY reached 5% engineering hoop strain 0.68 s later for P40HR28 and 1.28 s later for P80HR14, showing that agreement in rupture timing does not fully describe the accuracy of the preceding deformation response. For this assessment, time to a specified engineering hoop strain and strain-history RMSE provide useful complementary model-assessment metrics alongside rupture time. Rupture time alone is therefore an insufficient acceptance metric for high-temperature cladding deformation models. It is recommended that the time to a specified engineering hoop strain and the strain-history RMSE be adopted as complementary validation criteria alongside rupture time. The larger delay in the higher-pressure case provides additional assessment criteria for subsequent creep-model sensitivity analysis. Furthermore, future research could investigate the mechanisms underlying the observed variation in prediction error with heating rate.

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