

# RECENT VALIDATIONS OF THE ELESTRES CODE

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## ABSTRACT

Comparisons of experimental measurements to predictions of the computer code ELESTRES for specific fuel characteristics have been performed at Atomic Energy of Canada Limited. ELESTRES is a fuel performance code which predicts the behaviour of a CANDU fuel element under normal operating conditions. A database, which contains 133 irradiation histories with bundle powers and burnups as high as 124 kW/m and 470 MWh/kgU respectively, has been established to validate the ELESTRES code. This database provides the ability to compare experimentally measured fuel characteristics to ELESTRES predicted results. ELESTRES demonstrates a strong agreement for all the fuel characteristics examined: fission gas release percentage and volume, ridge strain, mid-plane strain, fission gas pressure, and centre-line temperature. Additional validations from past comparisons are also included for completeness; these validations to show the same trends. These validations demonstrate that the ELESTRES code is a quick and reliable tool for predicting CANDU fuel behaviour under normal operating conditions.

## 1. INTRODUCTION

### 1.1 Need

A nuclear fuel element consists of a cylindrical tube, called the sheath, containing sintered uranium dioxide pellets. The sheath provides a barrier against the release of radioactive gases to the surrounding coolant, thus, the integrity of this sheath is a very important factor in the design of these fuel elements. As pellets heat up in the reactor, their expansion can potentially push the sheath radially outwards. The resulting stresses can combine with chemical and metallurgical effects and contribute to potential failures during normal operating conditions.

The computer code ELESTRES\* models [1] the thermal and mechanical behaviour of an individual fuel element during the element's irradiation life under normal operating conditions. As the code evolves through improvements in the numerical methods and additional features are added, a testing method is necessary to help determine the effect these changes have on the code.

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\* ELESTRES: ELEment Simulation and sTRESses

Using a computer code COMPARE, a database which contains 133 irradiations has been established to validate the ELESTRES code. The database provides the ability to compare experimentally measured fuel characteristics to ELESTRES predicted results.

## 1.2 Definitions of Terms

Figure 1 shows the geometry of a CANDU fuel bundle, and Figure 2 shows a fuel element. Each figure illustrates the relevant terms. The bundle contains 20-40 fuel elements with each element having one sheath made of Zircaloy-4. Each sheath contains 20-40 pellets of uranium dioxide which generate heat in the reactor. R. Page [2] describes the fuel in more detail.

## 2. COMPUTER CODES

### 2.1 ELESTRES

The ELESTRES code [3] models the behavior of CANDU fuel elements under normal operating conditions. The focus of the code is on calculations of temperatures, pellet displacement and hourglassing, and fission gas release. The code models a single element by accounting for the radial and axial variations in stresses and displacements. The constituent models are physically (rather than empirically) based and include such phenomena as pellet-to-sheath heat transfer, temperature and porosity dependence of pellet thermal conductivity, burnup dependent neutron flux depression, burnup and microstructure dependent fission product gas release, and stress, dose and temperature dependent constitutive equations for the sheath. The interactions and feedbacks among these parameters are considered in a dynamic manner throughout the irradiation history.

The finite element model for the pellet deformation includes thermal, elastic, plastic, and creep strains. This model also includes fission gas swelling, densification, pellet cracking, and rapid drop of  $UO_2$  yield strength with temperature. The plasticity and creep calculations are based on the incremental theory of plastic flow, and employ the Von Mises yield surface in conjunction with the Prandtl-Reuss flow rule. The numeric implementations of plasticity and creep use the variable stiffness method along with a modified Runge-Kutta integration scheme for rapid convergence and accuracy.

The latest version of ELESTRES, M13A Cycle 4, was used for the validations.

### 2.2 COMPARE

The COMPARE code contains several plotting routines which allows for quick and easy comparison of experimentally measured values to the ELESTRES code predicted values. The COMPARE code generates plots containing several cases with predicted values plotted against measured values for the following fuel characteristics:

1. fission gas release (percentage and volume),
2. sheath ridge strain, and
3. sheath pellet mid-plane strain.

For these plots, the code calculates the following statistical values using their respective formulas.

$$\text{mean deviation} = \frac{1}{n} \sum_{i=1}^n |x_i - \bar{x}|$$

$$\text{standard deviation} = \sqrt{\frac{\sum_{i=1}^n x_i - n\bar{x}^2}{n-1}}$$

$$\text{correlation coefficient} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{[\sum (x_i - \bar{x})^2][\sum (y_i - \bar{y})^2]}}$$

$$\text{average difference} = \frac{1}{n} \sum_{i=1}^n x_i - \bar{x}$$

These statistical techniques provide a numerical description of the agreement between the predicted and measured values.

The code also generates several specialty plots which contain detailed predicted versus measured comparisons. Each specialty plot pertains to only one irradiation test case.

### 3. DATABASE

#### 3.1 Gas Release, Ridge Strain, and Mid-plane Strain

The first part of the database focuses on comparing the experimentally measured values against the ELESTRES predicted values for fission gas release (% and ml), sheath strain at the pellet ridge and mid-plane strain. The experimental data from the irradiations applied to a combination of these four fuel characteristics, 98 cases, 89 cases, 12 cases, and 14 cases respectively. Table 1 contains the key statistics of the data in the database.

The following data was instrumental in establishing the experimental data and the ELESTRES input files [3 and 4]:

- 1.) fission gas release data compiled by A. Ranger, L. Alvarez and J. Walsworth, and
- 2.) strain measurement data compiled by H. Wong and M-Z. Pindera.

The cases dealt with the end-of-life conditions, on-power strain measurements, and on-power measurements. Each validation plot contains dashed lines which represent the experimental error in the measurements.

#### 3.2 Specialty Validations

This part of the database contains cases which compare the experimentally measured fuel characteristics to the ELESTRES predicted values over each case's entire irradiation history. The following data helped establish the three specialty plots used for comparison [4]:

- 1.) ridge strain against linear power from Case 1: Experiment X-264 [5],
- 2.) gas pressure against element burnup from Case 2: Experiment X-9-107 Element ARZ [6], and
- 3.) centre-line temperature against element burnup from Experiment FIO-136 [7].

One plot was generated for each case which compares the experimental data to the predicted results.

The ELESTRES predicted values from source number three required slight adjustments to account for the unusually high enrichment used in this test. The experimental case involved an element fuel enrichment of 10% which exceeds 6%; the maximum enrichment ELESTRES can model. The predicted centre-line temperature for an enrichment of 10% was extrapolated from the centre-line temperature for the same case using enrichments from 0.71% to 6%. Figure 3 demonstrates how this extrapolation was performed.

## 4. VALIDATION RESULTS

### 4.1 Temperature

The centre-line temperature against burnup comparison, Figure 4, shows excellent agreement between the measured and predicted values at lower temperatures ( $\pm 2\%$ ). As the temperature begins to rise above 1900°C, ELESTRES under predicts this temperature slightly ( $\pm 5\%$ ). These discrepancies result from several factors. First, the power history which was used in ELESTRES is an average over the three-element bundle. During the post-irradiation examination, two of the elements had failed and the ELESTRES code does not model defected sheaths. Also, a central hole was not modelled.

### 4.2 Gas Pressure

The speciality plot, gas pressure against burnup, indicates a strong agreement between the measured and predicted values. This agreement is seen in Figure 5.

### 4.3 Gas Release

The gas release validation plots show a strong agreement between the measured and predicted values from ELESTRES. For percentage gas release (%), the mean deviation and average difference between the measured and predicted values is 4.5% and 1.7% respectively, 68% of the calculations are within 8% of the measurements. For volumetric gas release (ml), the mean deviation and average difference between the measured and predicted values is 8.1 ml and 5.1 ml respectively, and 68% of the calculations are within 18 ml of the measurements. Figures 6 to 9 demonstrate this agreement.

### 4.4 Ridge Strain

The speciality plot from the X-264 Experiment, Figure 10, demonstrates reasonable agreement between the predicted and measured results. The predicted results clearly demonstrate the major trends of the measured values.

Another comparison was previously performed [8] where the predictions of ELESTRES were compared against in-reactor measurements of ridge strains [9] from IRDMR element ACH. Figure 11 shows that the predictions are in good agreement with the measurements. Figure 12 also shows the ELESTRES predicted results demonstrating good agreement with the IRDMR measurements for another IRDMR irradiation, ACA. Figure 13 also shows the ELESTRES predicted results [8] compared to the measured data for a third IRDMR element, ABS.

A previous comparison was performed [10] which involved experiments covering various combinations of pellet lengths, diameters, central holes, chamfers and dishes. The experiments and the predictions show similar trends for ridge strain, as seen in Figures 14 to 16. The predicted strains are generally within the scatter of experimental data.

From the 1992 comparison for ridge strain (%), the mean deviation and average difference between the predicted and measured values is 0.6% and 0.2% respectively, and 68% of the calculations are within 1.1% of the measurements. Figures 17 demonstrates this agreement.

#### 4.5 Mid-plane Strain

Again, the previous comparison [10] which involved experiments covering various combinations of pellet lengths, diameters, central holes, chamfers and dishes also demonstrates excellent agreement between the experimental results and the predictions for mid-plane strain, as seen in Figures 16, 18 and 19. The predicted strains are generally within the scatter of experimental data.

From the 1992 comparison for mid-plane strain (%), the mean deviation and average difference between the predicted and measured values is 0.5% and 0.1% respectively, and 68% of the calculations are within 0.9% of the measurements. Figures 20 demonstrates this agreement.

#### 4.6 All End-of-Life Strains

All the comparisons (1989 and 1992) between the predicted and measured data for strains at the end-of-life, ridge and mid-plane, were combined. These results consisted 48 points and demonstrate a reasonable agreement between the measurements and predictions, and are shown in Figure 21.

#### 4.7 Element Length

A 1988 comparison of ELESTRES predictions against measurements of element lengths in experiment DME-187 involved the irradiation of 18 fuel elements containing short flat-ended pellets (length to diameter ratio of 0.5). The measured length changes due to the power ramp were between 0.17 and 0.27%. The calculated length changes were between 0.08 to 0.33%. Figure 22 illustrates this comparison.

### 5. EXPANSION

This database can easily be expanded by adding new cases to the database files. The data from these cases can pertain to any one of the comparisons. As well, only 5 out of a possible 20 specialty plots have been utilized, these five plots are:

1. linear power against burnup,
2. power against time,
3. gas pressure against burnup,
4. ridge strain against burnup, and
5. centre-line temperature against burnup.

Adding more specialty validation plots is quite simple.

The database can be easily updated as corrections or better information is provided on the existing cases. This database is by no means a permanent point of reference, but the database, like the ELESTRES code, should evolve to provide a continually improving validation standard.

## 6. CONCLUSIONS

Overall, the ELESTRES code demonstrates good agreement between its predicted values and the experimentally measured data. The following list summarizes the conclusions for each fuel characteristic based on the 1992 comparisons using the M13A.4 version of ELESTRES.

- Fission Gas Release (%):
  - mean deviation of 4.5%
  - standard deviation of 4.0%
  - average difference of 1.7%
- Fission Gas Release (ml):
  - mean deviation of 8.1 ml
  - standard deviation of 9.2 ml
  - average difference of 5.1 ml
- Ridge Strain (%):
  - mean deviation of 0.6%
  - standard deviation of 0.6%
  - average difference of 0.2%
- Mid-plane Strain (%):
  - mean deviation of 0.5%
  - standard deviation of 0.5%
  - average difference of 0.1%
- Temperature:
  - consistent with measurements
  - to  $\pm 2\%$  in the lower burnup range
  - to  $\pm 5\%$  in the higher burnup range
- Internal Pressure (MPa):
  - strong agreement with measured data
  - to  $\pm 0.1$  MPa in power ramps
  - to  $\pm 0.01$  MPa in constant power ranges
- Element Length (%):
  - strong agreement with measured data

Based on these results and the previous comparisons, the code appears consistent with the experimental data.

## 7. ACKNOWLEDGEMENTS

The authors would like to sincerely thank R. Sejnoha and M. Gacesa for their useful suggestions and discussions during this project. Thanks are also in order for the CANDU Owners Group (COG) for funding this endeavor. The many individuals which contributed to establishing the database are gratefully acknowledged including R. DaSilva and his work in the IRDMR experiments.

## 8. REFERENCES

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1982, pp. 203-212.

- (2) R.D. PAGE, "Canadian Power Reactor Fuel", Atomic Energy of Canada Limited, report AECL-5609, 1976.
- (3) M. TAYAL, "Modelling CANDU Fuel Under Normal Operating Conditions: ELESTRES Code Description", Atomic Energy of Canada Limited, report AECL-9331, 1987.
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TABLE 1: KEY STATISTICS FROM DATABASE

Parameter	Number of Irradiations	Minimum Value	Maximum Value
Power (kW/m)	133	0.1	124.0
Final Burnup (MWh/kgU)	133	0.07	467.7
Gas Release (%)	98	0.01	36.30
Gas Release (ml)	89	0.01	103.60
Ridge Strain (%)	12	0.33	5.02
Mid-plane Strain (%)	14	0.11	3.77
Internal Pressure (MPa)	1	0.145	1.014
Temperature (°C)	1	299.7	2100.1
Total Number of Irradiations in Database	133		

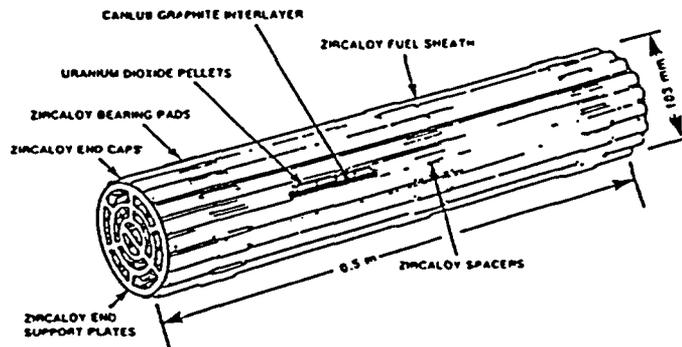


FIGURE 1: FUEL BUNDLE

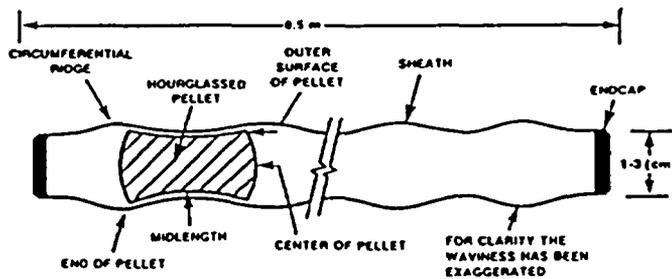


FIGURE 2: FUEL ELEMENT

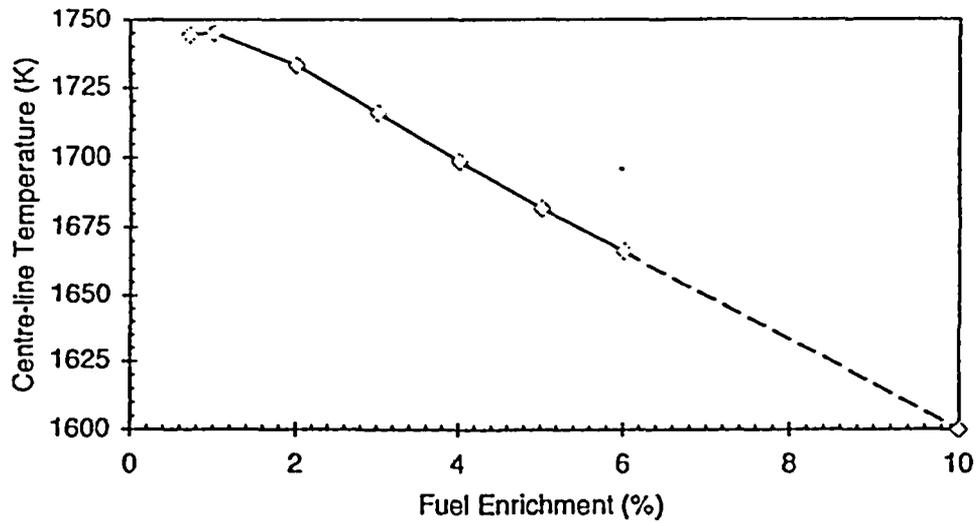


FIGURE 3: CENTRE-LINE TEMPERATURE VS. FUEL ENRICHMENT

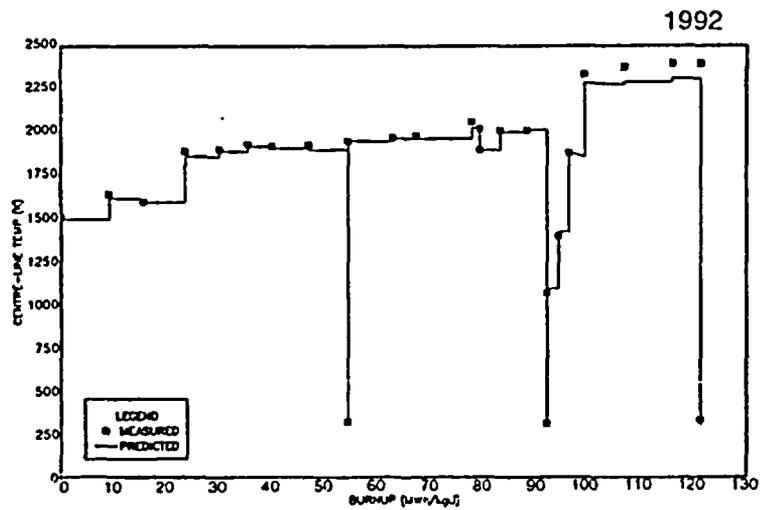


FIGURE 4: CENTRE-LINE TEMPERATURE FOR EXPERIMENT FIO-136

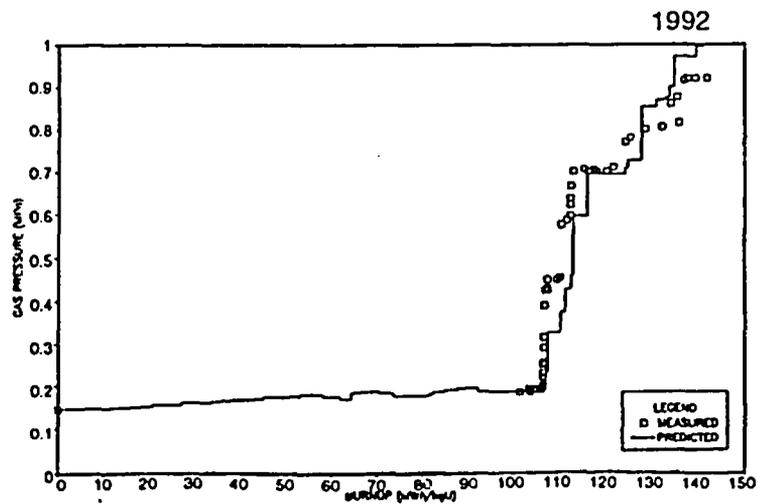


FIGURE 5: INTERNAL GAS PRESSURE FOR CASE 2: EXPERIMENT X-9-107

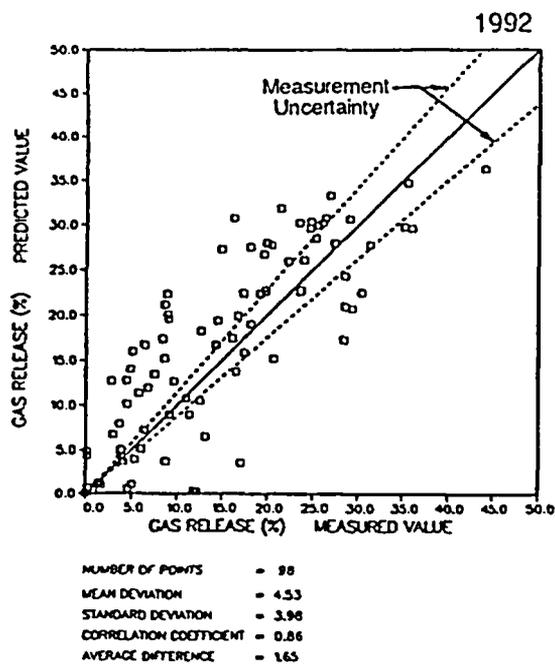


FIGURE 6: FISSION GAS RELEASE (%) AT END-OF-LIFE (LINEAR PLOT)

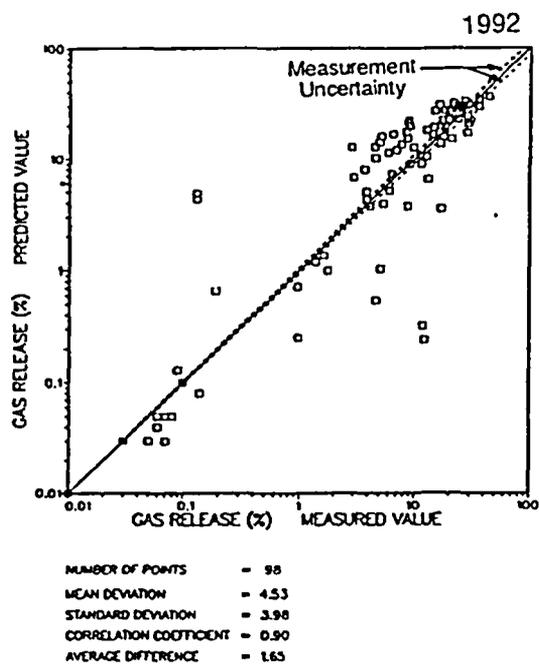


FIGURE 7: FISSION GAS RELEASE (%) AT END-OF-LIFE (LOGARITHMIC PLOT)

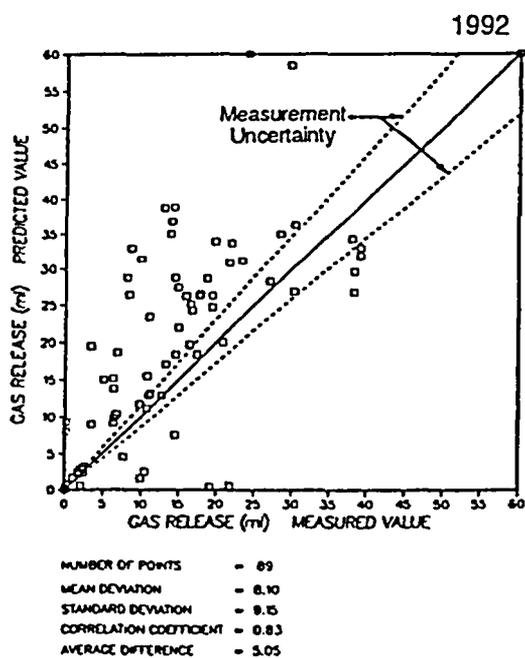


FIGURE 8: FISSION GAS RELEASE (ml) AT END-OF-LIFE AT 20°C / ATM. PRESSURE (LINEAR PLOT)

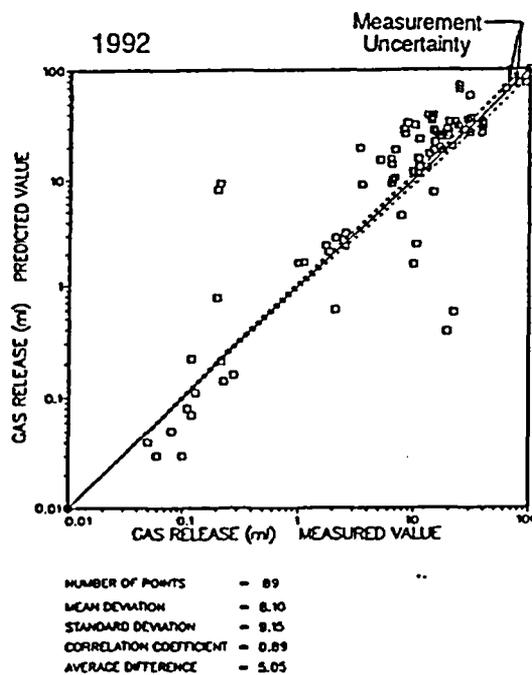


FIGURE 9: FISSION GAS RELEASE (ml) AT END-OF-LIFE AT 20°C / ATM. PRESSURE (LOGARITHMIC PLOT)

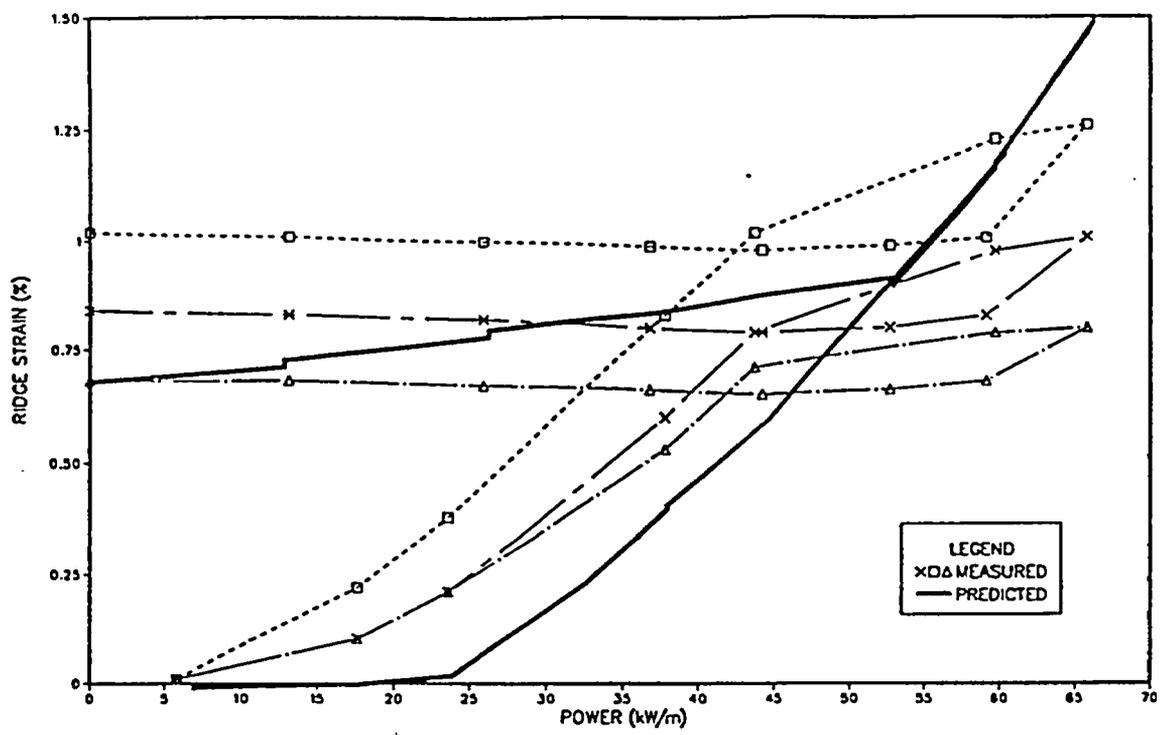


FIGURE 10: RIDGE STRAIN FOR CASE 1: X-264 EXPERIMENT

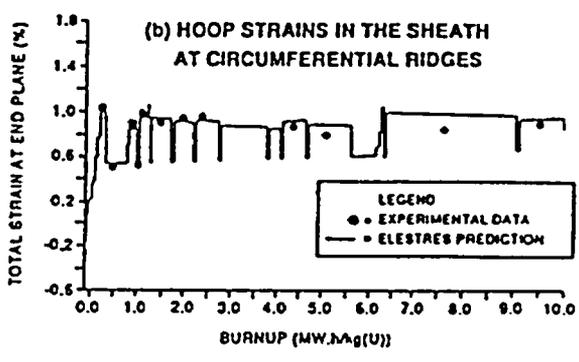


FIGURE 11: COMPARISON OF HOOP STRAINS IRDMR ELEMENT ACH

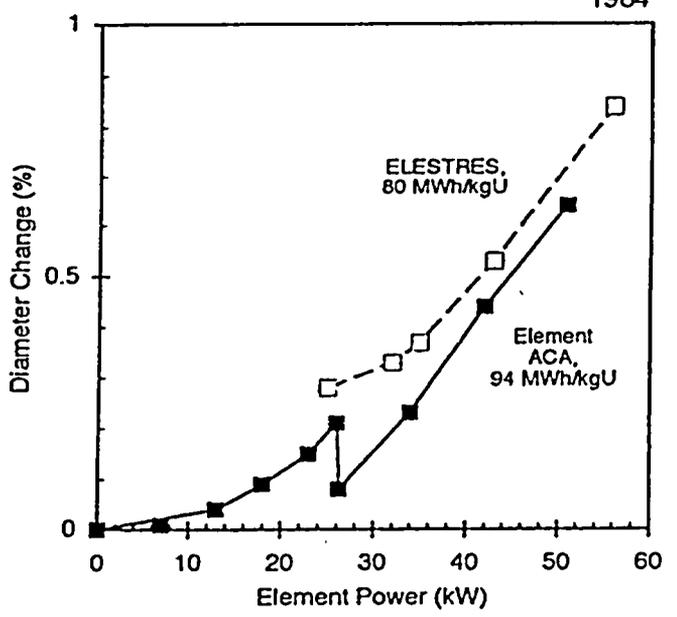


FIGURE 12: IRDMR MEASUREMENTS COMPARED TO ELESTRES CALCULATIONS FOR SHEATH STRAINS AT CIRC. RIDGES

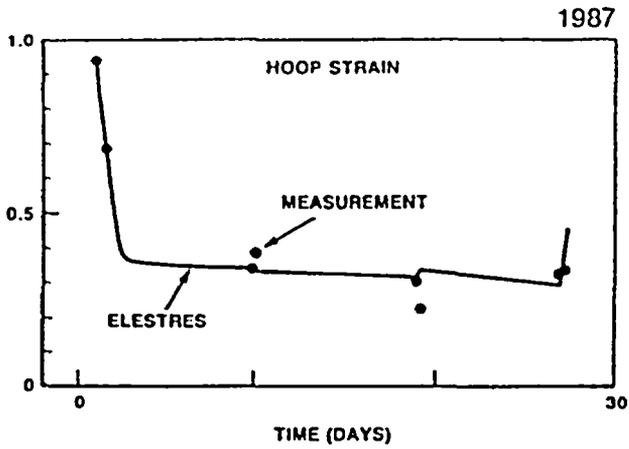


FIGURE 13: HOOP STRAIN AT THE RIDGE IRDMR ELEMENT ABS MEASUREMENT VS. ELESTRES

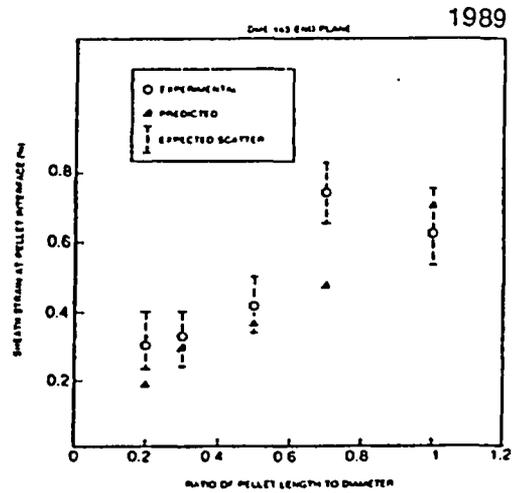


FIGURE 14: COMPARISON OF PREDICTED SHEATH STRAINS WITH MEASUREMENTS AT PELLET END PLANE

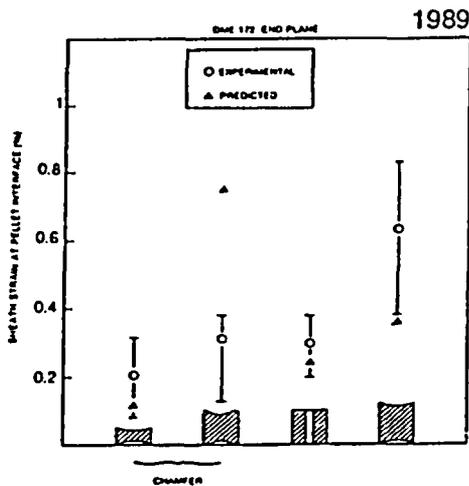


FIGURE 15: COMPARISON OF PREDICTED SHEATH STRAINS WITH MEASUREMENTS AT PELLET END PLANE

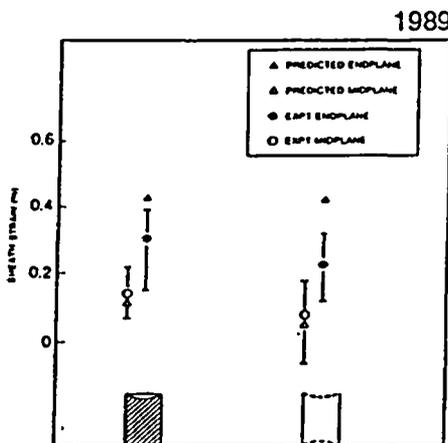


FIGURE 16: COMPARISON OF SHEATH STRAINS

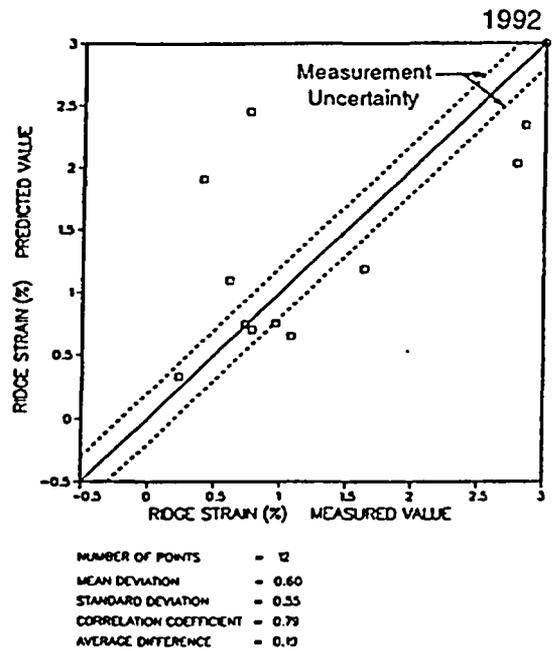


FIGURE 17: TOTAL RIDGE STRAIN (%) AT END-OF-LIFE

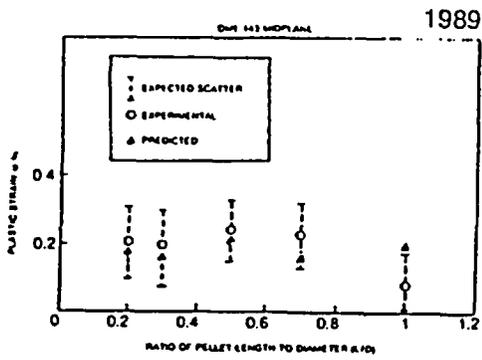


FIGURE 18: COMPARISON OF MID-PLANE SHEATH STRAINS

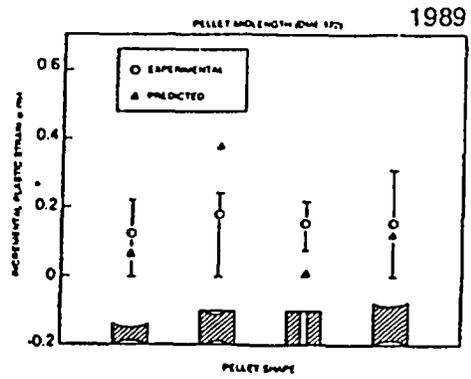
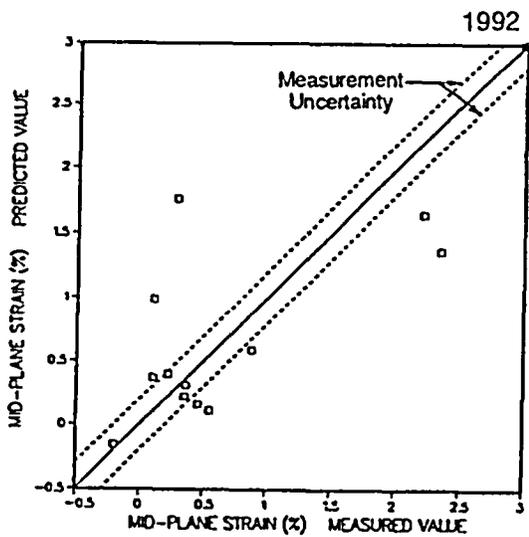
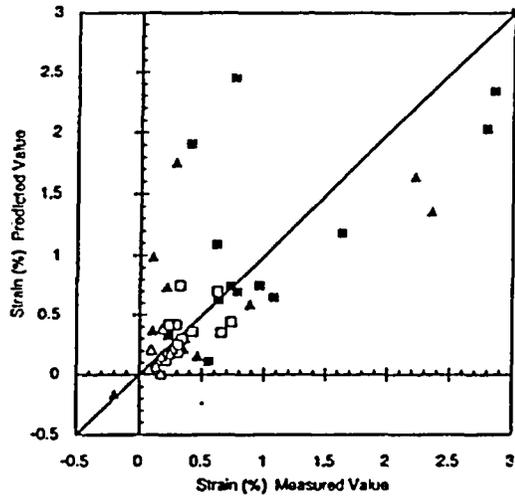


FIGURE 19: COMPARISON OF MID-PLANE SHEATH STRAINS



NUMBER OF POINTS = 14  
 MEAN DEVIATION = 0.48  
 STANDARD DEVIATION = 0.46  
 CORRELATION COEFFICIENT = 0.81  
 AVERAGE DIFFERENCE = 0.08

FIGURE 20: TOTAL MID-PLANE STRAIN (%) AT END-OF-LIFE



NUMBER OF POINTS = 48  
 MEAN DEVIATION = 0.33  
 STANDARD DEVIATION = 0.41  
 CORRELATION COEFFICIENT = 0.86  
 AVERAGE DIFFERENCE = 0.05

■ 1992 Ridge  
 ▲ 1992 Mid-plane  
 □ 1989 Ridge  
 △ 1989 Mid plane

FIGURE 21: ALL END-OF-LIFE STRAINS MEASURED VS. PREDICTED

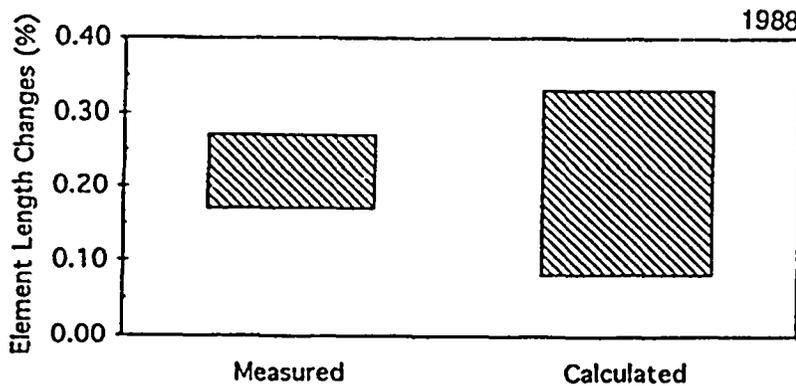


FIGURE 22: COMPARISON OF ELEMENT LENGTH CHANGES