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# A Semi-Mechanistic Approach to Calculate the Probability of Fuel Defects

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by M. Tayal, E. Millen, R. Sejnoha and  
G. Valli

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1992 October 4-8.

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# A Semi-Mechanistic Approach to Calculate the Probability of Fuel Defects

**AECL-10642**

by M. Tayal, E. Millen, R. Sejnoha and G. Valli\*

## **Abstract**

In this paper we describe the current status of a semi-mechanistic approach to calculate the probability of fuel defects. It expresses the defect probability in terms of fundamental parameters such as: local stresses, local strains, and fission product concentration. The calculations of defect probability continue to reflect the influences of the conventional parameters like: ramped power, power-ramp, burnup and CANLUB. In addition, the new approach now provides a mechanism to account for the impacts of additional factors involving detailed fuel design and reactor operation, for example: pellet density, pellet shape and size, sheath diameter and thickness, pellet/sheath clearance, coolant temperature and pressure, etc. The approach has been validated against a previous empirical correlation. An illustrative example shows how the defect thresholds are influenced by changes in the internal design of the element and in the coolant pressure.

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# Méthode semi-mécaniste pour les calculs de probabilité des ruptures de gaine

## **AECL-10642**

par M. Tayal, E. Millen, R. Sejnoha et  
G. Valli\*

### **Résumé**

Le présent document décrit l'état actuel des calculs de probabilité des ruptures de gaine réalisés à l'aide d'une méthode semi-mécaniste. Le document explique la probabilité de rupture en fonction de paramètres fondamentaux tels que : les contraintes locales, la déformation locale et la concentration des produits de fission. Les calculs de probabilité prennent toujours en compte les paramètres fondamentaux tels que : la variation de la puissance par rampes, la rampe de puissance, la combustion massique et le concept Canlub. En outre, la nouvelle méthode offre maintenant un mécanisme permettant de tenir compte des incidences de facteurs additionnels où entrent en jeu l'étude détaillée du combustible et l'exploitation du réacteur comme, par exemple : la densité, la forme et la taille des pastilles, le diamètre et l'épaisseur de la gaine, l'écart entre la gaine et les pastilles, la température et la pression du caloporteur, etc. On s'est servi d'une ancienne analyse de corrélation empirique pour valider cette méthode. On y présente aussi un exemple pour montrer comment les variations de pression du caloporteur et les modifications apportées à la conception des éléments combustibles influent sur les seuils de rupture.

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### ILLUSTRATIONS

## 1. INTRODUCTION

The performance record of CANDU\* fuel is excellent [1]. The cumulative defect rate to date is low: in over 800,000 bundles irradiated about 1000 bundles have defected in the power reactors. Most of the defects occurred during identifiable departures from the norm, and helped improve our understanding of the nature and level of defect probabilities. Surveys of the defects have shown that Stress Corrosion Cracking (SCC) is an important mechanism for fuel failures [1].

At present, empirical correlations [2,3] are used to define the limits of powers and of power-ramps within which CANDU fuel can be operated without risk of failure under normal operating conditions. However, the fuel engineers also need to be able to assess the impact of operating the fuel under conditions beyond the existing data-base. This can help guide the acceptance/loading of fuel (e.g., effects of manufacturing variations/flaws), or can guide reactor operation (e.g., effects of power cycles, extended burnups, non-routine startups, non-routine fuelling, etc.), or can aid in the evolution of advanced fuel designs [1] (e.g., High Burnup Fuel, Highly Advanced Core, Low Void Reactivity Bundle, DUPIC\*\*, etc.). This paper describes a semi-mechanistic approach that is a step in that direction.

In this paper we first provide some technical background relevant to SCC, followed by a discussion of the mechanistic equations and their validation. An illustrative example shows how the defect thresholds are influenced by changes in the internal design of the fuel element and in the coolant pressure.

Figure 1 defines some of the terms used in this paper. The nomenclature is given towards the end.

## 2. BACKGROUND

SCC of fuel element cladding occurs when the irradiation-embrittled sheath experiences high tensile stresses in the presence of a corrosive internal environment provided by the fission products. It may also be influenced by hydrides, which can provide sites for crack initiation and which can also blunt the growth of cracks [4,5].

The high tensile stresses occur mostly due to pellet expansion because of power-ramps. They can also be caused by excessive pressure of fission gas.

To date, the SCC defects in commercial CANDU fuel have been associated with circumferential ridges and with the reentrant corner near the sheath/endcap weld. These are locations of stress concentrations – please see Figure 2.

---

\* CANDU: Canada Deuterium Uranium

\*\* DUPIC: Direct Use of PWR Fuel in CANDU Reactor

There is convincing evidence [6] that the likelihood of SCC is influenced by the following factors: the local stresses and strains, the local concentration of corrodants at the crack tip, the duration of stress/strains, and the influences of microstructure, of hydrides, and of irradiation on the resistance of Zircaloy to SCC. The studies to date have focussed on iodine and on cesium as the likely corrodants.

We call these the mechanistic parameters pertinent to SCC.

The existing empirical correlations [2,3] generally express the defect probability as a function of operational parameters like: ramped power, power-ramp, and burnup. Sometimes, the effect of dwell time and of graphite thickness is also considered.

In these empirical correlations, the ridge stresses and strains are represented by the power-ramp. The corrosive internal environment is represented by the combination of ramped power, burnup and CANLUB. The resistance to SCC is represented by burnup.

Previous experiments have demonstrated that other design and operational features can also influence the fundamental parameters that affect SCC. For example, in the area of ridge stresses/strains, IRDMR\* experiments have demonstrated that lower density of UO<sub>2</sub> leads to reduced strain at the ridge [7]. Similarly, Carter has shown that pellets of smaller length also reduce the ridge strain [8]. These aspects are not reflected in the empirical correlations.

Likewise, in the area of corrosive internal environment, gamma-radiography has demonstrated that some fission products tend to concentrate at the interfaces between neighbouring pellets [9]. For example, Lysell and Schrire report [8] that the concentrations of I-131, I-133, Cs-134, and Cs-137 are a factor of 4-14 higher at the pellet interfaces compared to the midpellet positions. This means that the number of pellets in the stack can also affect the local concentration of corrosives.

The semi-mechanistic approach described in this paper is being developed to address factors such as these.

### 3. MECHANISTIC PARAMETERS

At this time we use the following methods to calculate the mechanistic parameters noted earlier.

#### 3.1 STRESSES/STRAINS

We use the computer codes ELESTRES [10], SHEATH, and FEAST [11] to calculate the axisymmetric stresses and strains at the inside surface of the sheath at the circumferential ridge, and at the re-entrant corner of the sheath/endcap junction.

The axisymmetric stresses and strains are multidimensional, and each consists of the following four components: radial, hoop, axial and shear. The peak stresses/strains are influenced by: the applied load, material properties of the sheath; stress/strain concentrations; degree of multiaxiality; and boundary conditions (ridge vs endcap).

---

\* IRDMR: In Reactor Diameter Measurement Rig

To cover the above factors, we combine the eight components of stresses/strains by calculating the total energy imparted to the sheath by the expanding pellet. The following equation is used:

$$W = \int \sigma_{11}d\epsilon_{11} + \int \sigma_{22}d\epsilon_{22} + \int \sigma_{33}d\epsilon_{33} + \int \sigma_{13}d\epsilon_{13}$$

Here, 'W' represents the work done by the pellet on the sheath per unit volume. It is called 'work density' and has units of MPa. The subscripts 1, 2, 3 represent the radial, circumferential, and axial directions respectively. The four terms on the right hand side represent the contributions of radial, hoop, axial and shear components respectively. The integration is taken over the total increment of strain due to the power ramp. The above calculations are done at the inner surface of the sheath at the circumferential ridges - this location is at high risk of failure.

### 3.2 CORRODANT CONCENTRATION

We start with the ELESTRES code to obtain the mass of fission products ( $\chi$ ) released by the pellets to the space between the pellets and the sheath. Only some fraction of the fission products are active species that participate in SCC. To be consistent with the experimental evidence noted earlier regarding iodine and cesium distribution, we allow the corrosive fraction of the fission products to concentrate in narrow rings at interpellet interfaces. Pellet cracking can further enhance the local concentration of fission products. We assume that the net effect of graphite is equivalent to a reduction in the amount of fission products that reach the surface of the sheath.

To account for these effects we use the following equations (Please see the nomenclature):

$$\alpha = \gamma k_1 k_2$$

$$\gamma = \left( \frac{\chi}{2\pi r q(N + 1)} - am \right)$$

Here  $\alpha$  is the local concentration of corrosive fission products in the fuel element.  $\gamma$  is a Fission Product Parameter, which is proportional to the local concentration of fission products at the sheath surface, and accounts for the effect of graphite through its mass  $m$ .

### 3.3 RESISTANCE TO SCC

Burnup is taken as the variable that governs the resistance of the sheath to SCC. This needs to be refined in future studies.

#### 4. APPROACH

Our efforts to date have focussed on SCC at circumferential ridges. Figure 3 illustrates the concept behind our approach, using the effect of power-ramp as an example. Larger power-ramps give larger displacements of the pellet and of the sheath, giving larger hoop strains at the ridge. Yield eventually levels the hoop stress at the ridge. Near the endcap weld, however, the components of stresses continue to increase past the uniaxial yield strength due to the high degree of multiaxiality. The trends in the work density are a composite of the trends of stresses and of strains.

As noted earlier, the above curves are specific to a particular fuel design. In Figure 3(d), 'base design' refers to the fuel design on which the existing empirical correlations for defect probability are based.

Let us suppose that we need to estimate the defect probability of an alternate fuel design - say, containing high density pellets - subjected to a power-ramp of  $\Delta P_1$  at a given burnup and ramped power. As noted earlier, the high density pellets will give higher strains and stresses in the sheath. Therefore the curve for work density will be different in the alternate design - see for example Figure 3(d). Hence an equivalence needs to be established between the two fuel designs.

Let the power-ramp  $\Delta P_1$  give a work density of  $W_1$  in the alternate design. To experience the same work density the base design needs to be subjected to a larger power-ramp, say  $\Delta P_2$  - see Figure 3(d). Thus, the probability of fuel defects in the alternate design due to a power ramp of  $\Delta P_1$  can be estimated by using  $\Delta P_2$  in the standard correlation for defect probability. Similar arguments can be constructed for the effect of ramped power.

To implement the above concept, we start with an existing empirical correlation - CAFE [3]. It expresses the probability of fuel defects in terms of operational parameters like power, power-ramp and burnup - for the standard design and operating envelope of fuel. Next we calculate the values of the mechanistic parameters for SCC associated with the above defect probabilities. In the final step, a relationship is found that expresses the probability of fuel failure in terms of the above mechanistic parameters.

#### 5. DEFECT THRESHOLDS

In terms of the mechanistic parameters, the defect threshold for work density is:

$$W^{\text{th}} = 2.6256 - 0.007082\omega$$

Here "W" is the density of work (MPa) done by the pellet on the sheath during the power-ramp at the inner surface of the sheath at the location of the circumferential ridge. The superscript "th" refers to defect thresholds. " $\omega$ " represents the element burnup (MW.h/kgU) at the time of the ramp. A similar threshold is obtained for the fission product parameter. Fuel defects are unlikely if either the fission product parameter or the work density is below its respective threshold.

## 6. DEFECT PROBABILITIES

If the defect thresholds are exceeded, then fuel defects can occur. Then, the defect probability,  $p$ , is given by:

$$p = (1 + e^{-A})^{-1}$$

where,

$$A = -6.109 + (139.4/\omega) + 0.012 \omega + (4.276 \gamma/\omega) + 0.527 W$$

The above equations express the defect thresholds and the defect probabilities in terms of mechanistic parameters, and can be applied to a variety of fuel designs and operating conditions. They are valid for element burnups between 75 - 220 MW.h/kgU. Fuel failures via SCC have not been observed at burnups below 75 MW.h/kgU in CANDU fuel containing thick graphite of good quality. The above equations are considered less precise at burnups above 220 MWh/kgU owing to a paucity of irradiation data.

## 7. VALIDATION

The validation of the computer codes ELESTRES and FEAST have been discussed previously [10,11]. Both codes show strong agreement with data and with other independent calculations.

We also note that for 37-element CANDU fuel, the defect thresholds and the defect probabilities predicted by our semi-mechanistic equations are identical to those given by CAFE – as illustrated in later figures. This is not surprising since the derivation of the mechanistic equations used CAFE in part. Nevertheless, the results are reassuring as a ‘quality assurance’ check. This approach ensures, and the QA checks confirm, that the predictions of the mechanistic equations are consistent with the experimental data on which the empirical correlation CAFE is based. It is noted here that the CAFE correlation is used by Ontario Hydro to calculate defect thresholds and defect probabilities of 37-element fuel during normal operation, and is consistent with data from NRU and Bruce reactors [3].

## 8. ILLUSTRATIVE EXAMPLE

For 37-element CANDU fuel, the mechanistic equations give the same results as CAFE, which is to be expected. This is discussed later via some graphs that illustrate the predictions.

The above equations were formulated in 1989 as part of a review of the integrity of fuel for the CIRENE reactor in Italy [12]. We used the above equations to help judge if the CIRENE fuel is strong enough to survive its intended operating conditions. A summary of that application is given in the following paragraphs.

The CIRENE fuel, though similar in many respects to 37-element CANDU fuel, differs from the latter in several details of fuel design and of operating conditions. The major differences pertinent to SCC are illustrated in Figure 4 and summarized below:

<u>FEATURE</u>	<u>CIRENE</u>	<u>CANDU</u>
a. Enrichment	some parts of core	none
b. Pellet diameter	larger	smaller
c. Pellet dish	deeper	shallower
d. Diametral clearance	higher	lower
e. Number of pellets	lower	higher
f. Sheath	thicker	thinner
g. Sheath yield strength	higher	lower
h. Graphite	thicker	thinner
i. Coolant pressure	lower	higher
j. Coolant temperature	lower	higher

These differences have consequences in fission product concentration and in sheath stresses/strains. For example, for a given element rating and burnup, the bigger pellets in CIRENE generate more fission products. Even accounting for the larger surface area of the CIRENE sheath, CIRENE contains more fission products per unit surface of the sheath. The smaller number of pellets in CIRENE mean that its fission products concentrate over a smaller length of the sheath, aggravating the previous effect. On the other hand the graphite layer is thicker in CIRENE, so the sheath is better protected. Regarding stresses/strains, the lower coolant pressure in CIRENE results in lower rate of creep collapse of the sheath during the low-power soak. This leaves a larger diametral clearance between the pellet and the sheath in CIRENE. Therefore, when the CIRENE pellet expands due to a power-ramp, it imparts less energy to the CIRENE sheath. Similarly, several other differences can also be identified.

Power-ramp testing of an earlier version of CIRENE fuel indicated that its defect performance is not consistent with that expected from the standard CANDU correlations. Hence the fuel design was improved, and the benefit in defect performance was quantified by using the preceding approach.

The many competing processes noted above can potentially have a complex impact on fuel integrity. The individual and the combined consequences of the above parameters were quantified by using the ELESTRES/SHEATH/FEAST codes in conjunction with the semi-mechanistic equations discussed earlier. Table 1 shows the combinations that were studied parametrically. Figure 5 illustrates the results.

Figure 5 shows that for a given power history, the larger diameter of CIRENE fuel results in a much higher level of fission products in the pellet/sheath gap. This tends to lower the defect thresholds for ramped power ( $P_{max}$ ). On the other hand, the thicker layer of graphite in CIRENE fuel provides it with a higher level of protection from the fission products. The two effects balance each other almost exactly, see Figure 6.

For a given power history, the much lower pressure of the CIRENE coolant results in a small gap between the pellet and the sheath at the beginning of the ramp. This means that when the pellet does expand due to the ramp, the sheath experiences smaller strains and stresses – see Figure 5. This increases the defect threshold for power-ramps by ~30%; see Figure 6.

Once the defect threshold is reached, the defect probabilities frequently increase more steeply in CIRENE than in 37-element CANDU fuel, owing largely to the larger diameter of CIRENE fuel. The net defect probability in CIRENE can be either higher or lower than in corresponding 37-element CANDU fuel, depending on the specifics of the power-ramp. Figure 7 is an example.

## 9. DISCUSSION

The semi-mechanistic equations discussed here do not replace the empirical correlations now in use. Rather, they provide a means of extending the range of applicability of the correlations, to conditions that are either not covered by the data base or are poorly represented.

The semi-mechanistic equations continue to reflect the influences of operational parameters that are currently used for defect thresholds/probabilities, viz: power-ramp, ramped power, and burnup. In addition, they provide a vehicle to account for the impacts of detailed fuel design parameters such as pellet density, pellet shape and size, sheath diameter and thickness, pellet/sheath clearances, etc. Additional operational parameters can also be covered, for example coolant temperature and pressure, etc. As noted earlier, previous experiments have already demonstrated that some combinations of the above features can have considerable impacts on factors such as stresses, strains and fission gas releases.

The example discussed earlier demonstrates how the methodology was applied to CIRENE fuel with its many similarities but also several differences from the standard CANDU fuel. We expect that the methodology can also be applied to obtain first-order estimates of defect thresholds and probabilities in other situations where sufficient empirical data may not exist to provide reliable guidance. With further evolution, some specific applications of the preceding concepts could include the following:

### 9.1 GUIDE THE ACCEPTANCE/LOADING OF NEW FUEL

Sometimes the as-fabricated fuel contains combinations of tolerances that are not sufficiently covered by the previous well-characterized database on ramp testing. One example is fuel of high mass, including high  $\text{UO}_2$  density and low clearances. Or, the fuel may contain manufacturing flaws whose impact is unknown from previous tests. The approach outlined here can help provide an interim guidance about the expected performance of such fuel.

### 9.2 GUIDE REACTOR OPERATION

Similarly, the approach can help guide reactor operation in new areas of operation, e.g., effects of power cycles, of extended burnups, of non-routine startups, of non-routine fuelling, etc.

### 9.3 AID EVOLUTION OF FUEL DESIGN

Some specific activities currently underway include [1]: High Burnup Fuel, Highly Advanced Core, Low Void Reactivity Bundle and DUPIC. Again, the approach outlined here can be applied in these evolutions.

## 10. CONCLUSION

A framework has now been established for a semi-mechanistic approach to calculate the defect probability of CANDU fuel. The approach consists of using the ELESTRES/SHEATH/FEAST computer codes to calculate the mechanistic parameters pertinent to stress corrosion cracking, and then correlating the results to the available experimental data. For 37-element CANDU fuel, the semi-mechanistic equations give the same results as the CAFE correlation. This is not surprising since the CAFE correlation was used in part to obtain the mechanistic equations. However, unlike the current empirical correlations, the semi-mechanistic equations can also be applied to other fuel designs and operating conditions. For example, an application of the mechanistic equations to the CIRENE fuel shows that the thresholds for ramped power ( $P_{max}$ ) in CIRENE are similar to those in the 37-element CANDU fuel. This is because the influence of the larger CIRENE diameter is balanced almost exactly by the influence of the thicker graphite in CIRENE. However, the defect thresholds for the power-ramps ( $\Delta P$ ) are ~30% higher in CIRENE than in 37-element CANDU fuel. This is mainly the result of the much lower coolant pressure in CIRENE. Once the defect thresholds are exceeded, the defect probability generally increases at a steeper rate in CIRENE than in 37-element CANDU fuel.

Further evolution of the technique can extend the range of its applicability.

## 11. ACKNOWLEDGEMENTS

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## NOMENCLATURE

a	Amount of fission products reacted/absorbed/adsorbed by graphite, per unit mass of graphite
A	Constant in the equation for defect probability
e	Exponential
$k_1$	Ratio of the mass of active species to the total fission products
$k_2$	Concentration factor for fission products due to pellet cracks
m	Mass of graphite
N	Number of pellets in the stack
p	Defect Probability (fraction)
$P_{max}$	Power after the ramp
$\Delta P$	Increase in power
q	Width of the ring into which the fission products concentrate
r	Inner radius of the sheath
W	Local density of work

Greek Symbols

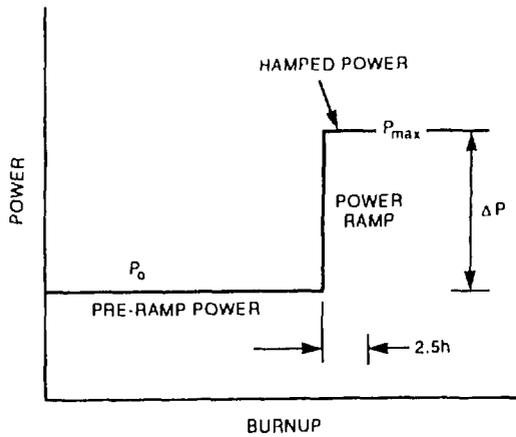
$\alpha$	Concentration of active species at the sheath surface
$\gamma$	Fission Product Parameter
$\epsilon$	Sheath strain
$\sigma$	Stress in the sheath
$\chi$	Mass of fission products released by the pellet
$\omega$	Burnup

Superscript

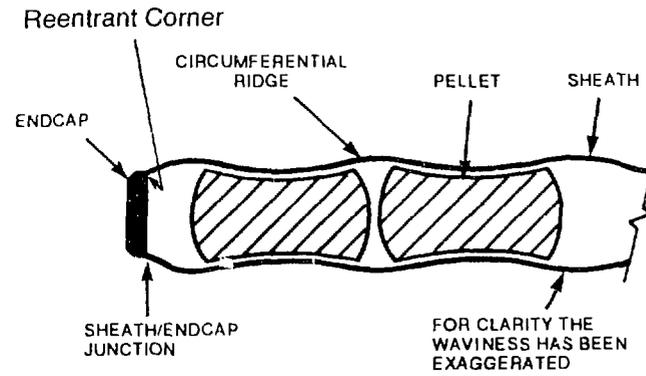
th	Threshold
----	-----------

Table 1  
 Parametric Study: Input Data

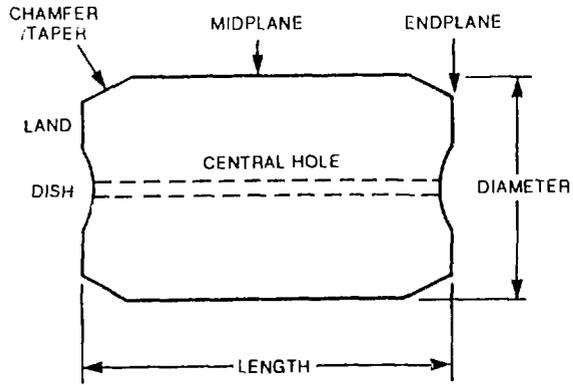
Permutation	Pellet Material	Pellet Dimensions	Sheath	Coolant and Plenum
#1		37-ELEMENT		
#2	CIRENE	37-ELEMENT		
#3	CIRENE	37-ELEMENT		
#4	CIRENE	37-EL		
#5	CIRENE			



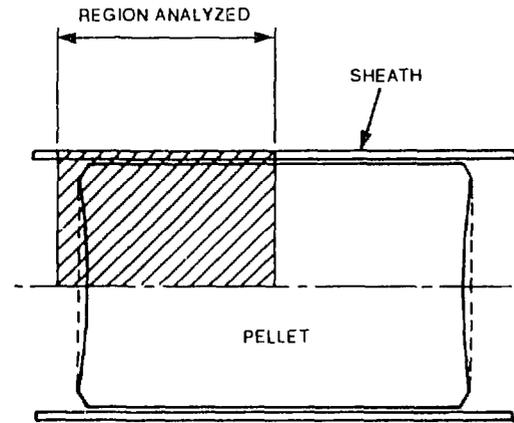
(a) POWER HISTORY



(b) FUEL ELEMENT



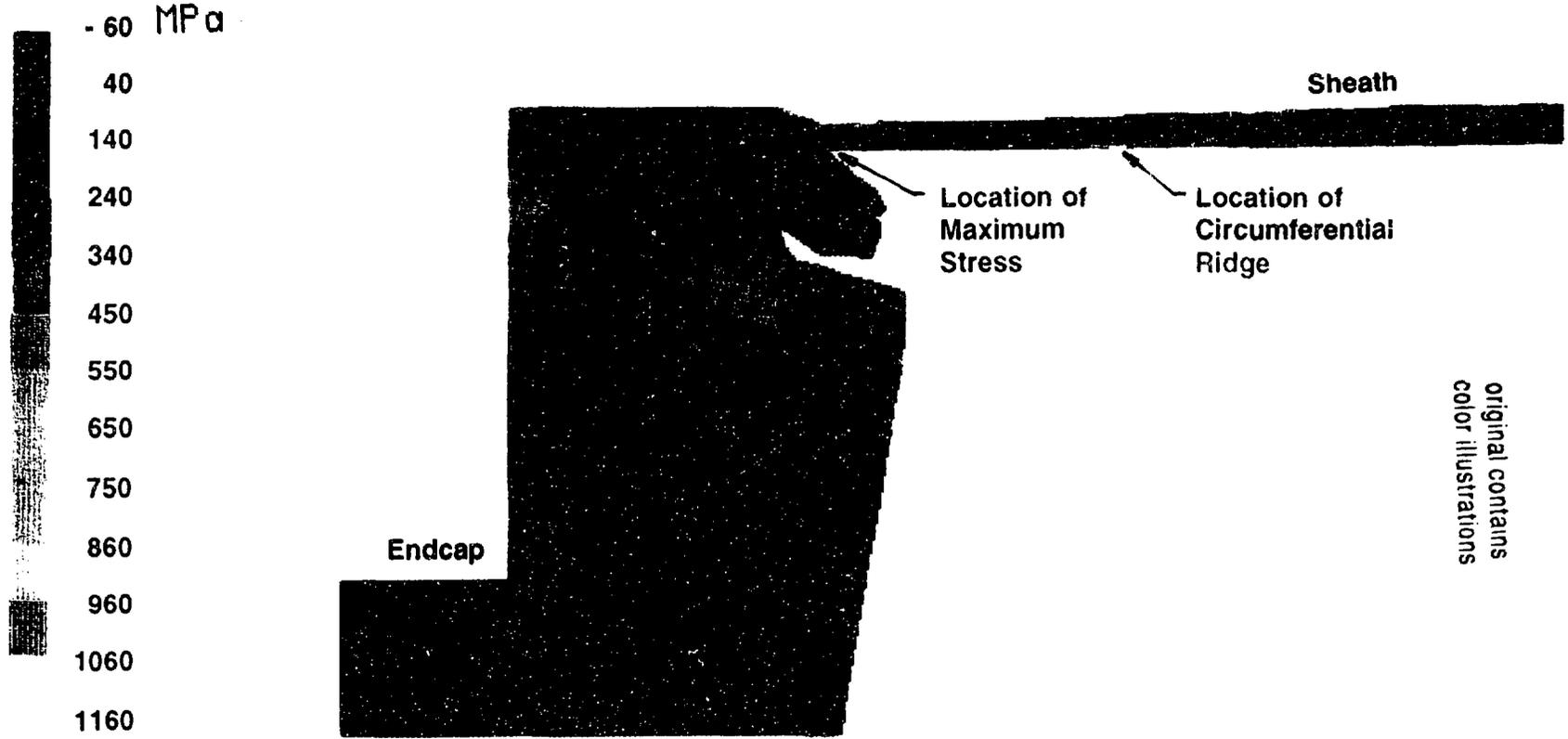
(c) PELLETT



(d) REGION ANALYZED

FIGURE 1 DEFINITIONS OF TERMS

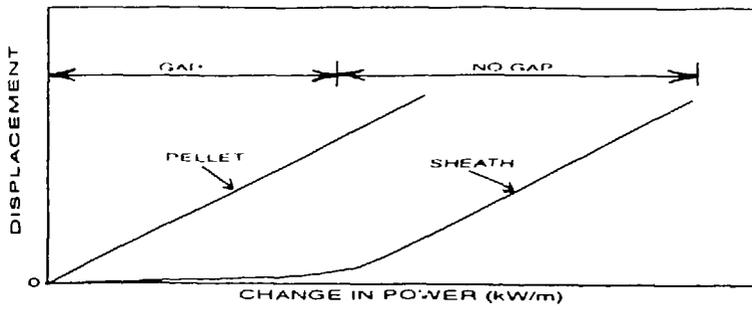
# Principal Stresses



0.6 mm Cold Axial Clearance  
0.2 MPa Internal Pressure  
0.04 mm Axial Displacement  
0.06 mm Radial Displacement

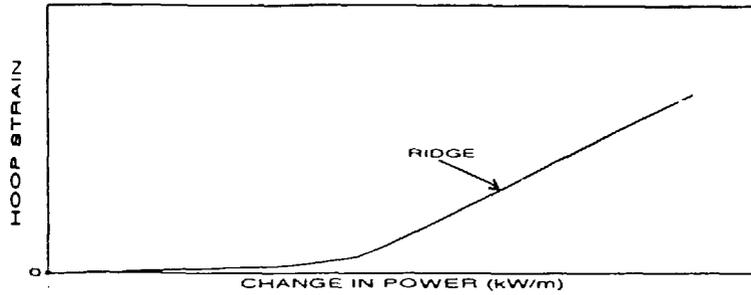
Elastic-Plastic Calculation

Figure 2 : Principal stresses near the endcap and near the circumferential ridge



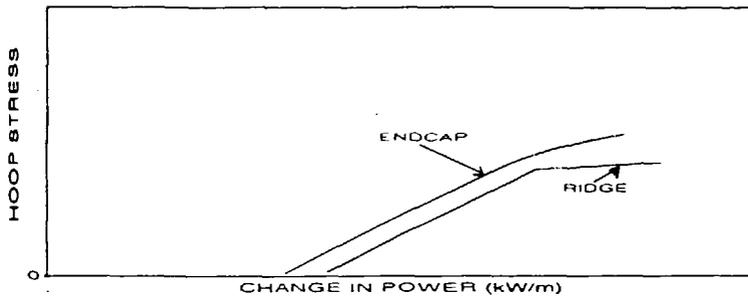
ELESTRES

(a) Displacement



ELESTRES

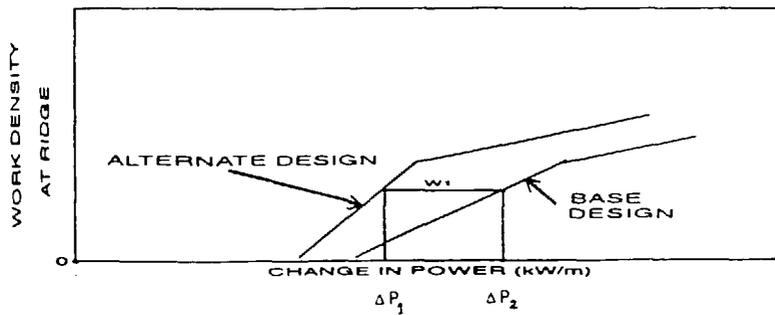
(b) Hoop Strain



SHEATH

FEAST

(c) Hoop Stress



SHEATH

FEAST

(d) Work Density

FIGURE 3: IMPACT OF A POWER RAMP

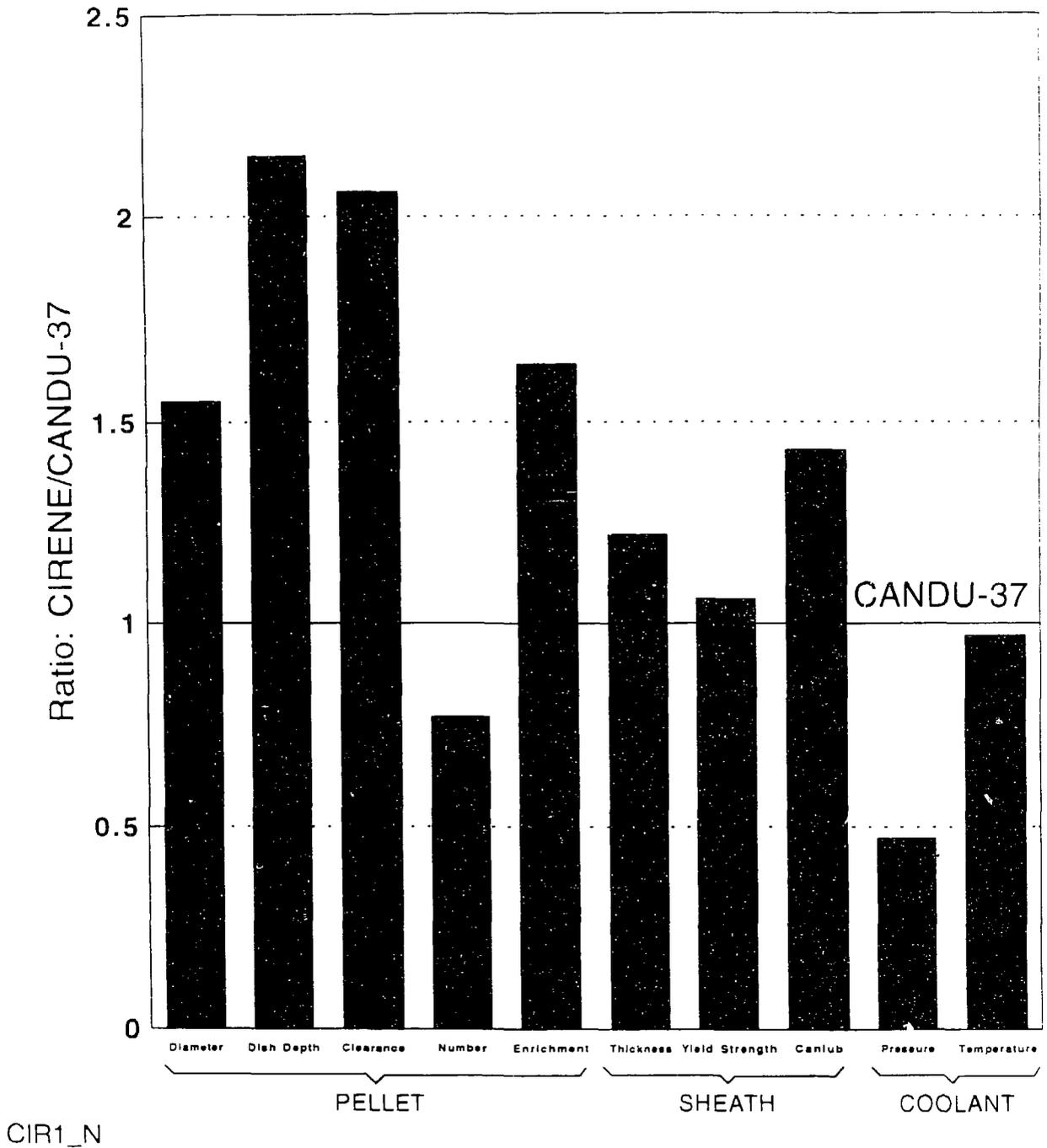
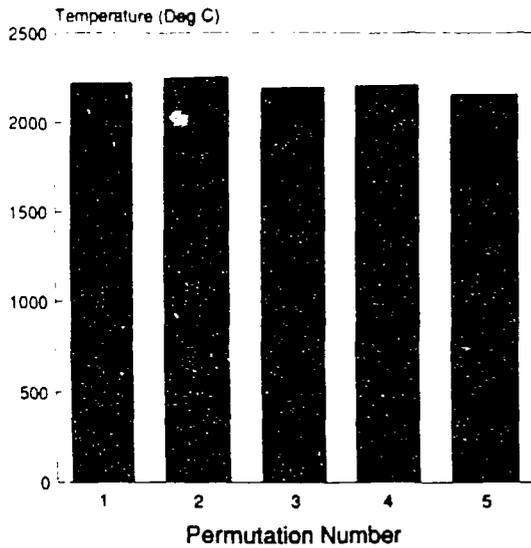
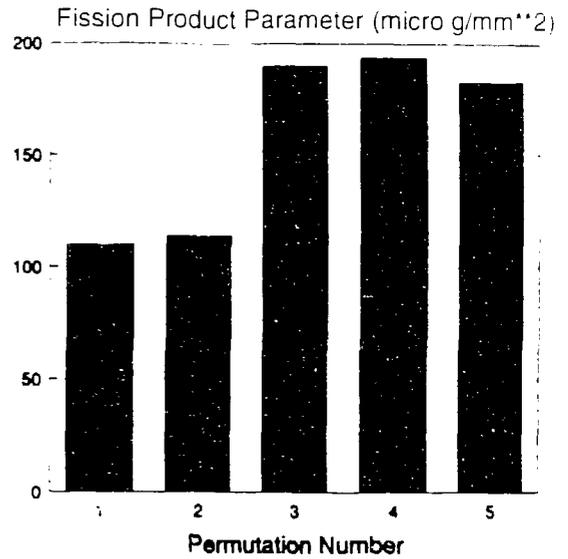


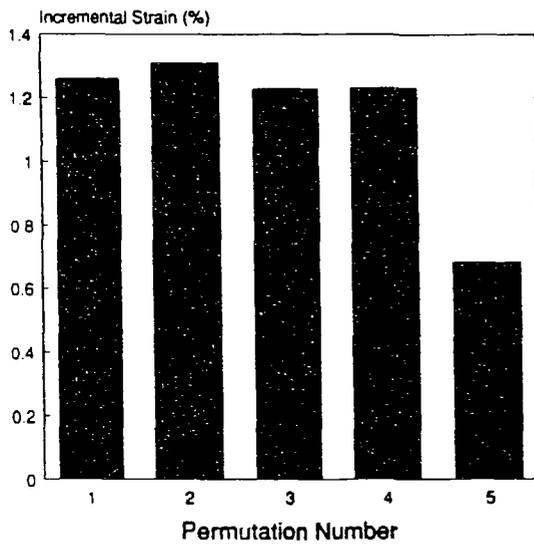
Figure 4 : CIRENE Parameters pertinent to SCC, as ratios of corresponding CANDU-37 parameters



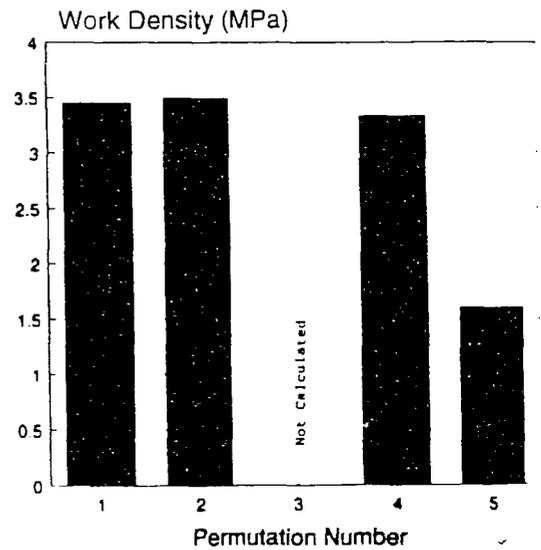
Central Temperature



Fission Product Parameter



Incremental Hoop Strain in Sheath

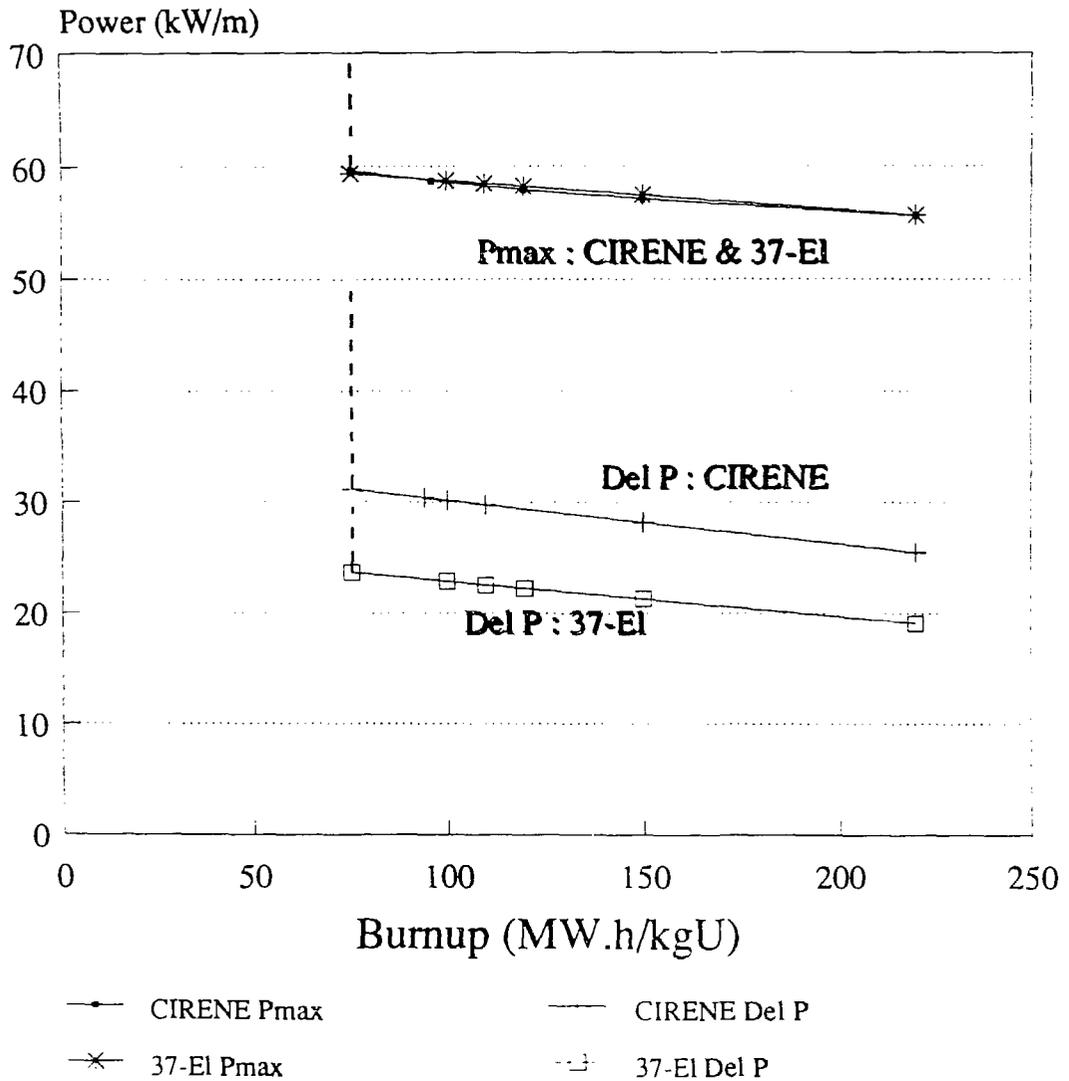


Work Density

900128

Figure 5 : Parametric Study : Results

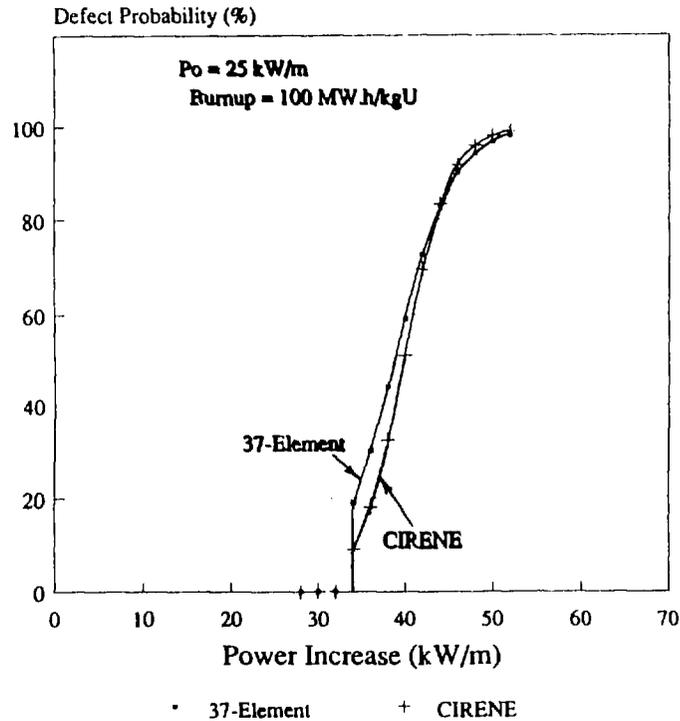
# Defect Thresholds CIRENE & 37-Element



900220

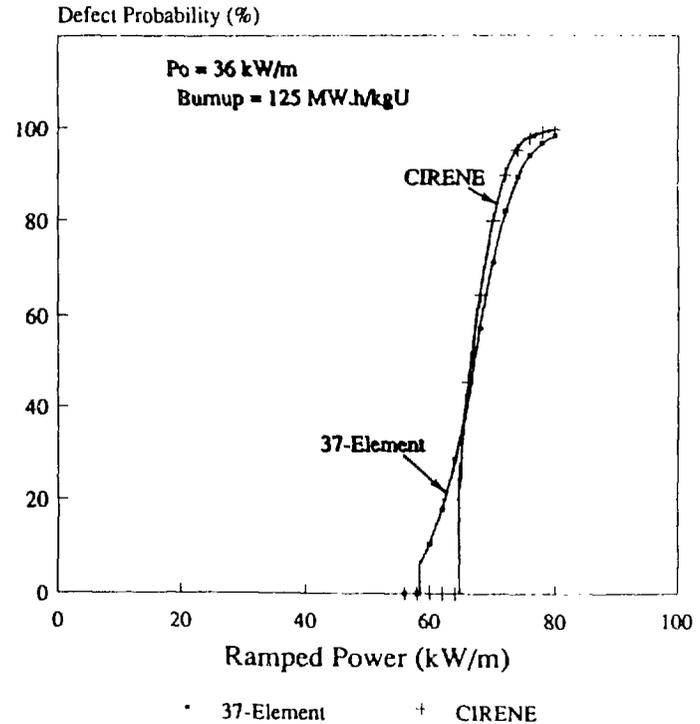
Figure 6 : Defect Thresholds

## Defect Probability CIRENE vs 37-Element



(a)  $P_0 = 25 \text{ kW/m}$   
Burnup = 100 MW.h/kgU

## Defect Probability CIRENE vs 37-Element



(b)  $P_0 = 36 \text{ kW/m}$   
Burnup = 125 MW.h/kgU

Figure 7 : Comparison of Defect Probabilities  
in 37-Element and in CIRENE Fuels