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AN INTRODUCTION TO CURRENT MODELING TECHNIQUES IN NUCLEAR FUEL PERFORMANCE ANALYSIS

Su Chiang Shu Faya*

ABSTRACT

~~This work provides~~ an overview of several important phenomena considered in fuel performance analysis, such as fuel restructuring, fuel swelling, fission gas release, pellet cracking, etc. All these phenomena are interdependent. For the purpose of illustration of integral fuel rod analysis the LIFE-1 computer code is discussed.

1 – INTRODUCTION

The achievement of good fuel cycle economics in both thermal and fast reactors requires the fuel element to achieve a relatively high burnup without failure. If fuel failure is defined at the point at which the fuel rod cladding ceases to form an impervious barrier between the fuel and coolant, then it is important to develop a means of predicting this failure point and the events which lead to that failure. The net picture is very complicated. Fuel materials with compositions which vary as a function of time and space operate for long periods of time at extreme temperatures in an irradiation environment. Many of the resultant effects are uncertain and are difficult to estimate with confidence. The problems, associated with the development of an accurate simulation of fuel element behavior under actual fluctuating reactor operating conditions for off-normal conditions, are tremendous.

Several areas of study may be defined. One group of investigators have primary interests individually in thermodynamics, in mathematical models of fission gas behavior, in fuel swelling and other problems related to the oxide fuel material itself. Fuel cladding specialists focus on the mechanical behavior of cladding materials in reactor environments, on the corrosion behavior of cladding and on solid state physics problems such as the behavior of voids in metals. Interrelated areas include both the chemical interaction and the mechanical interaction between fuel and cladding. All of these areas of activity must be integrated to arrive at comprehensive, valid performance models for complete fuel elements.

It is interesting to note that at present no scientist working in the field would dare to claim that a fully developed mathematical model with sufficient accuracy for design use is available. However, in recent years the efforts directed toward the attainment of fundamental data and toward the development of improved fuel performance computer programs have increased enormously.

The intent of this work is to provide an introduction to several of the important phenomena considered in fuel performance analysis. Areas of current interest in this field of endeavor are discussed. The discussion should provide an engineer who is new to this field with a solid information base for further study.

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2 – FUEL RESTRUCTURING

Material science is primarily concerned with the relationship between structure and properties. In oxide nuclear fuels, the structural changes are especially interesting. The bulk of existing fuel materials information consists of observation of these structural changes[4]. Studies of structural changes are predominant because these changes are easily observed.

2.1 – Fuel Regions

Any fine-grained aggregate of crystals processed by sintering will increase in grain size when heated at the elevated temperatures encountered in nuclear fuel operation. The driving force for this grain growth is the reductinon in surface energy by the reduction in grain boundary area. The higher the temperature, the more rapid the grain growth.

Figure 2.1 shows a typical microstructure of a highly rated oxide fuel pin with restructuring that results from a high thermal gradient. Four distinct regions are reccgnized:

1) Undisturbed region – the outer zone with a temperature range of ~ 700 – 1400°C, in which the grain size is unchanged compared with the as-sintered product;

2) Equiaxed grain growth region (~ 1400-1700°C);

3) Columnar grain growth region (> 1700°C); and

4) Central void.

2.2 – Columnar Grain and Central Void Formation by Migration of Fabricated Voids.

In any oxide fuel elements, there are pores present even before fissioning has produced inert gas bubbles. These bubbles are deliberately introduced in order to provide space to accommodate some of the fission gases and thus reduce the fuel element swelling, thereby decreasing the cladding strain. These voids may migrate along the temperature gradients existing in fuel clements. The migration of these voids are appreciable at temperature $\gtrsim$ 1900°K[14] but negligible for temperatures much balow this. This is the temperature range in which columnar grains are observed to form.

As the voids move inward, the axial and circumferential stresses become compressive which tends to force the voids into an elongated shape. The thermal gradient alters the shape in the same direction. The migration of elongated voids toward the center of the fuel could thus produce columnar grains with concomitant central void formation.

Wide columnar grains are observed in short-time exposures of low density elements and needle-like grains are noticed in long-time exposures. This seems to indicate that wide grains are formed by the migration of fabricated pores and the needle-like grains result from the migration of fission gas bubbles. The migration of fabricated pores at very short exposures will not affect any fission gas release, since no appreciable fission gas has been produced where the wide columnar grains have been established. After their formation, the columnar grains remain without change until long exposures, when elongated fission-gas bubbles obliterate them and form long, narrow, needle-like columnar gains.

Figure 2.2 shows the extent of columnar grain growth expected for UO_2 as a function of the centerline temperature of a cylindrical fuel element. Various exposure times are indicated and the effect of the amount of fabricated porosity on the size of the resultant central void is shown.

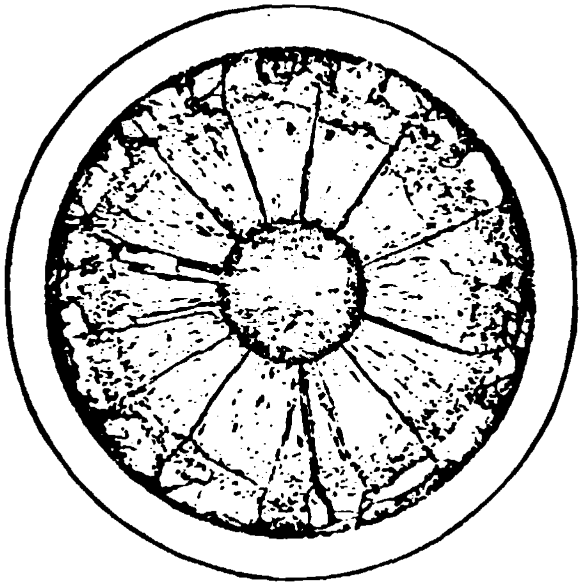

Figure 2.1 – Cross-Section of Highly Irradiated Mixed-Oxide Pin Showing the Central Void, Colummar Grain Zone, and Undisturbed Zone Next to the Cladding[8].

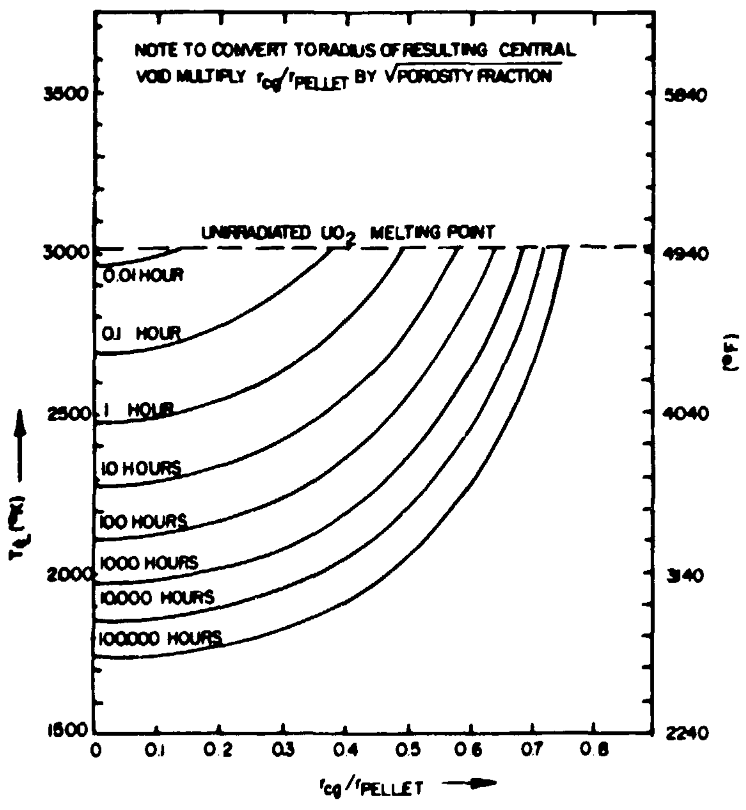

Figure 2.2 – Colummar Grain Growth Radius as a Function of Fuel Temperature and Time[14].

The density of oxide pellets is usually manufactured in the range of 90 – 95% of the theoretical density. This corresponds to a porosity range of 10 – 5%. The effect of porosity is to decrease the thermal conductivity of fuel material.

3 – FUEL SWELLING AND FISSION GAS RELEASE[14,12,20]

During the fission process in reactor fuels, many new atoms are formed. Some of these ($\sim$1.7 per atom fissioned) are generally regarded as "solid" fission products. An appreciable number ($\sim$0.3) per atom fissioned) are the inert gases Xenon and Krypton. As noble gases, both have low solubility in and a low chemical reactivity with the fuel. These gaseous fission products are responsible for the primary stresses imposed upon the fuel rod cladding. These stresses originate from two sources:

1) The fraction of gas which is released from the fuel increases the internal pressure which must be restrained entirely by the cladding.

2) The remaining fraction of gas which is retained in the fuel is by far the greatest contribution to fuel swelling which leads to the main stress on the cladding

3.1 – Mechanism of Fission Gas Swelling

Since the solubilities of Xenon and Krypton in oxide fuels are very low, fuel in an operating reactor quickly becomes supersaturated in these two elements. There will be a strong tendency for them to precipitate out as gas bubles in the fuel. As the gas atoms coalesce, the free energy change apperars as a stress of the growing gas bubble on the surrounding fuel matrix. This stress will be relieved by the flow of vacancies to the bubble until the internal pressure p is balanced by surface energy σ; that is, when the equilibrium is reached. The equilibrium pressure in the bubble is given by:

$$p = \frac{2\sigma}{r} \tag{2.1}$$

where

p = surface tension of fuel material

r = radius of bubble

The result of the bubble growth is the swelling of the fuel. This swelling from bubble coalescence has been explained physically by Barnes and Nelson [1]. If the gas obeys the perfect gas laws:

$$p = \frac{2\sigma}{r} = \frac{3mKT}{4\pi r^3} \tag{2.2}$$

where

m = number of gas atoms in the bubble.

K = Boltzmann's constant

T = gas temperature

If two bubbles of equilibrium size of radius r_1 and r_2 (containing m_1 and m_2 gas atoms, respectively) coalesce, the resulting bubble is not in equilibrium with the surface energy. To attain its equilibrium, the new bubble must have a radius R determined by:

$$(m_1 + m_2)\,KT = \frac{2\sigma}{\Gamma}\ \frac{4\sigma}{3} R^3$$

It is seen from (2.3) that m is directly proportional to the square of the bubble radius, so that

$$R^2 = r_1^2 + r_2^2$$

Consequently, the bubble of radius R has a greater volume at equilibrium than the sum of the volumes of the bubbles of radii r_1 and r_2. That is, to restore equilibrium, the new bubble must absorb still more vacancies. There is a net volume increase and the swelling increases.

3.2 – Mechanism of Fission Gas Release

Based on experimental observations Barnes and Nelson[1] developed a mechanism for bubble dynamics in oxide fuels. They described how bubbles coalosce and flow, and are held by obstacles such as dislocations and grain boundaries until large enough to escape from obstacles. Ultimately, they are released from the fuel. The forces acting on a bubble as a function of bubble size, r, are described as follows:

1) Forces due to a thermal gradient, $\frac{dT}{dx}$

$$F_T = \frac{4\pi}{\Omega} r^3\ K\left(\frac{dT}{dx}\right)$$

K = Boltzmann's constant

Ω = Atomic volume of the diffusion atom

2) Forces due to a stress gradient, $\frac{d\sigma}{dx}$

$$F_\sigma = 8\pi r^3 \left(\frac{d\sigma}{dx}\right)$$

3) Forces due to a stressed dislocation

$$F_d = \mu b^2 \cos\theta$$

where

μ = shear modules of fuel

b = Burgher's vector of a dislocation

θ = half angle between the ends of the dislocation where it emerges from the bubble surface.

4) Forces due to a grain boundary

$$F_{GB} = \pi r \sigma_{GB} \sin 2\varphi$$

where

σ_{GB} = grain boundary surface energy

φ = half angle of the cone defined by the intersection of the boundary with the bubble.

In Figura 3.1 various forces are plotted as a function of bubble radius. The force due to the temperature gradient dominates at large radius.

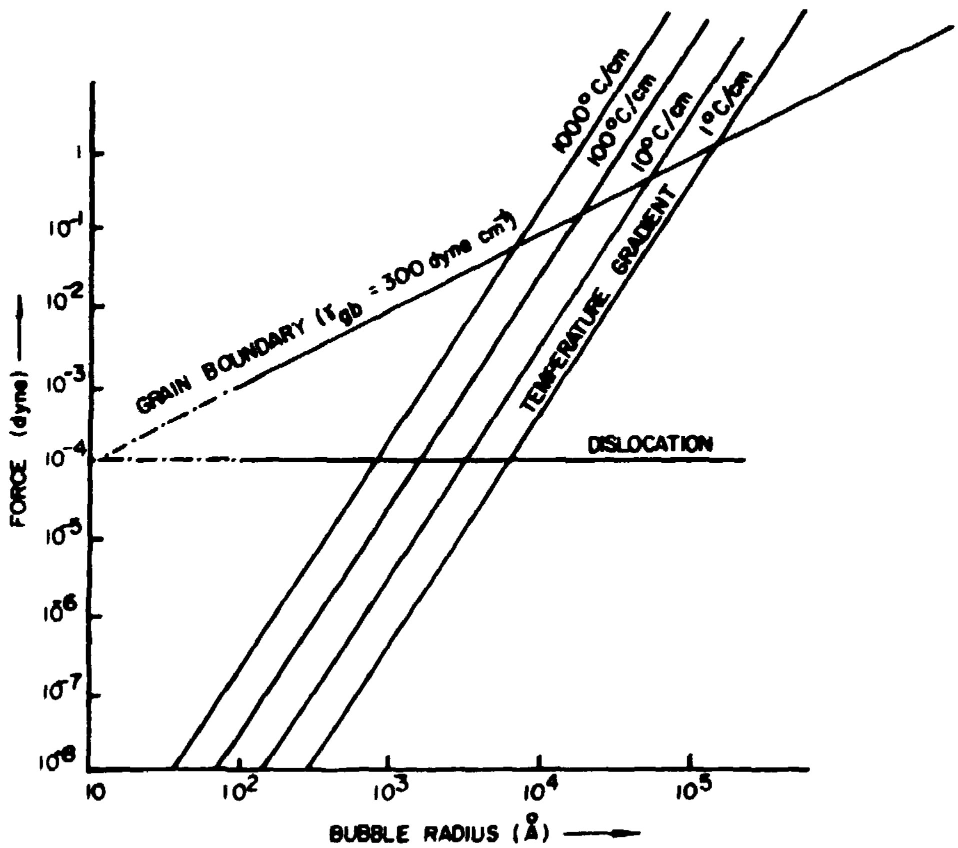

Figure 3.1 – The Forces Exerted on Bubble by Different Obstacles, as a Function of Bubble Radius[1].

Bubbles are nucleated on dislocations or within the matrix and migrate up the temperature gradient in the fuel until they encounter a dislocation. Here they may become attached. A dislocation exerts a retarding force on a bubble which has a maximum value of 10^{-4} dyne, independent of bubble size. A pinned bubble will grow by coalescence with neighboring bubbles until its radii reaches a critical size. At this point the temperature gradient provides a greater driving force than that of the dislocation and the bubble will leave the dislocation. Since bubbles all leave their dislocations at approximately the same radius, they have similar velocities and thus will encounter few collisions. The bubble will migrate up the temperature gradient until it reaches a grain boundary. Pinned at this grain boundary, the bubble will continue to grow until one of two things occurs: (1) the bubble will reach a new critical size, at which time it will be pulled from the grain boundary and migrate toward the fuel's central void, or (2) the bubble density on the grain boundary will increase to such an extent that interconnection of the bubbles to some free surface will occur and an immediate gas release will be effected. This latter phenomenon is known as breakaway and is considered to account for bursts of fission gas which occur in low temperature fuel operation.

Measurements of fission gas concentrations[3] within the columnar grain region indicate that between 70 – 95% of the gas produced in this region is released. In the equiaxed grain growth region 10 – 40% of the gas produced is released. Fission gas concentrations in the 1200 – 1400°C region indicate that less than 10% of the gas produced in this region is released. In the temperature region below 1200°C nearly 100% of the gas is retained.

High temperature gas release (>1200°C) from UO_2 fuel is an important consideration in steady-state reactor safety calculations because of its effect on the fuel-to-cladding gap conductance (and thus on the fuel temperature) and on the fuel rod internal gas pressure.

4 – FUEL PELLET CRACKINGS

The presence of radial and transverse cracks in ceramic fuel pellets has an important bearing on the stresses and strains produced in the cladding during in-reactor service. In some circunstances it appears that the endurance of the cladding is determined primarily by the tendency of strain to become concentrated in regions of cladding adjacent to pellet cracks.

Where a fuel rod is first brought to power, each fuel pellet will normally develop cracks due to the thermal stresses. The pellet center expands more than its periphery because of the centrer-to-surface temperature gradient. To accommodate this excess center expansion, radial cracks first form in the colder peripheral material. Then, with the continued increase in heat output further expansion of the pellet center causes the radial cracks to open further. Because of this expansion, the fuel pellet may encounter mechanical interaction with the cladding.

The resistance of pellet expansion due to the restraint provided by the cladding aided by the external coolant pressure will cause the hot pellet center to accommodate part of its thermal expansion by creeping into the central hole. This process will continue after full power has been attained. The restraint developed tends to deform the fuel, closing up the cracks. Crack closure begins in the weakest, hotter central region and then proceeds outward at a rate determined by the local fuel creep strength which varies as a function of temperature. Sintering processes at high temperatures may lead to healing of the closed cracks.

The crack distribution at full power can be represented as shown in Figure 4.1.

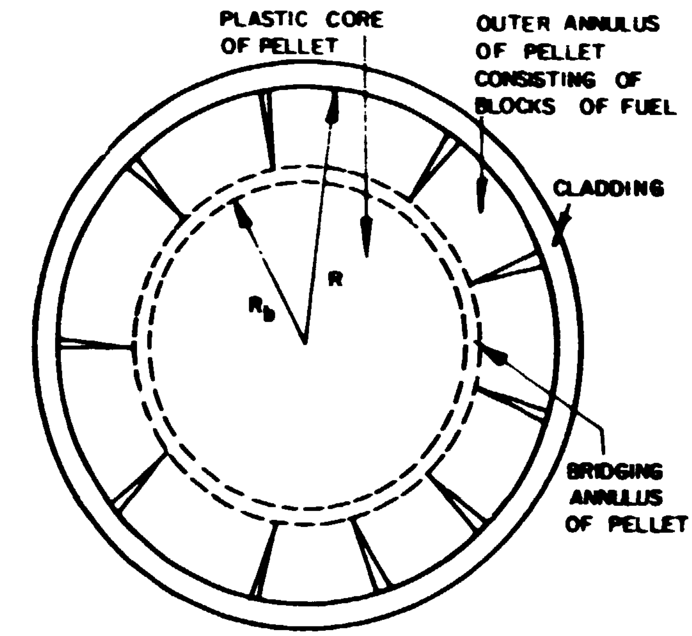

Figure 4.1 – Model Used for Crak Distribution in Fuel Pellet. R = Pellet Radius; R_b = Radius of Bridging Annulus[9].

The outermost rim of the pellet, consisting of fragments separated by open cracks, serves to transmit the restraint forces from the surface to the interior of the pellet. The reaction to this restraint is developed as a hoop stress which is concentrated in a ring designated as "bridging annulus". This load transmitting annulus is a narrow band at the base of the open cracks due to a rapid decrease of fuel strength with an increase of fuel temperature.

The position of the bridging annulus is an important factor in determining fuel-clad interaction on power cycling. At all times it exerts a major influence on the stress distribution in the pellet. Creep of the pellet under external restraint tends to move the brindging annulus towards the pellet surface. However, differential swelling within the fuel pellet may generate renewed opening of the cracks and offset their creep closure.

Under power cycling condition, pellet cracks are being generated during all phases. They will exist near the center of the pellet at low power and near the surface at high power, and the bridging annuls will move as a result of power cycling. Various computer programs have been developed to calculate the movement of the radius of briding annulus in terms of the fuel creep and swelling properties, the external restraint of the cladding, and the power generation history. During a reduction in power, for example, the rapid cooling central part of the pellet contracts. Since the power reduction is a relatively short process, the high tensil stresses set up by the contracting core are not relieved by creep processes, but cause the formation of a circumferential crack. By differential contraction radial cracks may be generated in the center of the fuel.

Figure 4.2 shows the fuel pellet cracking behavior during power cycling. The theoretical shape of a fuel oxide pellet during some phase of power cycling is shown in Figure 4.3.

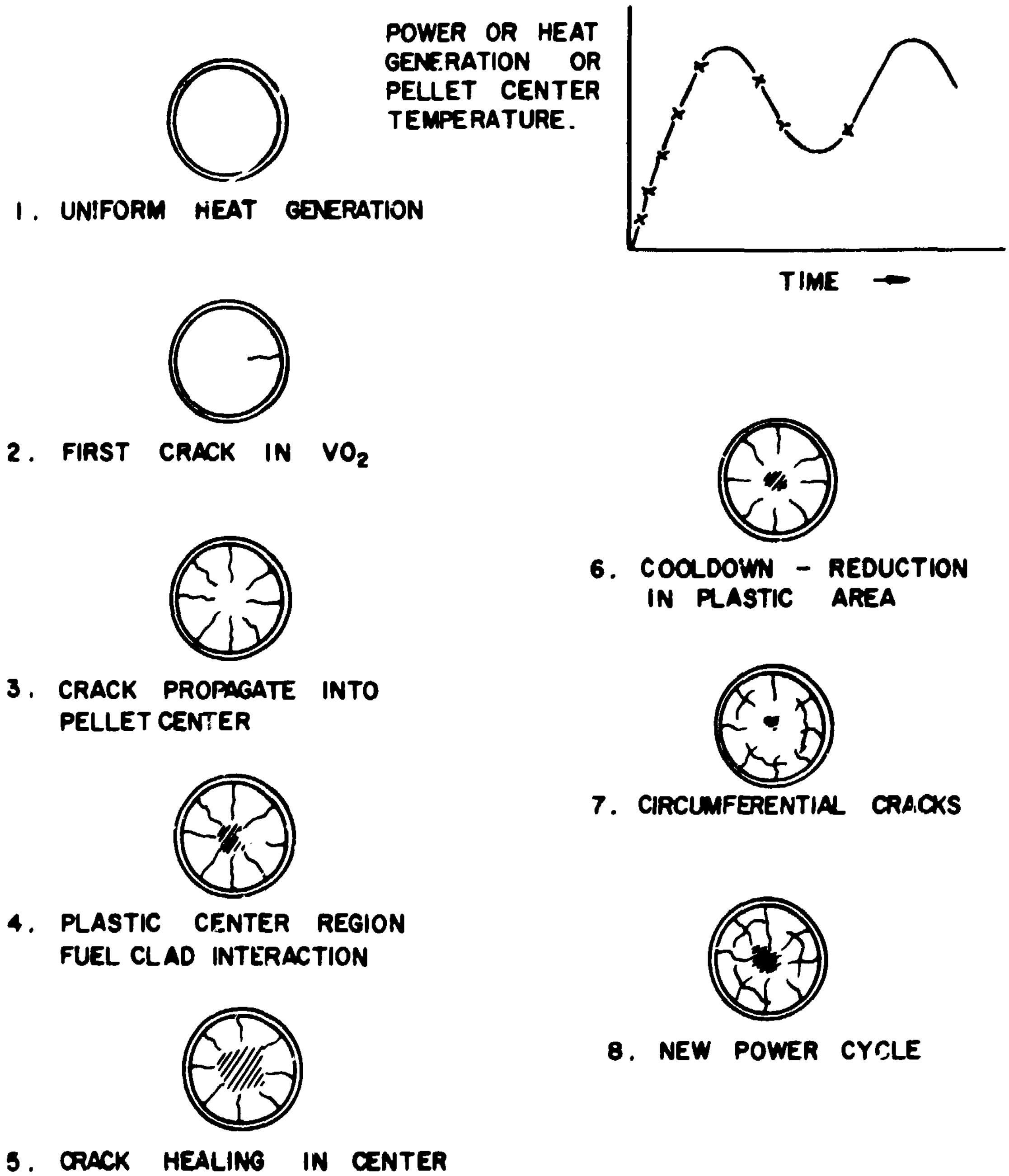

Figure 4.2 – Fuel Pellet Cracking During Power Cycling[11].

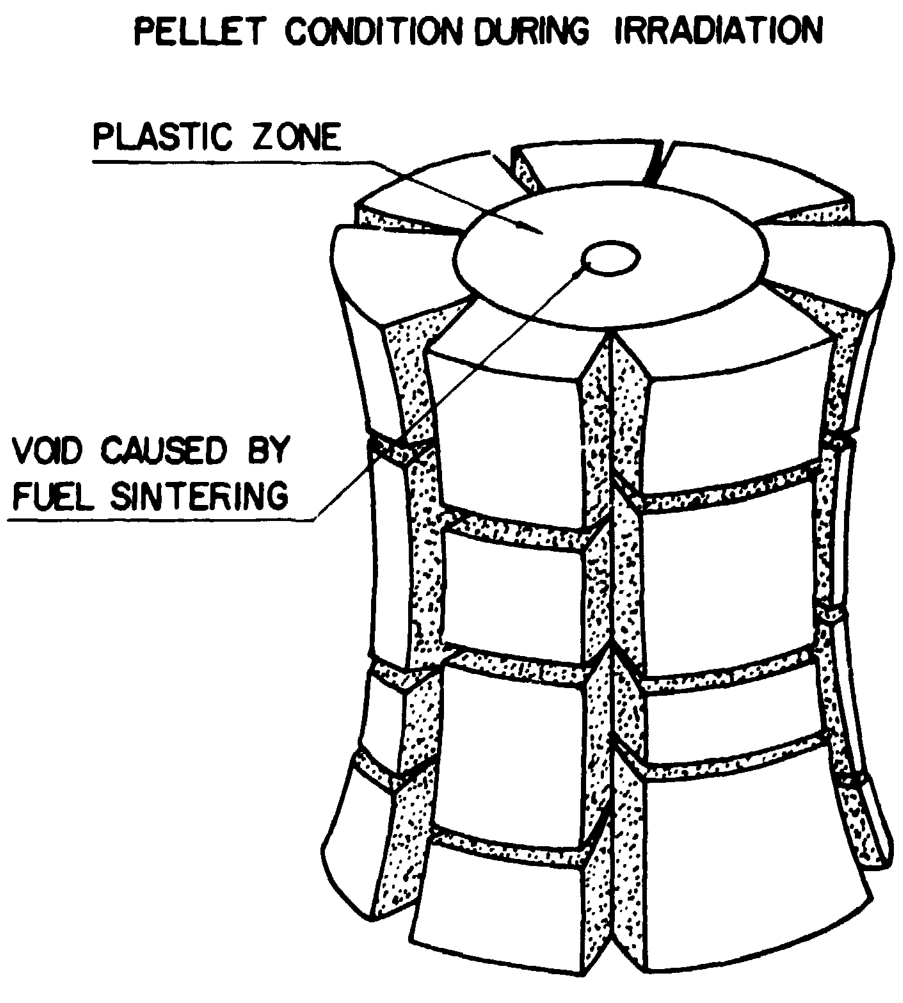

Figure 4.3 – Theoretical Shape of a Typical UO_2 Pellet During Irradiation[2].

The stress and strain distributions produced in nuclear fuel element cladding by the expansion of cracked pellets have been calculated both analytically and by numerical methods. As the radial and transverse pellet cracks open, the tendency of the cladding to stretch preferentially over them is reduced by frictional sliding at the pellet-clad interface. The magnitude of slippage is dependent upon the coefficient of friction between the pellet fragment and cladding, the angle between adjacent opening cracks, and the normal force across the cladding wall. The frictional forces opposing sliding are intensified by a high contact pressure, and thereby the strain concentration in the cladding over opening crack is increased.

Cladding strains due to thermal expansion and swelling of the fuel are concentrated by the pellet cracking and the pellet cladding interaction mechanism. This leads to a potential local thinning of the cladding which considerably reduces the endurance of fuel rods.

Numerical analyses have revealed the swelling of a pellet during a period at reduced heat rating increases its diameter so that when high heat rating operation is resumed and the pellet expands thermally, the cladding may suffer severe local strains and local thinning.

5 – AXIAL RATCHETTING OF FUEL AND CLADDING

The progressive extension or ratchetting of fuel rods has been observed under cyclic conditions of reactor power and system pressure. Ratchetting of fuel rods is essentially a two body interaction process consisting of the fuel and the cladding. A detailed study of governing mechanisms under which ratchetting can occur is complicated by the very diverse conditions under which fuel pellet interacts with the cladding. In the following section some important mecahnisms will be discussed in a qualitative manner.

Consider a long vertical fuel rod at same power level for which a gap exists between fuel and clad. The fuel is assumed to be a continuous rod in this simplified model. The clad may be assume to be at some constant temperature approximately that of the coolant. If the power level is increased causing the fuel to become hotter, it will expand axially and radially and interacting forces between fuel and clad can occur. The clad experiences circumferential and axial tension while the fuel experiences corresponding compression. The mutual axial forces are transferred by friction at the boundary.

If the road power is held at this level, these stresses begin to relax by high-temperature creep deformation. The clad creeps in tension and the fuel creeps in compression. However, due to the different creep characteristics of the fuel and cladding and nonlinear creep laws, residual axial forces may remain.

If after a certain history of power and system pressure either the power or the system pressure is reduced, the radial contact pressure between fuel and cladding can become sufficiently low so that the friction between fuel and cladding is overcome and irreversible relative axial movement can occur. The relative movement can occur as instantaneous elastic recovery of fuel and cladding as critical axial forces are suddenly removed, or it may happen gradually. The fuel will tend to consolidate by gravity as soon as the contact with the cladding is relieved.

In a new cycle fuel and cladding are again brought into contact by increase in power level or external pressure and will enter into contact at a new relative position. This cyclic relative movement between fuel and clad can be defined as a ratchetting process

The axial ratchet mechanism is shown in Figure 5.1.

There are many parameters which have an influence on the ratchetting characteristics of a fuel element. Some of these factors are: fuel geometry, such as pellet dishing; initial size of the fuel-cladding gap; factors affecting fuel or cladding creep, such as the porosity of fuel or the initial degree of cladding cold work; the tendency of the fuel to crack; and anisotropic properties of the cladding. The overall temperature and pressure conditions are primary parameters.

An additional factor indicated in Figure 5.1 is clad collapse. If the cylindrical clad shape is unstable at the operating pressures and temperatures, it becomes oval and is supported by the fuel at the minor axis. In this way some mutual axial forces can be generated even before the total fuel-cladding gap is filled by fuel expansion. The amount of ratchetting may be expected to increase as the critical pressure of cladding collapse decreases. Cladding collapse is discussed in detail in the next section.

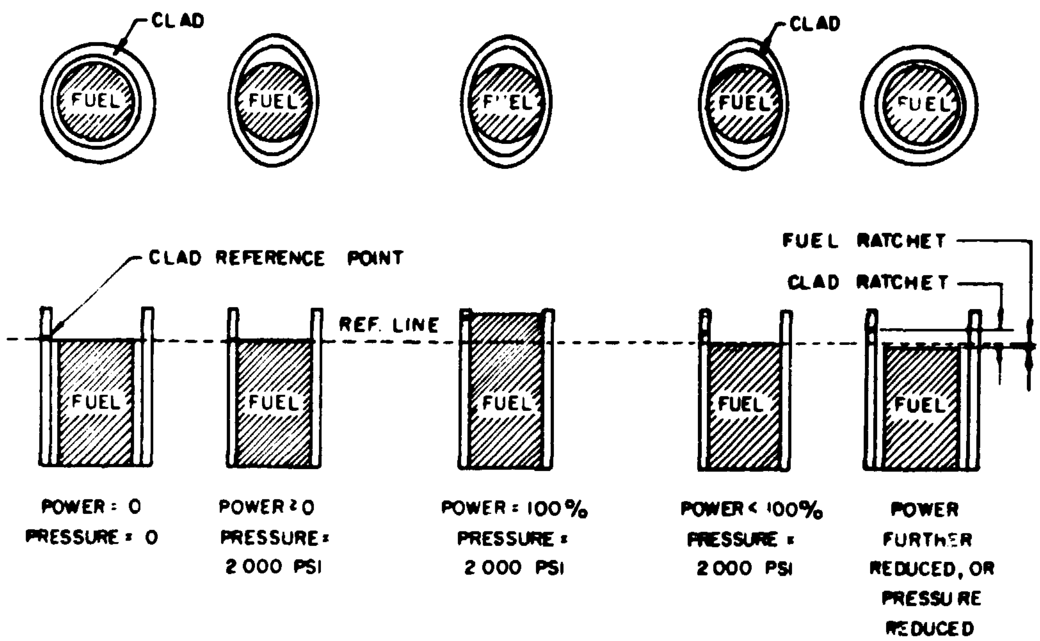

Figure 5.1 – Axial Ratchetting Mechanism[6].

6 – CLAD CREEP BUCKLING

A very important phenomena, particularly with fuel rod claddings which are designed for free-standing, non-iterative service, is creep-buckling (or creep collapse) of long thin-walled circular cylindrical shells under external pressure at elevated temperature. Creep is define as the slow deformation of solid materials under constant stress on load. At elevated temperatures all known materials experience a certain amount of creep, and this must be taken into account in structural strength calcualtions. Although creep is pronounced at elevated temperatures, it can occur within any temperature range[7].

A long, cylindrical tube subjected to a constant external radial pressure and to a reasonably high temperature for a sufficient length of time will eventually collapse, no matter how small the pressure is[19]. *Analyses show that the mechanism of this collapse is dependent on the presence of* initial deviations from perfect roundness in the shape of the cylindrical cross section. From the outset there exists a differential stressing of the fibers of the cylinder wall. A timewise change in ovality occurs as a consequence of creep deformations arising from tangential compressive and tangential bending stresses produced by uniform external pressures acting on the initially oval tube.

In virtually any production lot of cladding tubing, the most prevalent imperfection will be the "as fabricated" ovality. Standard cladding dimensional tolerances permit a small amount of ovality in each tube. This aspect provides a realistic basis for the use of ovality-creep relationships for calculating the time-dependent conditons for creep buckling instability.

7 – FUEL PERFORMANCE ANALYSIS COMPUTER CODES

Now that several important phenomena of the behavior of pellet-filled, long cylindrical fuel rods have been discussed, the integral fuel element analysis methodology will be examined.

The emphasis in the development of fuel element analysis computer programs is placed on predicting events such as: 1) cladding strains due to fuel thermal expansion and fuel swelling; 2) product gas release and fission product gas; 3) the effect of internal gas pressure on fuel-cladding interfacial pressures and heat transfer; and 4) the stress relaxation in the cladding. In brief, the fuel element computer programs attempt to examine the interactions between the various competing phenomena taking place in a fuel element under irradiation. The major quantity of interest is the strain and deformation of the fuel element cladding.

A simplified schematic of the interdependence of variables to be considered in computer programs for the analysis of pellet-filled fuel elements during irradiation is shown in Figure 7.1.

For the purpose of illustration, the LIFE-I computer code, developed at Argonne National Laboratory, will be discussed.

The LIFE-I computer code is designed to predict the in-pile thermal-mechanical behavior of cylindrical, fast-reactor fuel rods as a function of the reactor operating history. In particular, LIFE-I has been designed to predict the following as a function of time and axial position: 1) temperature distribution; 2) thermoelastic, creep, and swelling deformations of the fuel and cladding; 3) fuel restructuring and hol pressing; 4) fission product generation and migration; and 5) migration of plutonium in the mixed-oxide fuel.

The fuel element geometry is shown in Figure 7.2

The coolant pressure exerts an external load on the cladding. An additional axial force may also be specified. An initial gap between the fuel and cladding is allowed for pellet fuel, and the gap is allowed to open or close sequentially as a function of the specified reactor operating conditions. When the gap is open, the plenum pressure is exerted between the fuel and cladding. When the gap is closed, a finite coefficient of friction may be specificied for the fuel-cladding interface so that the axial elongation of the fuel column may be different from that of the cladding. The central void which develops in the fuel during operation is assumed to be open to the plenum so the plenum pressure loads the fuel internally.

A simplified flow chart of LIFE-I is shown in Figure 7.3.

The radial temperature distribution is obtained by dividing the fuel and cladding into any specified number of radial zones. For the gross mechanical analysis, the fuel is divided into three radial zones, corresponding physically to the temperature dependent different microstructure regions of the fuel. The cladding forms the fourth radial zone. For stress-strain calculations, the three fuel regions and the cladding region are treated as concentric cylinders with the average thermal and mechanical properties of each region determined by averaging and interpolation.

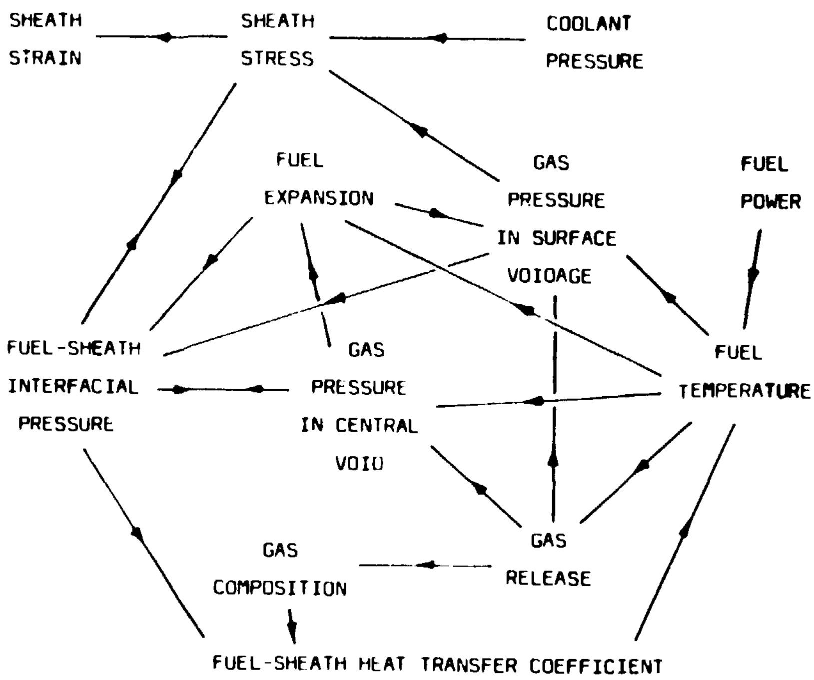

Figure 7.1 – Schematic of the Interpendence of Variables Considered in a Fuel Modeling Computer Program (A → B Denotes that a Change in A Affects B)[15].

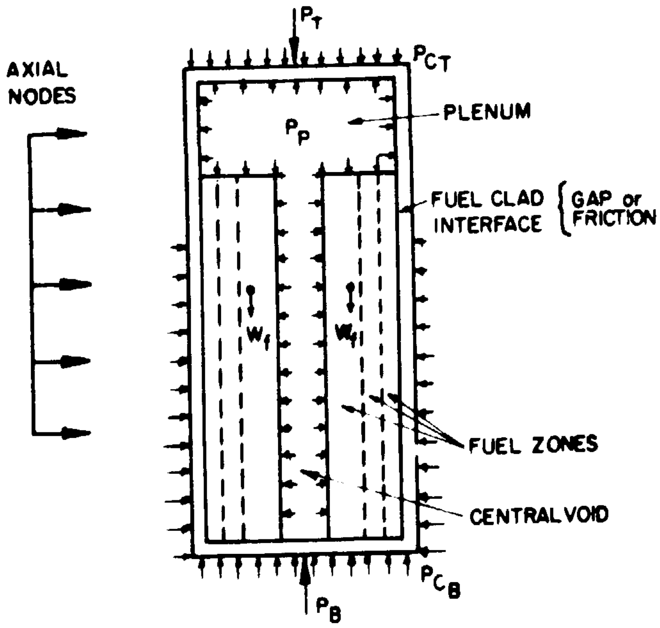

Figure 7.2 – Fuel Element Axial Cross-Section Model Utilized in the LIFE-I Computer Code[10].

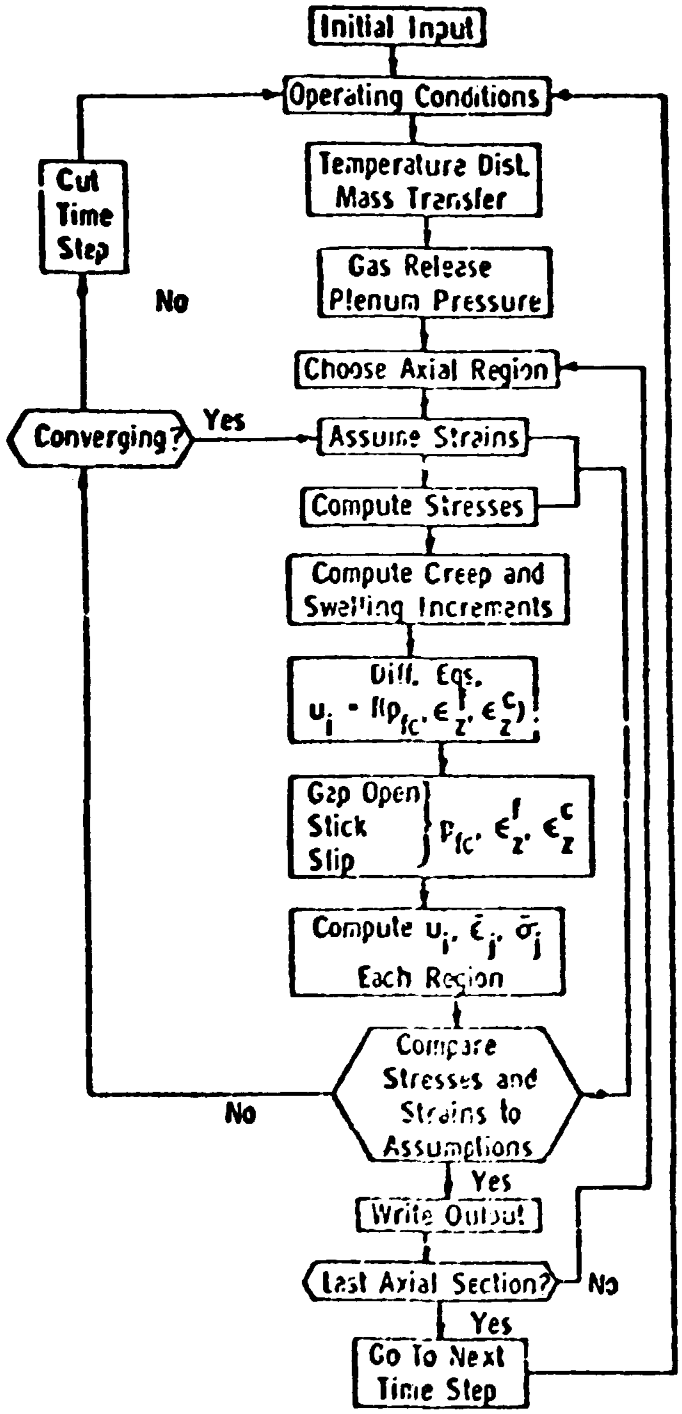

Figure 7.3 – Simplified Flow-Chart for the LIFE-I Compute Code[10].

RESUMO

Este trabalho apresenta uma visão geral dos fenômenos mais importantes considerados na análise do desempenho de pastilhas durante a operação de um reator nuclear. São considerados fenômenos tais como reestruturação e aumento de volume do combustível, liberação de gases de fissão, trincas radiais das pastilhas, etc. Todos estes fenômenos são interdependentes. A fim de ilustrar os métodos de an^lise dos diversos fenômenos o programa de computador LIFE-1 é discutido em detalhe.

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