THE BACO FUEL ROD ANALYSIS COMPUTER PROGRAM

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ABSTRACT

This contribution describes the fuel performance simulation code BACO("BArra COmbustible").The current version is mainly applied to predict the performance of a self standing fuel rod section in pressurized heavy water reactors;however it can be easily extended to every fuel rod type.The code includes models for the elastic,thermal,linear and non linear creep deformation as well as for the redensification,swelling and cracking of the oxide fuel pellet and for the anisotropic thermal,elastic and plastic deformation of the cladding. The temperature distribution and fission gas release pressure are also calculated at the different steps in the irradiation for the changing rod geometry.

A central finite difference method and the hypothesis of axial symmetry and modified plane strain allows to write the stress-strain increments at a time step as a finite system of non linear equations.The non linear system of equations is solved by linearisation and inversion of the resulting matrix at each time step.This approach provides an accurate and relatively fast solution if a sparse matrix inversion method is used.The stresses and the strain increments due to crack opening are used as the system unknowns.The boundary conditions and plastic laws are more easily written in terms of stresses rather than strains. Also the pellet-cladding contact pressure agrees with the calculated compressive radial stress at the interface.If this stress becomes tensile the contact is assumed to be broken

Some results representative of the code predictions are reported.These show the potentiality of the code to describe the stress and strain at different points of the rod and times of irradiation.The importance of using a pellet fracture model and an anisotropic description of the mechanical behaviour of a zircalloy cladding are discussed.The iso hoop stress loci at the cladding internal surface are plotted as a function of linear power and burn up.

1. INTRODUCTION

A fuel performance simulation code named BACO ("BArra COmbustible") has been developed. Elastic and plastic deformations as well as the thermal state of a fuel rod section are calculated by the code. The aim of its development is to provide a detailed description of the UO_2 - pellet / zircalloy - cladding system used in thermal reactors (i.e. the argentine power station Atucha). The numerical scheme of the code allows its extension to simulate the performance of any fuel pin; for example it is also being used to study LMFBR fuel pin capsule irradiations.

For the numerical modeling the hypothesis of axial symmetry and modified plane strain (constant axial strain) are adopted. Models for the elastic, thermal, creep, swelling and redensification strains as well as for the deformation due to axial and radial cracks are included in the description of the fuel pellet performance. For the cladding a model of the anisotropic thermomechanical behaviour is adopted, this includes elastic, thermal, plastic, creep and irradiation growth deformations. By using finite differences the stress - strain relations at the rod can be written as a finite system of algebraic equations. Some of the advantages of this scheme are: i) its application to a compose medium (i.e. fuel and cladding) ii) a simple treatment of the strain due to cracks, iii) an explicit inclusion of the material behaviour dependence on any physical parameters, including those self consistently calculated by the code as temperature, stress - strain state, etc , iv) the calculation of anisotropic distortions and v) a large numerical stability.

2. THERMAL AND MECHANICAL MODEL

The fuel pin irradiation life is divided into subsequent time steps. At a point of the fuel rod section the total strain increment in a time step is assumed to be:

$$\delta\varepsilon_i^T = \Sigma_j \delta\varepsilon_i^j + \delta\eta_i \qquad (1)$$

where i refers to any of the cylindrical main directions (i=r,θ,z) and j to the relevant distortions included (i.e. thermal, elastic, plastic, etc). Each $\delta\varepsilon_i^j$ is a explicit function of the main stresses and/or can also depend on other physical parameters as temperature, irradiation time, etc.

$$\delta\varepsilon_i^j = f_i^j \; (\sigma_k , T , t , - - -) \qquad (2)$$

The Prandtl - Reuss relations for the strains in isotropic media and Hill's equations{1} for the elastic, plastic and creep deformation of an anisotropic medium are used in order to express eq. (2) as a function of experimental data at the fuel and cladding respectively. $\delta\eta_i$, at the right of eq. (1), is the strain increment due to the eventual existence of a crack propagating normal to the i direction.

Under the hypothesis of axial symmetry and modified plane strain the distortions in the directions r and θ reduce to:

$$\varepsilon_r = \partial u / \partial r \qquad \text{and} \qquad \varepsilon_\theta = u / r \qquad (3),$$

where u is the radial displacement. In this case the equilibrium condition can be written

$$\partial\sigma_r / \partial r + (\sigma_r - \sigma_\theta) / r = 0 \qquad (4).$$

Besides eqs. (1) to (4) appropriate boundary conditions (i.e. constant external pressure over the rod) must be adopted for solving the stress - strain state of a heat generating rod

For the thermal problem steady state conditions are assumed. At each time step the Fourier equation

$$q = - 1/r \, d(rK \, dT/dr)/ dr \qquad (5)$$

is then solved for the temperature T at every point in the pin. In eq.(5) q is the heat generated per unit volume (a function of r within the fuel and null at the cladding) and K is the thermal conductivity, which is itself an explicit function of the temperature and other physical parameters.

3. CODE STRUCTURE

For the calculation the axial section of the rod is divided into circular concentric rings. Within a central finite difference scheme the eqs.(1) to (4) are written for the stress - strain at each ring as a function of the stresses at the circumferences which bound the rings (radial mesh points). Using eqs.(3) the displacements u are removed from the system and only the main stresses at the mesh points and the axial strain increment $\delta\varepsilon_z^T$ remain unknowns. At each time step (t - t+δt) a linear system of equations can be obtained for these stresses by Taylor expanding eq.(2)

$$\delta\varepsilon_i^j = \Sigma_{k'} \, \partial f_i^j \, (\sigma_k, T, t, -, --) / \partial\sigma_{k'} \Big|_{\substack{\sigma = \sigma(t) \\ T = T(t) \\ - - \\ - -}} (\sigma_{k'}(t+\delta t) - \sigma_{k'}(t)) \qquad (6)$$

This approach to the problem of linealization has been also proposed by Wilmore and Hayns{2}. The matrix that results by replacing (6) into (1) to (4) is sparse and can be inverted by using very efficient numerical methods {3}.

In order to introduce in the calculation the strain $\delta\eta_i$ due to cracking of the pellet, it is assumed that, when at a mesh point a predetermined fracture stress is attained in the θ or z direction, the inside ring is cracked in that direction (cracks normal to the r direction are not included in the calculation). The main tangential or axial stress at the point is now fixed as a boundary condition (i.e. gas pressure) and the increment in strain due to "cracking" must be determined from eqs.(1) to (4). This means at each time step the problem unknowns are the stresses σ_i at the uncracked rings external boundaries, the crack strain increments $\delta\eta_i$ at the cracked ones and the total axial strain increment, which under the hypothesis of plane strain is the same for each mesh point. If the accumulated crack width in a ring becomes negative the crack is assumed to have closed or healed depending on the local temperature. If the pellet has a fabrication dishing this can be simulated by an initial distribution of open axial cracks.

The boundary conditions over the fuel rod section are constant temperature and coolant pressure at the cladding external surface. Whenever there is a gap between fuel and cladding the calculated internal gas pressure is assumed to act over the internal cladding and external pellet surfaces. During the irradiation this gap may close and those surfaces touch each other. The stresses at the fuel and the cladding are now coupled through an unknown contact pressure (p_c). The fuel - cladding system is now solved with the conditions of equal normal stress σ_r over the last mesh point of the pellet and the first one of the cladding ($\sigma_r = -p_c$) and equal radial displacement u of these points (by (3) this is equivalent to impose the equality of ε_θ).The gap is assumed to open if the contact pressure at a given step becomes tensile.

For obtaining the temperature distribution eq.(5) is integrated with the boundary condition of constant temperature at the external cladding surface and with the rod geometry which results from the distortion calculation at the last succesful time step{4}.

The stability and convergence of the numerical scheme obviously depend on choosing a sufficiently small time step.As usual there is a compromise between accuracy and computer time for the calculation.In BACO the step length is automatically determined by: i) the creep rate,ii) the velocity of the crack tip penetration (no more than one ring can change from being"cracked" into "uncracked" or viceversa in a single step), iii) the percentage of variation of the contact pressure, iv) the plastic deformation rate of the cladding and v) the power rate.

As several codes for simulating fuel behaviour are based on a finite difference scheme {2} it is worthy to end this section by remarking some aspects of the method not thoroughly discussed in the literature.We have in a previous work {5} compared the central finite difference scheme with forwards or backwards differences alone against the analytic solution of a thermoelastic problem.There it was concluded that central differences give the most appropriate solution from the point of stability and convergence.This scheme allows then for a relative small number of points being necessary for an accurate calculation.However a last word of caution is necessary:the central differences must be formulated insuring that the equilibrium condition (4) and the strains in eqs.(1) to (3) when expressed in finite differences correspond to a point located inside each ring.In the previous work {5} we have expressed those at the mesh points.There as one of the points agrees with the pellet or cladding external radius a backward difference must be performed at this point.This in turn introduces spurious radial oscillations in the solution for long times of irradiation.

4.APPLICATIONS

Some characteristic results will be shown in this section.In the first example the importance in the code predictions of including a fuel fracture model will be discussed.We shall afterwards stress the influence of including the mechanical anisotropy in modeling the cladding.This can be of paramount importance in thermal reactors with zircalloy cladding.

A pre-pressurized rod of UO_2 fuel with zircalloy cladding is simulated.No central fabrication hole nor dishing is supposed to exist in the fuel pellet and its external radius at room temperature is of 5.31 mm.The cladding external radius is of 5.95 mm and the internal one of 5.40 mm,leaving an initial cold gap of .09 mm.The rod has an initial internal He pressure of 17 Atm at room temperature and the coolant pressure is of 120 Atm with a temperature of 305C. A power cycle as sketched in Figure 1 is simulated as a function of the fuel stay in the reactor or equivalently its burn up.This cycle resembles the one suffered by a fuel rod at the Atucha reactor where the fuel is changed from one channel to another during operation.For the calculations that follow W_1 (Figure 1) is fixed at 250 W/cm and Bu_1 at 2500 MWxd/Ton.

In Figure 2 the radial dependence of the calculated hoop stress at the fuel pellet is compared for a run where no pellet cracking was allowed against a normal one.Two residence times are chosen for the comparison,t_1 at 88% of the initial power up ramp and t_2 at the end of the fuel stay in the second channel (Figure 1).Much larger,irrealistic stresses are always found when no cracking is allowed.In this case at the end of the stay (t_2) the creep at the fuel relaxes part of the stresses built into it,compare for example the dotted line ($t=t_2$) in Figure 2 with the full one ($t=t_1$) at the center of the fuel.However if cracking is allowed at t_2 the stresses are fully relaxed to almost a hydrostatic condition,not only in the cool,cracked,external region but in every region of the pellet.

Two different runs of the code are performed for W_2=550 W/cm (Fig.1),in one isotropic mechanical behaviour is assumed for the cladding while in the other the cladding is anisotropic.Anisotropy is assumed in the thermal expansion,the elastic distortion,the creep and plasticity laws and an irradiation growth law is adopted {6}.For plasticity and creep the same laws,

$$\varepsilon_{eq}=f(\sigma_{eq}) \qquad \text{and} \qquad \dot{\varepsilon}_{eq}=g(\sigma_{eq}) \qquad (7)$$

where ε_{eq} is the equivalent strain and σ_{eq} the equivalent stress defined in Table I,are adopted in either approximation.The coefficients of anisotropy as well as the thermal and elastic coefficients are reported in Table I. In Figure 3 the hoop stress at the internal cladding surface and the permanent radial displacement(creep+plastic) of the external cladding surface are plotted as a function of fuel burn up.It is seen that before the fuel-clad gap closure a larger creep down of the cladding results in the anisotropic approximation than in the isotropic one;this determines an earlier contact in the first case.On the other side,after contact and a relatively long residence time,a larger relaxation of the tensile hoop stress takes place in the anisotropic approximation.

It is frequently asserted that the amount of data emanating from a code calculation is formidable.There is always the problem of how to transfer those data to a design engineer or to a reactor operator.This is the reason for the increasing popularity of graphical approaches to the fuel performance predictions {7}.Within an equivalent approach we have drawn the predicted iso hoop stress loci for the internal cladding surface of a fuel which goes through a power cycle like the one in Figure 1. The idea is that,if there is some chance of fuel failure by pellet clad interaction,a value of hoop stress can be defined below which the probability of failure is practically null.These loci provide then the residence time for which the code predicts that a given hoop stress value is reached at the internal cladding surface as a function of the power at the second reactor channel.The input parameters to use the plots are power at the first channel and burn up at that channel.These same loci plots are useful to show the difference in hoop stress predictions within the isotropic and the anisotropic cladding approximations.In Figure 4 the resulting loci for different W_2 values and for the power cycle previously described are reported within either approximation.

5.SUMMARY AND CONCLUSIONS

In this paper we have described the mathematical framework of the code BACO.This code has proved to be numerically stable,rapidly convergent and to predict the mechanical behaviour of a fuel rod section in an acceptable physical form.This mechanical description is a very detailed one considering the restrictions imposed by the axial symmetry and plane strain approximations necessary for reducing the amount of computer time.The advantage of the finite difference numerical method adopted is that space or temperature dependent laws for the rod mechanical and thermal behaviour are explicitly included in the calculation and the complex links between these laws are automatically dealt by the code. It is then very efficient for evaluating the relative importance in the fuel performance of the different phenomena taking place at the rod components during irradiation.

Some demonstrative results are shown in section 4. In Figure 2 the importance of including in the calculation a self consistent fuel fracture mode is shown. The model proposed predicts a large relaxation of the stresses in the whole pellet, these reach almost the hydrostatic value after some residence time. The influence of allowing for the cladding anisotropy is shown in figures 3 and 4. It is seen that the use of anisotropic mechanical laws for the calculation which are consistent with a zircalloy cladding predicts a much larger creep down and a smaller value of the cladding hoop stresses than the equivalent isotropic approach for the same cladding material.

References

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Table I

	Thermal Expansion Coefficients $\{10^{-5}/K\}$			Young Moduli $\{10^3$ MPa$\}$			Poisson Ratio	Coefficients of Anisotropy{8}#		
Model	α_r	α_θ	α_z	E_r	E_θ	E_z	$\nu_r=\nu_\theta=\nu_z$	a_r	a_θ	a_z
Anisotropic	.871	.4441	.6721	82.32	68.6	65.17	.325	.52	.48	.87
Isotropic	.66	.66	.66	68.6	68.6	68.6	.325	.50	.50	.50

$$\varepsilon_\alpha=\frac{\varepsilon_{eq}(\sigma_{eq})}{\sigma_{eq}}\{a_\beta(\sigma_\alpha-\sigma_\gamma)+a_\gamma(\sigma_\alpha-\sigma_\beta)\} \qquad \alpha,\beta,\gamma=r,\theta,z$$

$$\sigma_{eq}=\{a_r(\sigma_\theta-\sigma_z)^2+a_\theta(\sigma_r-\sigma_z)^2+a_z(\sigma_r-\sigma_\theta)^2\}^{0.5}$$

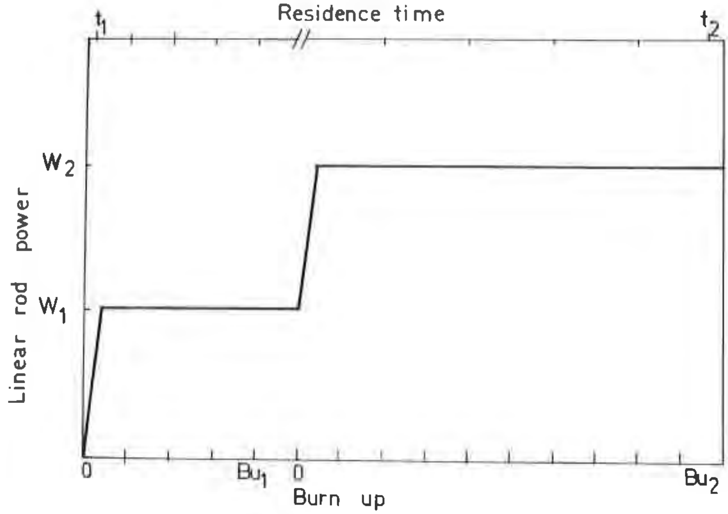

Figure 1: Power cycle

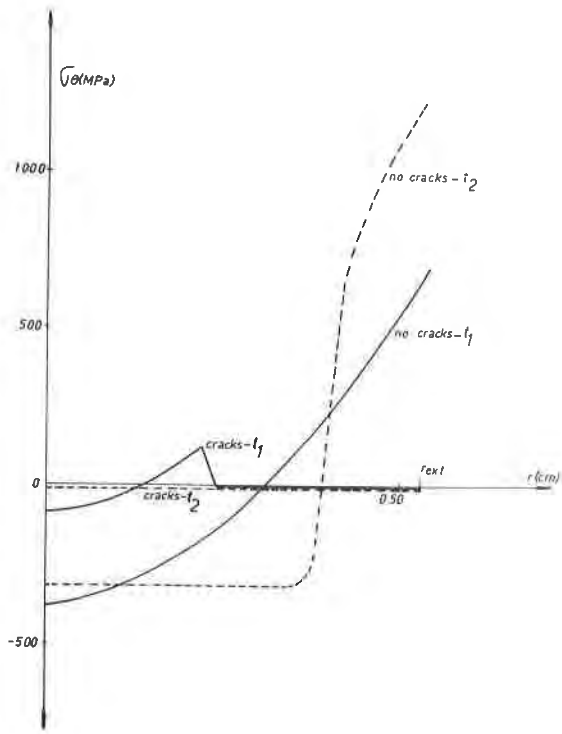

Figure 2: Hoop stress(with and without a fuel fracture model) as a function of the pellet radius at two different residence times.

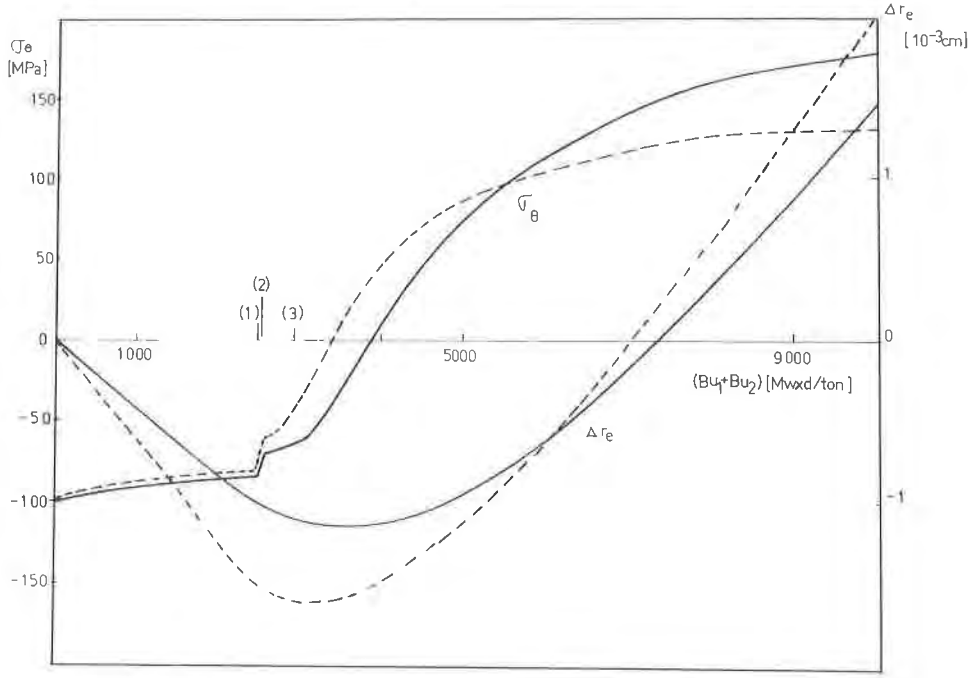

Figure 3: Hoop stress σ_θ at the internal cladding radius and permanent radial displacement Δr_e of the rod radius as a function of total burn up. Full lines correspond to the isotropic model for the cladding and dotted ones to the anisotropic description.
(1) Power rise from W_1 to W_2.
Contact: (2) in the anisotropic case and
(3) in the isotropic.

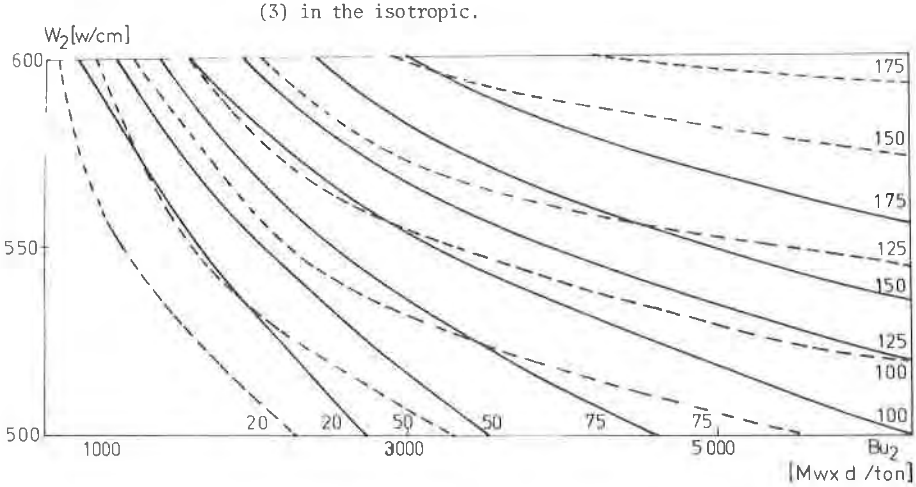

Figure 4: Iso hoop stress loci against linear power at the second fuel location in the reactor and fuel burn up at that location. Full lines: isotropic model for the cladding; dotted lines: anisotropic.
The parameters of the curves are the values of σ_θ in MPa.