SIMULACIÓN DEL COMPORTAMIENTO DE BARRAS COMBUSTIBLES MEDIANTE EL DESARROLLO SIMBIÓTICO DE CÓDIGOS QUASI 2D EN DIFERENCIAS FINITAS Y HERRAMIENTAS 3D DE ELEMENTOS FINITOS

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Key words: Nuclear fuel, Fuel modeling, BACO, MECOM.

Abstract. La geometría de una barra combustible nuclear con pastillas de UO_2 es un compromiso entre la intención de maximizar el contenido de UO_2 y minimizar el perfil de temperatura teniendo en cuenta el comportamiento termo-mecánico, la economía y la seguridad en la operación del combustible nuclear durante y después de su irradiación. El código BACO es utilizado para la simulación del comportamiento de una barra combustible en condiciones de irradiación. La última versión fue desarrollada en la División DAEE (CAB, CNEA). Mejoramos los resultados de BACO usando un conjunto de herramientas desarrollados en la División MECOM (CAB, CNEA). La dupla BACO, código quasi 2D basado en un esquema de diferencias finitas, y las herramientas 3D de MECOM que emplean el método de elementos finitos, constituye un sistema completo para el análisis 3D del estado tensión-deformación de una pastilla bajo irradiación. Usamos combustibles CANDU y PHWR MOX para ilustrar el acuerdo cualitativo entre cálculos y datos experimentales. El objetivo de este trabajo es optimizar la geometría de la pastilla combustible.

SIMULATION OF THE NUCLEAR FUEL RODS BEHAVIOR BY MEANS OF THE SYMBIOSIS OF FINITE DIFFERENCES QUASI 2D CODES AND 3D FINITE ELEMENTS TOOLS

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Abstract. The geometry of a nuclear fuel rod with UO₂ pellets is a compromise among the intention to maximize UO₂ content and minimize the temperature profile taking into account the thermo-mechanical behavior, the economy and the safety of the fuel management during and after irradiation. The BACO code is used for the simulation of a nuclear fuel rod behavior under irradiation. The last versions were developed at the DAEE Division (CAB, CNEA). We enhanced the findings of BACO by using the complete set of tools developed at the MECOM division (CAB, CNEA). The coupling of BACO, a quasi 2D code based on a finite differences scheme, and the 3D MECOM tools based on the method of finite elements constitutes a complete system for the 3D analysis of the stress-strain state of the pellet under irradiation. CANDU and PHWR MOX fuel will be used to illustrate the qualitative agreement between experimental data and calculations in order to optimize the shape of the pellet.

1 INTRODUCTION

A fuel element is a set of fuel rods assembled with structural components like "grids" and "spacers". Each fuel rod is a tube (or "cladding") made of Zircaloy filled with UO₂ pellets. The starting point for the design of an UO₂ pellet is a simple cylinder. However, that shape for a pellet under irradiation leads to a "bamboo" way for the fuel rod due to the temperature profile (see Figure 1). The pellet l/d relation (length / diameter) is optimized in order to minimize that geometric behavior. A few modifications in the cylinder are introduced in order to reduce the pellet to pellet axial stresses and the PCMI (Pellet-Cladding Mechanical Interaction) at the top and at the bottom of the cylinder. Those stresses are reduced by using "dishings", "shoulders" and "chamfers" in the cylinder (see Figure 2). In fact, we reduce stresses by sectioning the parts of the pellet where the maximum deformations are present, obtaining an optimized UO₂ pellet. The study of conic, flat and/or hollow pellets under irradiation were presented in several papers plus the study of the relative influence of the variation of l/d and the size of dishing, chamfer and shoulder. We intend to maximize the UO₂ content, minimize the temperature profile and reduce the PCMI (Pellet-Cladding Mechanical Interaction) and PCI-SCC (Pellet Cladding Interaction - Stress Corrosion Cracking) effects taking into account the economy and the safety of the fuel management during and after irradiation.



Figure 1: I) As fabricated nuclear fuel rod, II) fuel rod under irradiation at a low power (and low temperature profile), III) fuel rod under irradiation at a high power (and high temperature profile).

Figure 2 : Fuel rod pellets parameters.

Diameter gauge measurements of the rods have revealed the presence of increased dimensions at the pellet ends during and after power ramps resulting from the wheatsheaf of hourglass or bamboo shape adopted by the pellets. A detailed diameter measurement reveals the presence of a secondary ridge at the middle of the pellet (see Figure 3 where a good example of the diameter change during power ramp at the pellets is presented)¹. The change is due to the poor thermal conductivity of the UO₂ fuel and the differential thermal expansion caused by radial temperature gradient of the pellets. Ridge formation to a greater or lesser extent is found in all small gap rods when power ramped. The axial displacement of the

pellets and the changing in the axial power profile of long fuels as PWR and BWR could lead to the formation of ridges at different heights of the rod (ratcheting). Figure 4 shows the PIE (post-irradiation examination) of the fuel pellets after irradiation. The small length of CANDU and experimental fuel rods guaranties a good positioning of pellet ends with the ridge due to the absence of ratcheting. We could expect the presence of clear ridges in these types of fuels when the gap is closed due to power ramping, swelling, creep-down or a combination of them. This particular situation is the usual condition under irradiation for the CANDU fuel rods where the cladding is collapsible and no gap is present.



Figure 3 : Real radial deformations profile of nuclear fuel rod. "Ridges" and "secondary ridges" are clearly shown¹

Figure 4: Transversal and axial macrographies of an irradiated fuel rod ¹.

The thermo-mechanical behavior of a nuclear fuel rod under irradiation is a complex process where too many coupled physics and chemical phenomena are present. The BACO code (BArra COmbustible, Spanish expression for "fuel rod") was developed at the Atomic Energy National Commission of Argentina (CNEA, "Comisión Nacional de Energía Atómica") for the simulation of the behavior of nuclear fuel rods under irradiation. BACO uses a quasi two-dimensional approach and with its use several 3D (three dimensional) topics as the stress-strain state can be explained. Nevertheless, we enhance the BACO code results by using "ad hoc" tools based on a finite elements scheme developed at the MECOM and DAEE Divisions (Bariloche Atomic Center, CNEA). The temperature profile and the boundary conditions, among others, are calculated with BACO to be inserted as input data in the MECOM tools. Then we calculate the 3D stress-strain state and the deformations of the UO₂ pellet. The MECOM tools include the same laws for elasticity and thermal expansion than the BACO code. We find the shape of the pellet under irradiation showing the stress profiles, the bamboo effect and others 3D effects as the presence of the secondary ridge and the radial profile of a fuel rod.

We will show the symbiosis between BACO and MECOM tools by using CANDU, and PHWR MOX fuels as input data. The results will show the good agreement between experimental data and calculations particularly for the radial profile of pellet after irradiation. The coupling of BACO $^{2, 3, 4, 9, 18, 19 \text{ and } 20}$ and MECOM $^{5, 6, 7 \text{ and } 8}$ tools constitutes a powerful system for the analysis and design of nuclear fuel pellets taking into account the best combination of l/d and the dimensioning of dishing, shoulder and chamfers. Innovative or

unusual pellet shapes can be analyzed by using these "ad hoc" tools against the actual tendency to use commercial software adapted for nuclear applications.

2 THE BACO CODE

2.1 BACO code description

The BACO code structure and models have already been described in the reference [2], including steady state and transient thermal analysis. Nowadays, the number of instructions is about twelve thousand FORTRAN 90 lines. Data post-processing and the coupling with 3D calculation using finite elements improve the output of BACO and the analysis of results. The last versions of the code were developed in the DAEE Division (CAB, CNEA). We participated in several international programs of comparisons between codes and experiments²¹. At present we are participating in the Co-Ordinated Research Project on Fuel Modeling at Extended Burnup II organized for the International Atomic Energy Agency (IAEA)²².

On modeling the UO_2 pellet, elastic deformation, thermal expansion, creep, swelling, densification, restructuring, cracks and fission gas release are included. For the Zry cladding, the code models elastic deformation, thermal expansion, anisotropic plastic deformation, and creep and growth under irradiation. The modular structure of the code easily allows us to add different material properties. It can be used for any geometrical dimensions of cylindrical fuel rods with UO_2 (or MOX) pellets (either compact or hollow, with or without dishing) and Zry cladding.

A special feature of the BACO code is to include a complete treatment of the fuel with or without mechanical contact of the pellet surface and the clad, in any irradiation stage, and then could be fully used to model self standing clad sheets (like LWR and Atucha fuel rods)³ or collapsible clad sheets (like CANDU and Embalse fuel rods)⁴, without special changes in the physical models triggered by the user input. BACO includes excellent compatibility for PWR²¹, BWR²¹, WWR²², MOX¹³ and experimental fuels²¹.

Fuel rod power history and either cladding or coolant outside temperatures must be given to the program. Rod performance is numerically simulated using finite time steps (finite differences scheme). The code automatically selects time steps according to physical criteria. Temperature profiles within pellet and cladding, main stresses at pellet and cladding, radial and axial crack pattern in the pellet, main strains and hot geometry of pellet and cladding, change in porosity, grain size and restructuring of the pellet, fission gas release to the free volume in the rod, trapped gas distribution in the fuel and in the UO₂ grain boundary, internal gas pressure and current composition of the internal gas, dishing shape evolution, are calculated. The output of the code contains the distribution along the rod axis of these variables.

2.2 Numerical treatment

Summary of assumptions made in the numerical treatment implementation:

- Cylindrical symmetry.
- Pellet and clad are divided into circular concentric rings.
- Axial symmetry and modified plane strain (constant axial strain) is adopted. The threedimensional stress-strain problem is reduced to a quasi-two-dimensional problem.
- Behavior equations integrated with a finite difference scheme.
- Fuel pin irradiation life is divided into subsequent finite time steps for the temporal integration.

2.3 Mechanical treatment

It is assumed that during the time interval $(t_0, t_0 + \delta t)$, the strain-stress increments can be expressed as the superposition of the strain-stress increments due to the different existing deformation mechanisms. Thus, the strain-stress state at $t_0 + \delta t$ can be obtained as,

 $\epsilon = \epsilon_0 + \delta \epsilon$

where:

 ε_0 : is a stress-strain magnitude at t_0 , and

 $\delta\epsilon;$ is the corresponding variation during the small time step δt

The equations to be integrated are, essentially, the compatibility equation of each ring, the equilibrium equation, and the Hook's generalized equations, subject to the appropriate boundary conditions. That means a system of seven coupled differential equations. The finite differences approximation leads to a non-linear system of algebraic equations, which is linearised through a Taylor expansion. The previously described system for a given time increment can be solved for the main stresses by direct matrix inversion.

2.4 Thermal treatment

The temperature distribution in the pellet or cladding for the strain state results from solving Fourier equation for steady state heat transmission. The boundary condition is a fixed temperature at the cladding external surface and the heat source is known.

The details of the mechanical and thermal treatment and the pellet, cladding and constitutive equations are available in reference [2].

3 MECOM TOOLS

The 3D finite element (FEM) calculations were performed with a set of tools developed at the Computational Mechanics (MeCom) Division at the Bariloche Atomic Center (CAB), CNEA. Basically, these are grouped in two software packages, "acdp95" ⁵ and "gpfep99" ⁶, kindly made available to us by its main developers.

The package "acdp95" includes tools for mesh generation and optimization⁷ and a complete collection of visualization programs. Non structured meshes composed of tetrahedral elements for arbitrary geometries can be obtained. Visualization tools for viewing meshes and the FEM solutions over these meshes (scalar and vectorial) are available.

The package "gpfep99" is the FEM solver. In fact, it is a system to generate FEM solvers. It is distributed in source form (written in FORTRAN 77). It is possible at the user to write a block in a subroutine to implement the physical model under study. In our case, we wrote no more than three hundred lines of code (100 for the elasticity problem, 100 for the stress calculation and 100 for the Von Mises stress calculation). "gpfep99" can handle time dependent and non linear problems and there are several types of elements (not only linear tetrahedral) implemented. There is also a paralellizable version⁸. The solutions obtained with "gpfep99" can be visualized with the "acdp95" tools.

4 BACO + MECOM

A first approximation of the fuel rod behavior is made using the BACO code. The treatment is quasi-bidimensional at this stage but using the complete set of models and options of BACO mentioned above. We generate the input data for the MeCom Tools, in particular the geometry of the pellets and the boundary conditions for a particular time of the irradiation. The geometry of the pellet includes the dishing evolution⁹, the shoulders and the deformations calculated by BACO. The boundary condition is the gas pressure. The temperature profile field is an input data. Porosity, crack pattern and thermal conductivity can be included into MeCom for a best estimation of its thermal behavior. The result is the 3D deformed geometry of the pellets and the 3D maps of stresses and strains. At present we are just including elasticity and thermal expansion into the FEM solver. It is not included a way for stress release like creep, cracks opening and/or plasticity. The stress-strain state results in an extreme condition of behavior with the highest stress in the pellet more than the most demanding condition. BACO runs and is developed under a Windows environment by using Digital FORTRAN and/or Lahey FORTRAN compilers. MeCom tools runs under LINUX operative system. "Cygwin" makes the coupling of them. "Cygwin" is a Linux-like environment for Windows. Then, we do not need to change the system to use both sets of codes.

5 A 3D CANDU FUEL PELLET SIMULATION APPROACH

We analyze the 3D behavior of a normal CANDU fuel pellet without chamfers for illustrative purposes. We use the temperature profile of figure 5 and other parameters calculated with BACO for a CANDU fuel during high demanding conditions of operation. The mesh for finite elements calculation is included en figure 7. We are using more than 15000 elements. The von Mises stresses are included in figure 7 where three different views facilitate the analysis. The stress state obtained shows high values due to the absence of a mechanism to relax them, as crack opening and/or creep. The highest stresses are located at the shoulders of the pellet where more cracks are usually present.



Figure 5: CANDU pellet temperature profile.



Figure 6: 3D CANDU pellet calculated with BACO + MeCom tools. Radial deformations are emphasized.



Figure 7: Mesh and von Mises Equivalent stress of the pellet.



Figure 8: Radial deformations in a CANDU Fuel Pellet.

Figure 8 presents the radial deformations of the CANDU pellet. Here, the highest deformations are located at the shoulders where the ridges are usually present. Figure 8 includes a plot with the radial profile of the pellet. The calculated way follows the way of the experimental radial profile of CANDU fuels. We assume that the cladding profile is the same than the pellet profile. This is a strong assumption but it is sustained for the collapsibility of the CANDU fuels. The height of the ridges has a smaller value than the ones reported in the literature but it keeps a high qualitative value¹⁰. Finally in figure 6 we draw the 3D pellet by using the previous calculation.

6 PHWR MOX EXPERIMENTAL SUPPORT

The irradiation of the first prototypes of PHWR MOX fuels fabricated in Argentina began in 1986. These experiments were made in the HFR-Petten reactor, Holland. The six rods were fabricated in the α Facility (CNEA, Argentina)^{11, 12, 13}. This set of irradiations is included in the IFPE of the OECD¹⁷. We use one of those irradiations as experimental support of the codes. An irradiation of PHWR extended burnup was performed with the MOX fuel rod named A.1.3. The burnup of extraction was 15000 MWd/tonUO₂, three times the usual burnup at end of life of a PHWR NPP, including a demanding power ramp at EOL (End Of Life). The radial power profile during the base irradiation, before the power ramp, presented a maximum value at the bottom of the fuel rod. The temperature profile calculated with the BACO code is sketched at figure 9. The maximum value of temperature was achieved at the bottom of the rod. The power ramp was performed at the Pool Side Facility of the HFR-Petten Reactor. We flip the position of the MOX fuel, thus the maximum value of power and temperature are located in the opposite side of the rod. The new temperature profile is included in figure 10.



Figure 9: Temperature profile of the MOX fuel A.1.3 before ramping at EOL (End Of Life), section 1 at the bottom of the fuel rod.



Figure 10: Temperature profile of the MOX fuel A.1.3 at the top of the power ramp at EOL (section 1 at the top of the fuel rod).



Figure 10: Pellet profile of five axial sections of the MOX fuel A.1.3 before ramping at EOL.



Figure 11: Pellet profile of the five axial sections of the MOX fuel A.1.3 at the top power ramp at EOL.



Figure 12: Fuel rod profile of the MOX fuel A.1.3 before and after the power ramp. Experimental (top curves) and calculated (lower curves) values.

We calculate the stress-strain state of the MOX fuel rod before and after the final ramp by using the previous temperature profile and the calculated inner pressure. The radial deformations of the pellets are included in figures 10 and 11. Here we observe the "bamboo"

effect and the presence of an expected small secondary ridge in the 5 sections of the rod.

Figure 12 includes the fuel rod profile of the MOX rod after the power ramp and the representation of the stack of pellets. It is a strong assumption to correlate the experimental deformations of the MOX fuel with the pellets profile calculated with BACO + MeCom. Nevertheless, there is a strong correlation from a qualitative point of view and the clad wall thickness had only a small effect on the ridge height as was experimentally observed¹⁴.

7 CANDU FUEL EXPERIMENTAL SUPPORT

At this point we will analyze several fuel pellets with real and/or unusual geometric shapes. The pellet of figure 7 will be used in this analysis and it will be named (a) "normal" pellet, a CANDU fuel pellet with a shoulder and without "chamfers". Figure 13 includes the following pellets: (b) a flat pellet without dishing, (c) a hollowed pellet without dishing, (d) a standard CANDU fuel pellet, (e) a conic pellet with a dish at the top, and (f) a "barrel" (double conic pellet) with one dish. We include the radial deformation as the difference between the present radius and the original one for each pellet.



Figure 13: The meshes of experimental CANDU fuel pellets of Ref [10] and their radial deformations. ΔR is the difference between the present radius and the original one.

The radial pellet profile of the pellet with the dishing (see pellet (a) of figure 7) presents more deformation than the "flat" pellet without dishing (see pellet (b) of figure 13). This agrees with experimental evidence included in reference [15] (see figure 14).

The presence of "chamfers" in the pellet (see the standard CANDU pellet (d) of figure 13)

disables the presence of the zone of the pellet with the highest deformation. In fact, the chamfers reduce the radial deformation along the entire pellet as we expect by design.



Figure 14: Fuel rod diameter profile before and after the experimental irradiations of type (a) fuel pellets with one dishing and type (e) fuel pellets ¹⁰.

The presence of a central hollow in the pellet (see pellet (c) of the figure 13) reduces the bamboo shape and the radial deformation along the pellet.

The most radical pellets as the (e) and (f) of figure 13 reduce the ridging but there is a no contact with the cladding at the end of the conic sections. These pellets reduce the content of UO_2 and they do not keep the concept of a collapsible cladding for CANDU fuels. The radial fuel rod profile after irradiation of type (e) pellets shows the depression of the cladding in the conic section and the ridges in the cylindrical zone of the pellet (see figure 14). Cladding depression calculations are beyond the scope of this work, however the cylinder and the middle position of the pellet agree with them.

These observations among others agree with the experimental observations^{10, 16}.

8 AN APPROACH TO A 3D PELLET CRACKS SIMULATION

An approach to a cracked pellet analysis can be initiated with the two cracks defined in figure 15: (a) a single crack at the top of the pellet, and (b) a single crack crossing from the

top to the bottom of the pellet. The radial profile of the single cracked pellet (a) shows a maximum value of the radial deformation close to the crack. The minimum deformation is present in the opposite side of the crack (see figure 15). The case of a full crack (b) presents the maximum deformation close to the cracks but, the minimum value is located at $\pm 30^{\circ}$ of the crack. These curves of minimum values for the radial deformations looks equivalents in both types of cracked pellets. The maximum value of the deformation reaches the same value for both type of cracked pellets. However, the type (a) pellets present that maximum at the top and there is a strong decrement of its deformation along the height of the pellet.



On the other side, for type (b) pellets, the radial deformation near the crack is greater than the deformation 30° apart from the crack along the full length of the pellet. In this case, both deformation profiles looks very similar with an increment of the secondary ridge close to the middle of the pellet. It is clearly shown that the presence of the "real" cracks in type (a) pellets increases the ridging at its location but it reduces the deformation along the rest of the pellet. This point of view is in agreement with the previous radial profiles calculated for different pellet types without the presence of cracks where the ridges were underestimated. Figure 17 shows the von Mises equivalent stress for three type (a) cracked pellets with different penetration values. We observe stresses concentration at the vertices of the cracks. It is clearly shown a stress release effect due to the presence of the crack. This analysis could be continued with the inclusion of several cracks in the pellet in order to reduce stresses. The inclusion of these cracks in the previous shapes is beyond the qualitative purpose of the present analysis.



Figure 17: Top view of the von Mises equivalent stress for three cracked type (a) cracked pellets with different penetration values.

9 PELLET DESIGN

We mentioned above that the optimization of a fuel pellet geometry could be approached with the finding of the best l/d relation. This is in agreement with several experimental results presented in the literature^{10, 16}. Figure 16 includes two types of pellets with l/d = 0.5(a) and l/d = 1.5 (b). We find that the ridging is reduced when l/d is reduced with a perfect agreement with experimental observation. Figure 18 includes the experimental values and our calculations with different l/d values. There is not a clear correlation between experimental results and BACO calculations because the experimental evaluation of the fuel ridging was not clearly explained in the measurements performed in the references, however for a qualitative purpose we see that the global trends of the measurements of the mean ridge height are the same than the radial deformations of the pellets. We extend the qualitative agreement by varying shoulders and chamfers as it is shown in figure 18. The increment of l/dover more than 1.3 produces the maximum value of deformation. The decrement of l/dproduces a convergence to the lowest values for the radial deformation. These trends are present in all the BACO calculations.



Figure 18: Correlation between experimental mean ridge height and radial deformation (ΔR) calculated by varying the *l/d* relation.

10 PRESENT STATUS

The present situation of the BACO + MECOM tools development is defined in Figures 19 and 20. The figure 19 corresponds to a standard CANDU fuel pellet (type (d) in figure 13). The plot includes the fuel rod profile after irradiation (see figure 14), the BACO + MECOM calculation for the equivalent pellet and a reference line with no change in the radius profile (before irradiation). The experimental fuel profile is more steeped than the calculated pellet profile. However, the secondary ridge and the bamboo shape are presents in the plot with comparable values. The experimental ridges at the pellet tops are greater than the calculated one because we are not taking into account the effect of pellet cracking and we are just including elasticity. The pellet and the cladding are in contact due to the collapsibility of the CANDU fuel rods, then we expect an equivalent result from calculation and experiments.

The figure 20 is a CANDU fuel pellet with a conic section (type (e) in figure 13). We can define two zone in the pellet profile: the cylinder and the conic section. We repeat the previous behavior at the cylinder (top side of figure 20). The radial profile at the conic section presents a depression due to the forced no contact situation and the collapsibility of the cladding, here we are out of the scope of this work. However the qualitative and quantitative values obtained for the BACO + MECOM are in good agreement.





Figure 19: Type (d) pellet radial profile calculated with BACO+MECOM and the fuel rod radial profile of an equivalent fuel before and after experimental irradiation.

Figure 20: Type (e) pellet radial profile calculated with BACO+MECOM and the fuel rod radial profile of an equivalent fuel before and after experimental irradiation.

11 CONCLUSIONS

We presented the symbiosis between BACO and MECOM tools using CANDU and PHWR MOX fuels as input data. At present, we are including elasticity in the 3D evaluation and all the set of models of BACO. The results show a good agreement between experimental data and calculations particularly for the pellet radial profile after irradiation. The coupling between BACO and MECOM tools constitutes a powerful system for the analysis and design of nuclear fuel pellets taking into account very different shapes, the best combination of l/d, dishing, shoulder and chamfers parameters. The influence of the cracks was established appointed as a way to increase ridging and to release stresses. We mention: a) the reduction of the deformation of hollowed pellet, b) the absence of ridging when conic shapes are used for the pellets, c) the increment of ridging when a dishing is present in the pellet, d) the reduction of ridging due to chamfers, and e) the trends of radial deformation by the variation of l/d, as interesting examples by using BACO + MECOM. Innovative or unusual pellet shapes can be analyzed by using these "ad hoc" tools against the actual tendency to use commercial software adapted for nuclear applications. Typically we calculated a pellet ridge height of ~10 µm in good agree with the PWR fuel¹ of the figure 3 and the CANDU fuels of the l/danalysis. However the MOX fuel and the "unusual" CANDU pellets has a reported ridge height of more than the double size of the calculated ones but in a good qualitative agreement. A complete pre-characterization and detailed irradiation history are needed for an improved result. We emphasize the economical aspect of these tools where a few running of the codes can reduce the number of irradiations in an expensive programme. They also provide a frame for the analysis of the experiments.

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