AN APPROACH TO THE SIMULATION OF THE BEHAVIOUR OF ACCIDENT TOLERANT FUELS

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ABSTRACT

The BaCo code for the simulation of the behaviour of a nuclear fuel rod under irradiation conditions is presented by taking into account the initiative called "Accident Tolerant Fuels" (ATF). The need of a safer fuel design using new materials is emphasized. These materials mean a complete new set of parameters and models for each new fuel design. The evaluation of these properties is provided by the "Multiscale Modelling of Materials" methodology (M³), in particular the BFS method, within an international cooperation environment. Excellent agreement between experimental results and M³ calculation were found for FeCrAl and SiC. Preliminary results of the expected behaviour of several ATF are presented. In particular, it was found that the integrity of solid SiC claddings could be compromised when substantial mechanical interaction with the fuel pellet occurs during the irradiation. Finally a neutronic approach of a PHWR ATF fuel is done.

1. Introduction

The Fukushima accident in 2011 increases the need of better alloys and/or materials for Fuel Elements (FFEE) in order to have greater tolerance to failures as established in Nuclear Power Plant (NPP) design bases, including Loss of Coolant Accident (LOCA) and other serious accidents. These challenges also incorporate the use of other FFEE materials and design as carriers of fissile isotopes. These goals should be achieved without abandoning the concepts of assembly of cylindrical rods and of each fuel rod as a tube or sheath containing cylindrical pellets. Other concepts such as dispersed or spherical fuels are not precluded in principle, but the licensing can be much more difficult and expensive. From these requirements arises the initiative called "Accident Tolerant Fuels" (ATF) whose challenges can also be exploited by Gen-IV (Generation IV International Forum) designs.

A relevant stage in the development of this type of fuel is the need of new models and simulation codes of its behaviour under normal conditions and under irradiation together with advanced calculation techniques and computational tools that effectively assist the design of conventional fuels and new ATF designs.

The scarce experimental information of the proposed new materials can be complemented with first principles or *ab initio* calculations that enable a deep theoretical support comparable to the one usually intended for experimental support, producing an authentic synergy between experiments and theoretical models. The disadvantage of these studies is the absence of reliable data in comparison with the current available database for UO_2 and Zr alloys. The methodology of Multi-Scale Modelling of Materials ("M³") was proposed as a way to partially fill the gap between the empirical codes and the needs for new materials data.

Theoretical research using *ab initio* computational codes is important not only for benchmarking against available databases but also to predict the thermo-mechanical properties of new fuel structures and cladding materials. In this context, material parameters

obtained from M³ are being included in the structure of the BaCo code to incorporate those ATF materials in the simulations for preliminary assessments. So far the gathered information is promising and useful for future designs of fuels more tolerant to accidental scenarios.

The onset of experimental validation is based on demanding cases presented in IAEA coordinated research projects ("CRP") such as D-COM, CRP FUMEX I, II and III, CRP FUMAC, CRP ACTOF [1-4] and the IFPE ("International Fuel Performance Experiments") [5] of the NEA/OECD among others, providing a selection of cases of experimental irradiation supporting the validation of codes and models. It is clear that international cooperation is convenient, if not mandatory, for the proposal of new safer fuels.

2. The BaCo code

BaCo is a code for the simulation of the thermo-mechanical and fission gas behaviour of a cylindrical fuel rod under operation and storage conditions. The modelling of the UO_2 pellet includes elastic deformation, thermal expansion, creep, swelling, densification, restructuring, cracks and fission gas release [6, 7]. For the Zry (Zirconium alloy) cladding, the code models elastic deformation, thermal expansion, anisotropic plastic deformation, creep and growth under irradiation.

Originally centred on PHWR fuels as the CANDU [8] and Atucha [9], BaCo's capabilities also extend to PWR [2-4], BWR, WWER [10], MOX [11], experimental advanced prototypes and unusual fuels. The evolution of the code was historically oriented to the Nuclear Programme led by the Argentine National Atomic Energy Commission (CNEA), namely the fuel of the Integral PWR CAREM [12-14], PHWR MOX fuels [4, 10] and advanced PHWR ones (as the CARA fuel) [15].The BaCo code can be used for any geometrical dimensions of a cylindrical fuel rod with UO_2 pellets (either compact or hollow, with or without dishing) and Zry cladding. The modular structure of BaCo is compatible with different material properties for all components of the fuel rods (as SiC and FeCrAl for the cladding and USi and UN for the fuel, provided there are available data).

The code includes additional tools such as the software package for finite elements 3D calculations and the statistical analysis for advanced fuel designs by taking into account the as fabricated fuel rod parameters and their statistical uncertainties. BaCo allows for the calculation of a complete set of irradiations as for example the calculation of a full reactor core. BaCo 3D tools [20, 21], statistical analysis [28], full core calculations [9] and graphical data post-processing improve the code performance and the analysis of the calculations [7].

The BaCo code can simulate the storage conditions in order to obtain most safe fuel designs [16-19], by continuing the calculation after the irradiation period, taking into account the new conditions, in particular the change of cooling temperature and external pressure.

3. ATF ("Accident Tolerant Fuels")

Currently, the nuclear industry has begun to require the development of new fuels that are resistant to severe accidents while maintaining high operational performance. New materials and new designs of fuel elements converge in the ATF initiative.

We analyse the physical properties of the proposed materials for fuels and claddings. In addition, the parameters of these materials are obtained by *ab initio* and M³ methods, in particular for SiC, which are incorporated into the BaCo and BaCo3D [21] codes for the preliminary assessment of an ATF under irradiation and dry storage.

From the point of view of the performance of the services and the conditions of the FFEE, the most important properties are related to the heat transfer and their mechanical properties. If we increase the resistance to corrosion and oxidation, we decrease the generation of heat and hydrogen, among others, and then we are increasing the tolerance of a fuel element to those severe accidents. That is, it aims to strengthen the aspects that will significantly delay

the start of a failure or an advanced accidental stage. From the point of view of thermal conductivity there are clear disadvantages of UO_2 versus UC and UN, on the other hand offset by its high melting temperature.

4. M³ ("Multi-Scale Model of Materials") support

For non-traditional fuels, in particular ATF and Gen-IV fuels, available data for the development of new materials can be obtained through the M³, a methodology that provides the theoretical approximation to the modelling of the properties of the materials through *ab initio* methods, molecular dynamics, Kinetic Monte Carlo and finite element calculations.

5. M³ Methodology applied to β-SiC

Silicon carbide is presented as a large family of crystalline structures called "polytypic". This manifests the ability of this compound to crystallize in numerous modifications that can be described as different stacking sequences of the same unit layer. Reference [24] describes and analyses the calculations of the elastic constants and the thermal properties of the β-SiC in particular the Young's modulus, the specific heat and the linear thermal expansion coefficient. Reference [24] shows a good agreement with other authors.

6. M³ Methodology applied to FeCrAl

6.1 BFS method for alloys

The BFS method is a quantum approximate method suitable for applications to multicomponent systems [26, 27]. The method is based on the notion that the energy of formation of a given atomic configuration (with unrestricted number and type of elements) can be defined as the superposition of the individual atomic contributions, $\Delta H = \Sigma\varepsilon_i$. Each individual contribution ε_i consists of a strain energy term, ε_i^S, which accounts for the change in geometry relative to a single monoatomic crystal of the reference atom *i*, and a chemical energy term, ε_i^C, where every neighbour of the reference atom *i* is in an equilibrium lattice site of a crystal of species *i*, but retaining their chemical identity. To completely separate the effect of changes in geometry (strain energy) from changes in chemical composition (chemical energy), a reference term, $\varepsilon_i^{C_0}$, is added in the calculation of the chemical energy, computed in the same way as ε_i^C, but where the neighbours of the reference atom have the same identity as the reference atom. A coupling function, g_i, ensures the correct volume dependence of the chemical energy contribution (i.e., the chemical energy vanishes at large interatomic distances). The net contribution ε_i to the total energy of formation is then

$$\varepsilon_i = \varepsilon_i^S + g_i(\varepsilon_i^C - \varepsilon_i^{C_0}) \qquad (3)$$

The parameters needed for the calculation of the different contributions are easily determined using the Linearized Augmented Plane Wave method [28]. The single element parameters (for Fe, Al, and Cr) are obtained from the zero temperature equation of state of the pure bcc solids, while the interaction parameters needed for the calculation of the chemical energy are obtained from the energy of formation as a function of volume curves for each and every one of the bcc-based binary combinations of all the elements. A full description of the steps needed to compute the different terms in Eq. 3 can be found in Ref. [29]. Finally, temperature effects are obtained from large scale Monte Carlo simulations, described in detail in Ref. [26]. Previous relevant applications of the BFS method to nuclear fuels can be found in Refs. [30-32]. BFS was used in order to obtain basic material parameters as the linear thermal expansion coefficient, specific heat, bulk modulus and others.

7. M³ and Material Properties for the BaCo code

M³ provides BaCo with the required material parameters and theoretical support the experiments (see for example Figures 5 and 1). The parameters and their dependency with temperature are included in the BaCo code in order to get a preliminary assessment of the expected behaviour of nuclear fuel rods with ATF materials. The Figures 5 and 6 show the calculated values for SiC with QE (Quantum Espresso) and experimental measurements for the coefficient of linear expansion and the Young's modulus. The Figure 5 shows the BFS calculation for FeCrAl of the coefficient of linear expansion and the comparison with experimental values and our measurements for our first FeCrAl alloy developed in CAB-CNEA [22, 23, 35]. Excellent agreements were found for those materials in particular in the temperature range of operation of the nuclear fuel.

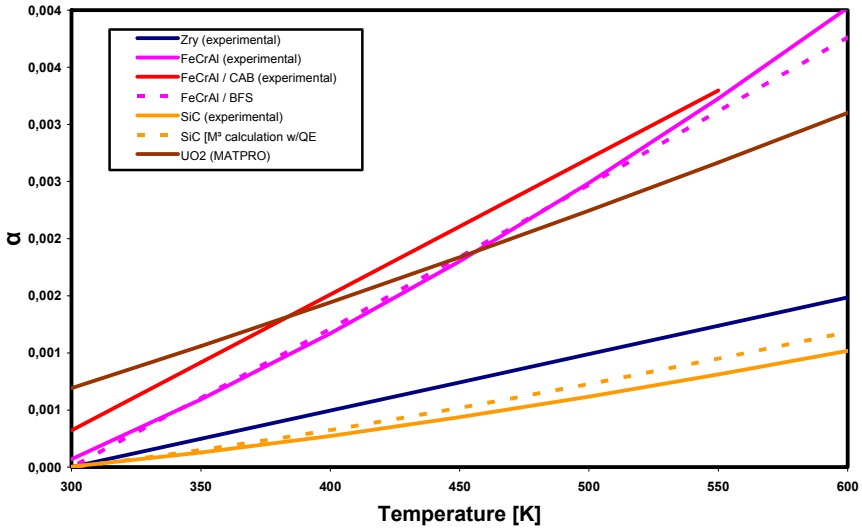

Fig 5. Coefficient of thermal expansion (α = ΔL/L(300K)) as a function of temperature for materials currently under study for ATF including our calculation with BFS for FeCrAl and QE for SiC).

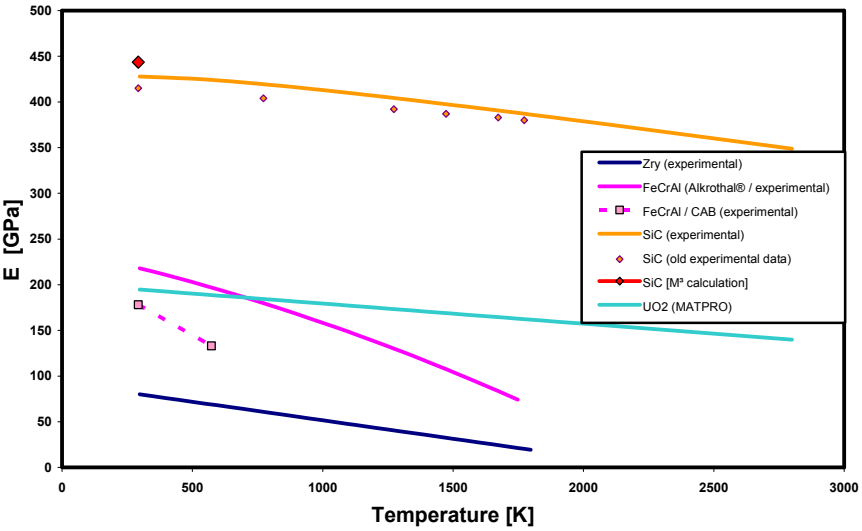

Fig 6. Young's modulus as a function of temperature including our calculation by M³.

7.1 An ATF with alternate claddings (SiC, FeCrAl)

The simulations were performed with a version of BaCo by using cladding material parameters from the open literature and the properties of SiC and FeCrAl calculated by the *ab initio* methods described in the previous section

As an example of these calculations, Fig. 7 shows the influence of the burnup on the central temperature of the fuel pellet of UO_2 with different cladding materials subject to a steady irradiation of 200 W/cm. This exercise is based on the proposals of the CRPs FUMEX I, II and III [2-4] of the IAEA where a very good agreement was found among the codes of the participants. The reduction in temperature for the case of Zry-4 from ~3 MWd/kgU is due to the PCI ("Pellet-Cladding Interaction") which improves the thermal conductivity and the transfer of heat from the pellet to the coolant. In Figure 8 we see the evolution of the pellet and clad radii using a SiC cladding, obtaining PCI to EOL ("End Of Life").

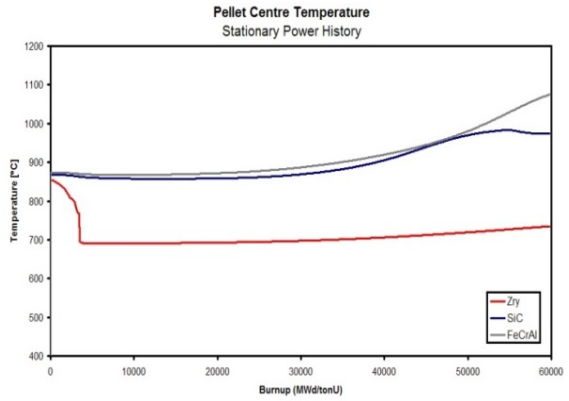

Fig 7. Central temperature of the UO_2 fuel pellet under steady state irradiation (200 W/cm) using three different cladding materials.

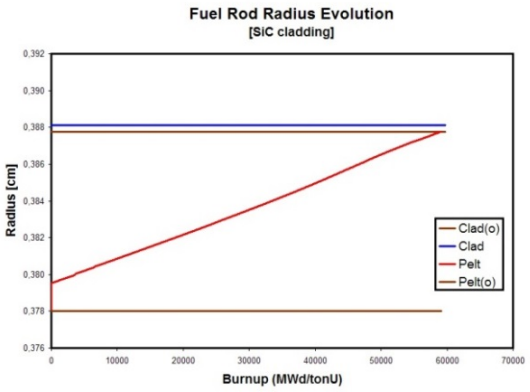

Fig 8. Evolution of the outer radii of a UO_2 pellet and internal radii a SiC cladding, where **Clad** is the "cladding inner radius", **Clad(0)** is the "as fabricated cladding inner radius", **Pelt** is the "pellet radius" and **Pelt(0)** "as fabricated pellet radius".

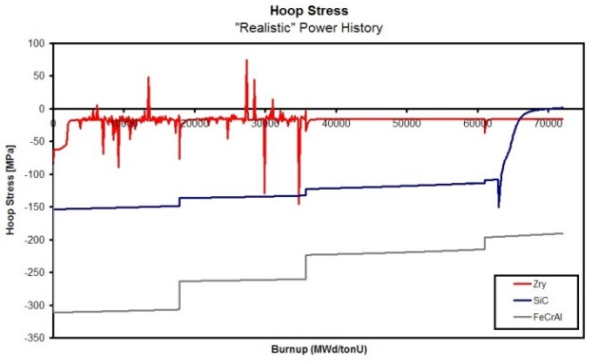

Fig 9. "Hoop stress" in Zry, SiC y FeCrAl claddings. CRP FUMEX II, Case 27(2d), provided by FANP.

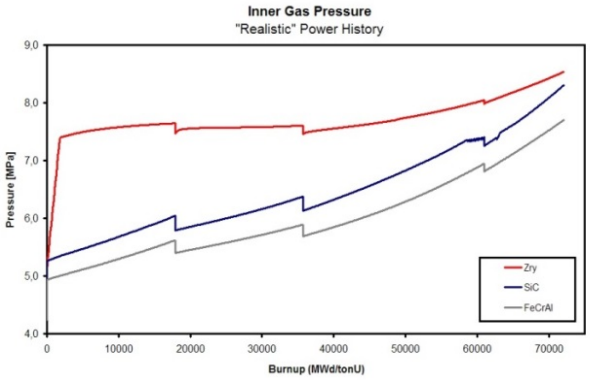

Fig 10. Internal pressure produced by the fission gases in the fuel rods with Zry, SiC y FeCrAl claddings.

A more realistic example corresponds to the "hoop stress" in Fig. 9, where the irradiation corresponds to a generic, conservative PWR power history, of an irradiation data provided by FANP ("Framatome Advanced Nuclear Power, Inc.", Case 27.2d) within the FUMEX II (Coordinated Research Project on Fuel Modelling at Extended Burnup II) of the IAEA [2-3]. The modelling starts at an average power of 350 W/cm followed by four power cycles at a decreasing level. The irradiation time is from ~1700 days to an extraction burn of ~70 MWd/kgU. Figure 10 shows the curves of the internal pressure of the free gases in the sheath (filling gases -He and gaseous fission products, Xe and Kr-). Thermal and mechanical interactions are important specially to take into account the influence of the free space inside the sheath on the pellet temperature. The highest pressure is obtained for Zry, which due to the PCI eliminates the free spaces between the pellet and the cladding due to cladding creeping down and the thermal expansion of the fuel pellet.

For comparison, the simulation was repeated for a fuel under dry storage conditions by using a WWER 440 fuel rod type from FUMEX II CRP (Case 9) irradiated in Kola 3 NPP, BC 007 of the FA 222 and assuming a SiC cladding. Figure 11 shows good agreement with previous calculations and similar general conclusions can be drawn. It can be seen that if using SiC cladding PCI should be avoided to ensure that the gap remains open. Alternatively, this failure can be prevented by using a cladding type SiC/SiC (inner solid tube covered with fibres). Figure 12 shows the evolution of the gap in which PCI is reached until EOL where it can be seen that the gap opens when storage starts.

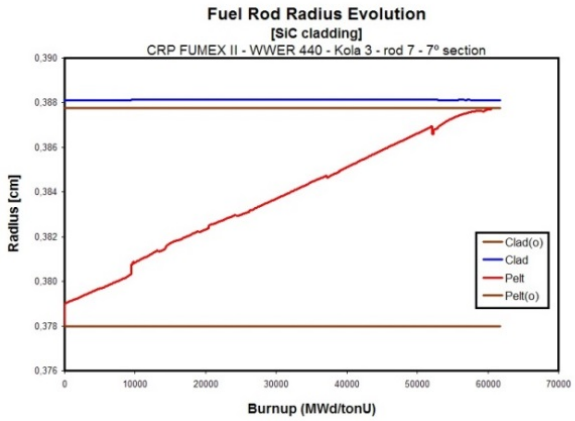

Fig 11. Evolution of radii of the pellet and the cladding in the most required axial section for a SiC fuel rod cladding.

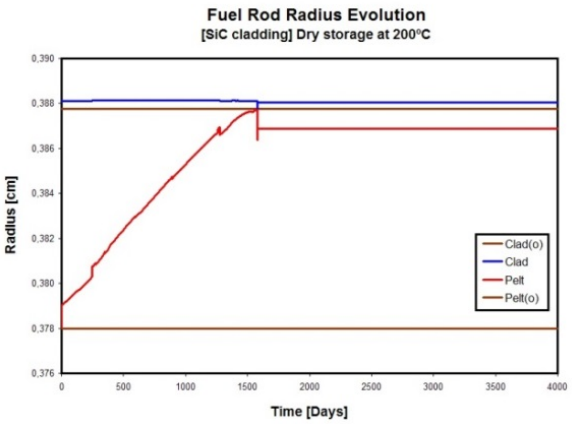

Fig 12. Evolution of radii of the pellet and the cladding during irradiation and in dry storage conditions at 200ºC. SiC cladding. Case 9 of the CRP FUMEX II of IAEA.

Figure 13 shows the gas pressure inside the fuel rod during irradiation. The outside pressure of the fuel rod corresponds to the coolant pressure. The inner pressure of the rod is lower than the pressure of the coolant during the irradiation stage as it is required for safety reasons. In turn, after irradiation the fuel rod is stored at normal pressure (1 atm) and a temperature of 200ºC is estimated.

The calculations plotted on Figs. 7-13 were performed by using the data input corresponding to the nominal parameters of the fuel rod and the reactor.

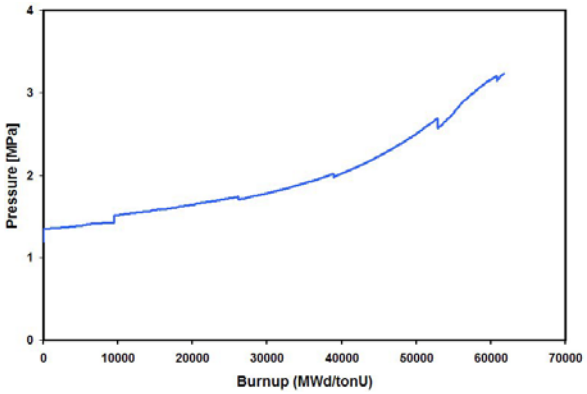

Fig 13. Gas pressure inside the fuel rod during the irradiation.

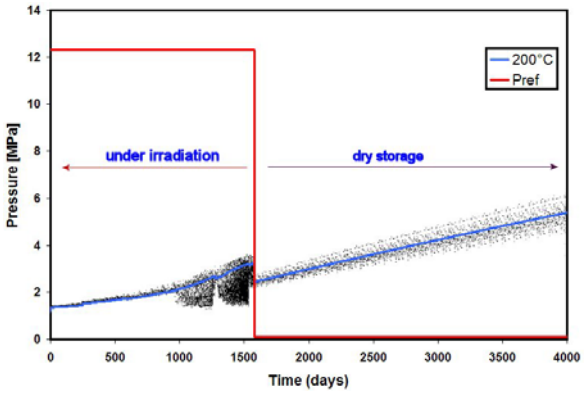

Fig 14. SA of the gas pressure calculation in the fuel rod including the boundary conditions (coolant pressure and ambient conditions) plus the nominal calculation and dispersion.

Figure 14 shows the dispersion of the results after the SA (Statistical analysis) is performed by using the Monte-Carlo technique taking into account the manufacturing tolerances. The rise of the gas pressure during the dry storage stage is due to the release of the fission

gases retained in the fuel pellets. Figure 15 shows the hoop stress of the cladding (tangential stress at the inner surface). A compressive and conservative tensile stress is found during irradiation whereas stress reversal is achieved at EOL. Figure 16 shows the statistical assessment of the pellet centre temperature. The big dispersion at high burnup up to EOL is due to the uncertainties in the PCI event.

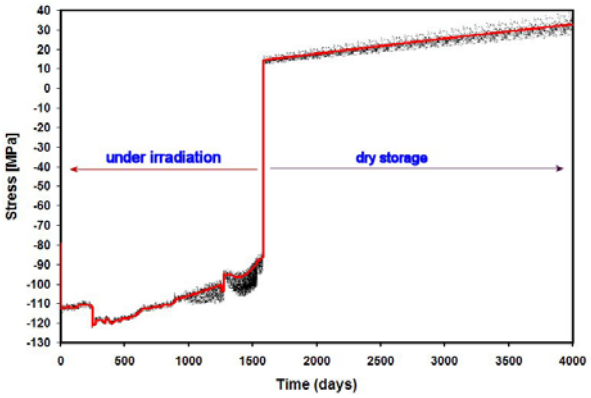

Fig 15. Statistical analysis of the hoop stress (tangential stress at the inner surface of the cladding). Nominal value and dispersion are plotted.

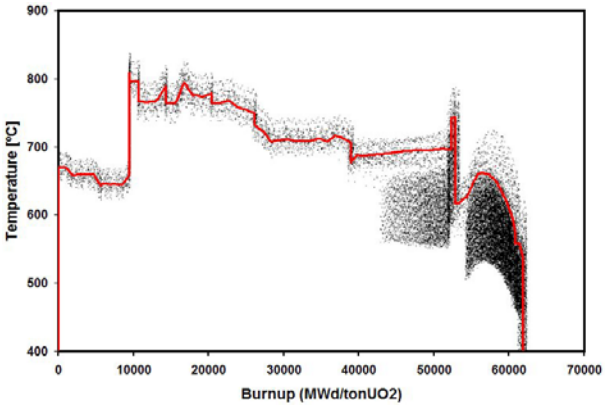

Fig 16. Statistical analysis of the pellet centre temperature at the most demanding axial segment of the fuel rod. Nominal value and dispersion are plotted.

7.2 An ATF with different fuel pellet materials

Some of the various new materials proposed in the literature for ATF are UN, UC, U_3Si_2, ThO_2 and ThC. As an illustrative example, Fig. 17 shows the BaCo simulation of the radial profile of pellet deformations for each material using the same temperature and pressure boundary conditions. Figure 18 shows the deformations of a solid chip and a chip with a central hole WWER type [27]. It can be seen that the presence of the hole improves the releasing of tensions and reduce the PCI.

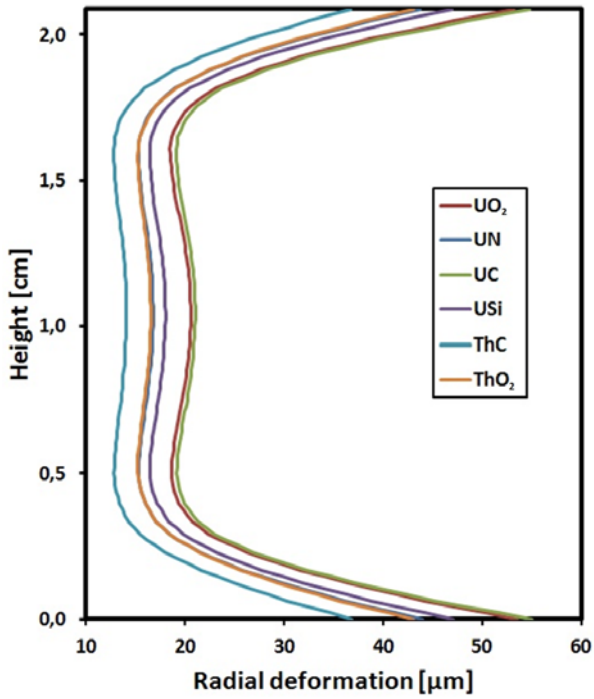

Fig 17. Radial deformations of fuel pellets with different materials under equivalent behavioural conditions of irradiation.

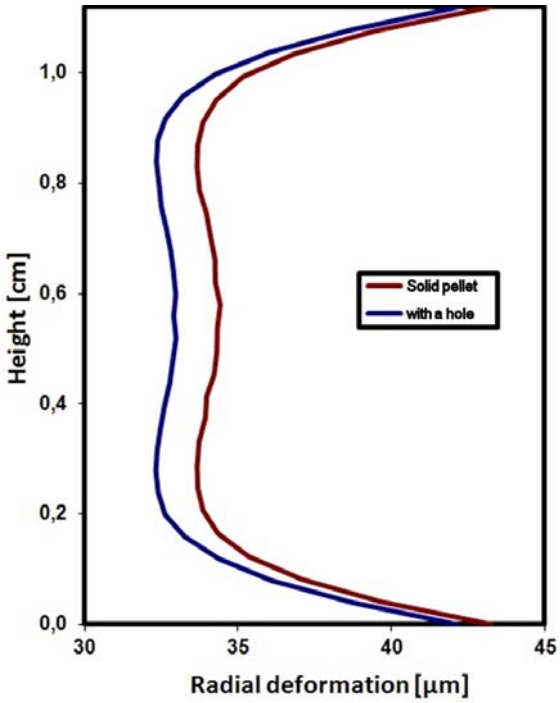

Fig 18. Radial deformations of UO_2 fuel pellets irradiated in equivalent conditions with and without a central manufacturing hole.

8. A proposal for an alternate ATF CANDU

8.1 Neutronic calculation of an ATF with a FeCrAl cladding

For the analysis of the feasibility of new fuel designs, either by implementing new materials or by improving the current irradiation cycles, the analysis of the neutronic of the system in question is required.

It was decided to implement the use of the DRAGON cell code [33] which allowed the first results to be generated within the project.

The analysed cladding material is FeCrAl, one of the alternatives that are being proposed to replace the current Zry clad commonly used in the nuclear industry. Its advantages are associated with the enormous experience in the steel industry, since it belongs to this family.

The implementation of a steel-based alloy in a CANDU reactor can improve the thermo mechanical properties of the cladding making possible an extension of burnup of the fuel element in a safe way.

The ATF initiative not only enhances the safety of the reactor operations but also could increase the burnup making each of them more profitable giving more gaining to the utility.

8.2 DRAGON code

DRAGON is a neutronic calculation code used to simulate the behaviour of neutrons at unit cell level or a fuel rod arrangement (a complete fuel element or a fraction of it). It is of the "Open Source" type and has all the functions that characterize a cell code [34].

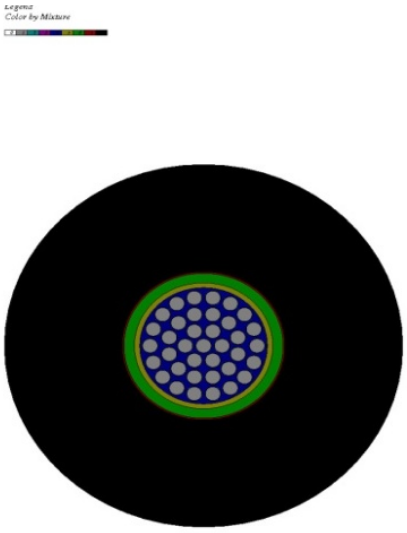

Fig 19. Post Script from DRAGON Code of the CANDU Lattice

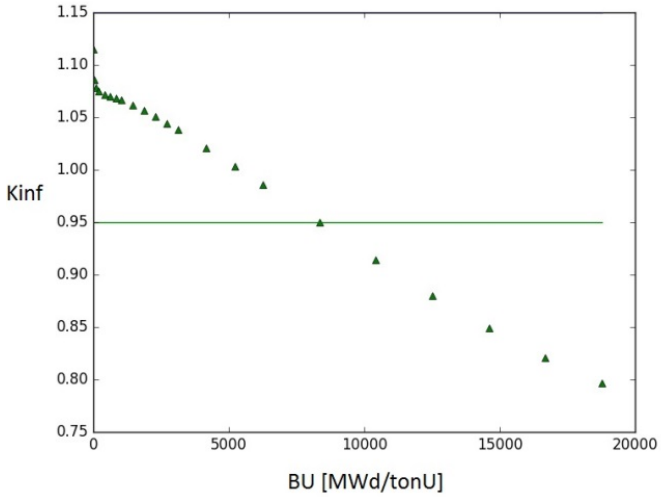

Fig 20. K_{inf} with an enrichment of 1.3% with FeCrAl clad.

8.3 FeCrAl in PHWR Reactors

The performance of the new materials in PHWR reactors should be evaluated, so, in order to do that, a comparative analysis of the results with different enrichments was done to a typical CANDU FE in a pressure tube as can be seen in Fig. 19.

As a result of the optimization, we found that the enrichment to maintain the same burnup as in the original design (that means that we just compensate the absorptions of the new alloy), is 1.3% of ^{235}U. In Fig. 20 the evolution of K_{inf} vs burnup is shown.

If we consider the possibility of decreasing the thickness of the cladding, we can obtain an extension in the life of the fuel element as we stated at first, or from another point of view, decrease even more the enrichment to decrease the cost of the fuel element.

The results obtained for this proposal, that is, with fixed enrichment in 1.3% and varying the thickness can be seen in Fig. 21.

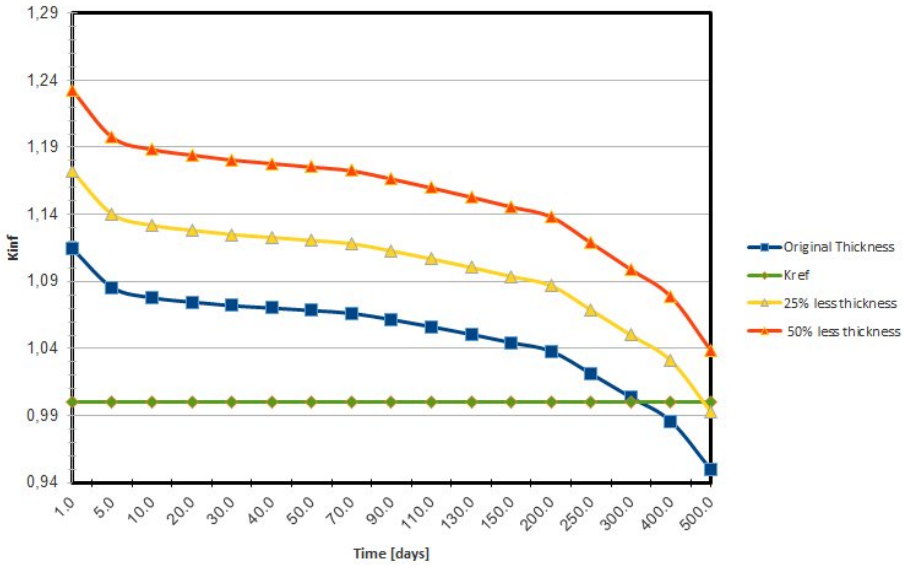

Fig 21. K_{inf} vs Burnup for different thickness of cladding for an enrichment of 1.3%.

9. Conclusions

The BaCo code is a powerful useful tool for the assessment of the behaviour of a nuclear fuel under irradiation conditions and dry storage. It was shown that the probabilistic sensitivity analysis is the appropriate method for understanding the influence of the uncertainties and as-fabricated tolerances of a nuclear fuel. We emphasized the role of the CRPs organized for IAEA as D-COM, FUMEX, FUMEX I, FUMEXII, FUMAC and ACTOF in order to promote the international cooperation into the field of nuclear fuel modelling and the development of fuel behaviour codes.

The M³ approach became a powerful tool in order for obtaining the data that at present is absent. M³ synergically provides a strong support for the nuclear fuel materials development as it was shown in the case of SiC and FeCrAl claddings. The basic calculations show a good agreement with the present data. A particularly relevant result is the importance of minimizing pellet-cladding interactions when solid SiC claddings are used.

It is reasonable to propose a first longer cycle of LEU (“Low Enrichment Uranium”) for a CANDU reactor with the benefits of making it more profitable and then start to change its cladding material to completely modify its fuel cycle introducing the enrichment technology but with new safety standards.

10. References

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