

ECONOMIC AND SAFETY IMPROVEMENT OF NUCLEAR FUEL CYCLE BY USING NUCLEAR FUEL CODES

Armando C. Marino^{1,2}, Edith L. Losada¹, Gustavo L. Demarco^{1,3}

¹ Comisión Nacional de Energía Atómica, Centro Atómico Bariloche, Av. Bustillo 9500, Bariloche, Río Negro, 8400, Argentina, marino@cab.cnea.gov.ar

² Instituto Balseiro, Universidad Nacional de Cuyo Av. Bustillo 9500, Bariloche, Río Negro, 8400, Argentina

³ Universidad Tecnológica Nacional, Facultad Regional Villa María, Córdoba, Argentina

ABSTRACT: *The developing of computer codes for the simulation of the behaviour and design of nuclear fuels is a wide field where the safety and the economy are evolved taking into account the basic issues of physics and direct engineering application. The BaCo code was developed in order to assist the nuclear fuel cycle in the area of nuclear fuel modelling, fuel designs, improvements in the performance of the nuclear power plants, fuel failures and safety analysis. The common sustenance of the code are the confrontation among experimental irradiations and other codes particularly into the research programmes of the IAEA as the CRP FUMEX I, II, III and ACTOF. Advanced materials and designs require the use of special techniques as the Multiscale Modelling of Materials (M³). Nevertheless a proper use of the old information of irradiation tests stored in databanks could assist those new developments. A basic description of the BaCo code and the use of present and historical experimental data plus Multiscale Modelling of Materials (M³) for new materials are presented.*

KEYWORDS: Nuclear Fuels, Fuel Behaviour, Codes, BaCo, M³.

I. INTRODUCTION

It is of crucial importance nowadays the developing a better experimental and theoretical knowledge of the processes related with the evolution of the fuel during the commercial irradiation and the evolution of defects and the accumulation of fission products for modelling the fuel behaviour under different operating conditions and the evolution of a spent fuel over long period of time. The current experimental database could be enough to support empirical correlations and modelling for current fuels. Nevertheless, new approaches are required if the actual fuel computer codes will be used to simulate new materials and extreme situations as ultra high burnup. There are at present new requirements of experimental data about the present developments and the new challenge of nuclear plant designs in particular for the ATF ("Accident Tolerant Fuels") and the Generation IV initiatives. Those experiments would be extremely expensive and they would require long periods of time. Part of the data needed for new fuels development, partially unavailable, could be obtained through extensive historical databases of fuel irradiations not completely analysed waiting to be the support of new fuel improvements. From the other side there are new methodologies that will provide a theoretical approach to model the properties of materials as Multiscale Modelling of Materials (M³), through ab initio, molecular dynamics, kinetic Monte Carlo and finite elements calculations over the relevant length and time scales of each method.

The BaCo code ("BArra COMbustible" -Spanish expression of "Fuel Rod"-) was a usual participant of a series of Coordinated Research Projects ("CRP") of the International Atomic Energy Agency ("IAEA") generically named FUMEX ("Fuel Modelling at Extended Burnup") and at present in the CRP ACTOF. The D-COM and the CRP FUMEX I, II & III were a series of comparison among experimental irradiations and code calculations. The development of BaCo begins at the end of the 70's at the Atomic Energy National Commission of Argentina (CNEA) in order to cover the study of the fuel rod ("FR") behaviour under irradiation conditions.

BaCo is focused on PHWR fuels as the CANDU and Atucha ones but we keep a full compatibility with PWR, BWR, WWER and PHWR MOX, plus advanced, experimental, prototypes and/or non usual fuels. At present CNEA are developing

the CAREM reactor where the fuel element has a hexagonal array as the WWER fuels. BaCo was strongly involved in the design and test of that innovative Argentinean PWR fuel and advanced PHWR fuels (as the CARA ones).

The code includes additional tools 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 the calculation of a complete set of irradiations as for example the calculation of a full reactor core.

II. THE BaCo CODE

The BaCo code was developed at CNEA for simulating nuclear fuel rods behaviour under irradiation (1, 2). The development of BaCo was focused on PHWR fuels, as CANDU (8) and Atucha ones (13), under irradiation and during storage conditions (17 18) also, by keeping a good performance with PWR fuels and also it keeps a good convergence with advanced fuel materials, as the proposed ones for the ATFs and Generation IV fuels, at least the most advanced designs for illustrative and comparative purpose.

The BaCo modelling of UO₂ pellets includes elastic deformation, thermal expansion, creep, swelling, densification, restructuring, relocation, cracks and fission gas release. For the Zry cladding, the code models elastic deformation, thermal expansion, anisotropic plastic deformation, creep and growth under irradiation. The modular structure of the code easily allows us to input different material properties. It can be used for any geometrical dimension of cylindrical fuel rods pellets (either compact or hollow, with or without dishing) and Zry cladding. A special feature of the BaCo code is its complete treatment of the fuel with or without mechanical contact to the pellet surface and the clad, at any irradiation stage.

Fuel rod power history and either cladding or coolant external temperatures must be given to the program. Rod performance is numerically simulated using finite time steps (a 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 and dishing shape evolution, are calculated. The output contains the distribution along the rod axis of these variables. The details of the mechanical and thermal treatment and the pellet, cladding and constitutive equations are available in reference (1) and an extended description of the code is included in reference (2).

BaCo assumes azimuthal bi-dimensional symmetry in cylindrical coordinates for the fuel rod (1). Although angular coordinates are not considered explicitly, angular dependent phenomenon, as well as radial cracking, are simulated through the angular averaging method (20). Also axial pellet cracking and relocation are included in BaCo. The hypotheses of axial symmetry and modified plane strains (constant axial strain) are used in the numerical modelling. The fuel rod is separated in axial sections in order to simulate its axial power profile dependence. Rod performance is numerically simulated using finite time steps (finite differential scheme). The modular structure of the code easily allows the description of phenomena observed in the UO₂ pellet and the Zry cladding behaviour. The current version of BaCo can be applied to any geometrical dimensions of cylindrical fuel rods mainly with UO₂ pellets (either compact or hollow, with or without dishing) and Zry cladding. However, the code allows us to calculate fuel rods with other materials for the pellets and the cladding as metallic uranium, uranium carbide, uranium nitride (for pellets) and silicium carbide (for cladding), at least for illustrative and comparative purpose, due to the simplicity of the modelling of these materials included in BaCo (15, 16).

III. ADVANCED FEATURES OF BACO

BaCo 3D tools (11), statistical analysis (12), full core calculations (13) and graphical data post-processing improve the code performance and the analysis of the calculations (2).

Although the BaCo code uses a quasi-two-dimensional approach, the use of several three dimensional (3D) finite element features allow a complementary analysis of 3D properties, as for example the stress-strain state at a specific period of time during the irradiation (11). The BaCo code results were enhanced by using “ad hoc” tools developed at the MECOM and SiM³ Divisions (Bariloche Atomic Centre, CNEA) (20). The temperature profile, the crack pattern and the boundary conditions (as the inner pressure, pellet stack weight, etc.), among others, are calculated with BaCo as the input data to the 3D stress-strain state and the deformations of the UO₂ pellet.

For a better understanding of the uncertainties and their consequences, the mechanistic approach must therefore be enhanced by the statistical analysis (12). BaCo includes a probability analysis within their code structure covering

uncertainties in fuel rod parameters, in the code parameters and/or into the fuel modelling taking into account their statistical distribution. As consequence, the influence of some typical fabrication parameters on the fuel cycles performance can be analyzed. It can also be applied in safety analyses and economics evaluation to define the operation conditions and to assess further developments. These tools are particularly valuable for the design of nuclear fuel elements since BaCo allows the calculation of a complete set of irradiations.

IV. THE NEEDS OF SIMULATIONS AND EXPERIMENTAL DATA

Experimental data are the common need for fuel design, fuel performance analysis and fuel modelling. These experiments are very expensive and lengthy in time. Due to those reasons it was implemented the IFPE in order to share data of irradiation of nuclear fuels (7). The simulation with computer codes is the key in order to close the bridge between the fuel design and the needs of experimental results.

The codes will provide a frame to define the power history and the parameters of the experiments after the analysis of similar irradiations and simulations. It is a useful tool to reduce the number of experiments which, together with the code results, will constitute the complete description of the fuel behaviour, in particular the PIE.

V. M³ (MULTISCALE MODELLING OF MATERIALS)

There has been a considerable interest in actinide nitrides and carbides during the last years due to the Generation IV reactor initiative and the wide scope of materials analyzed to be used in the ATF fuels. The current experimental database could be enough to support empirical correlations and modelling for current fuels. New approaches are required if the actual fuel computer codes will be used to simulate if new materials and extreme situations as ultra high burnup in future research programs. The Multiscale Modelling of Materials (MMM or M³) allows the study of complex phenomena such the behaviour of new fuels and cladding materials and could provide a theoretical methodology to obtain the required information. The M³ methodology is based on the electronic structure calculations through ab initio codes and allow the study of structural, electronic and elastic properties at T = 0 K, followed by the development of effective or model potentials to be used in molecular dynamics and kinetic Monte Carlo codes. However, molecular dynamics simulations requires an intensive use of powerful computers and therefore the inter-atomic potentials to be used must be computationally efficient as well as physically appropriate for the description of the properties of the required new materials to be used in the Generation IV reactors and the ATF fuels.

With these techniques, algorithms and software we can obtain the basic parameters of materials as Young modulus, Poisson's ratio, thermal expansion coefficients, elastic constants, lattice parameters, lattice constants, Bulk modulus, shear modulus and Debye temperatures, among others, with an impressive physical support based on the main laws of physics. References (15, 16) include a wide explanation of the usage of that methodology in the field of nuclear materials.

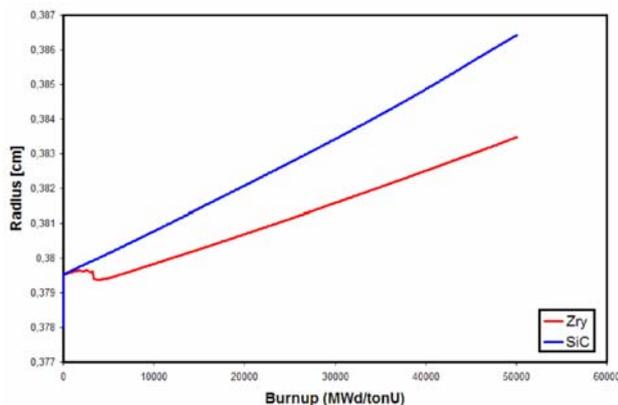


Figure 1: Pellet radius evolution of two fuel rods with Zry-4 and SiC cladding irradiated in PWR conditions and at constant power.

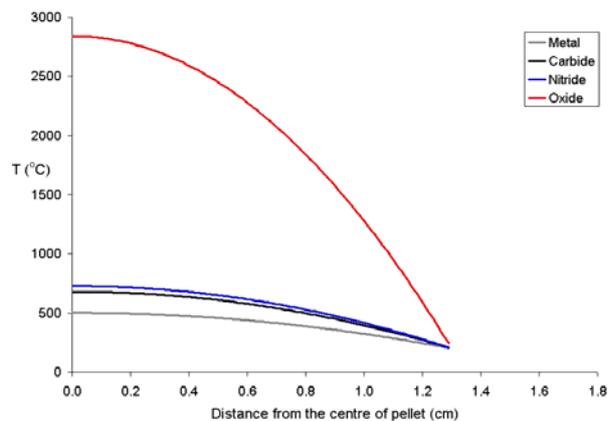


Figure 2: Fuel pellet centre temperature of a 26 mm diameter CANDU pellet with a power density of 250 W per cubic meter.

VI. NEW MATERIALS WITH PRESENT CODES

The symmetry of revolution adopted for the fuel rod and the modular structure of the code allows us to include new materials for the fuel pellet, the cladding and/or the filling gases by taking into account the requirements of the new reactors defined in the Generation IV initiative and the proposal of new designs taking into account the ATF concepts. Two examples of the use of BaCo are presented as an approach of the behaviour of SiC claddings, Figure 1 includes a comparison of the evolution of the UO_2 pellet radius by using a Zry-4 and SiC claddings in PWR conditions. The difference of behaviour is due to that Zry is a metallic alloy and SiC is a ceramic. Figure 2 shows the temperature radial profile by using different materials for the pellets (metallic U, Uranium Carbide, Uranium Nitride and UO_2). It is clearly shown the strong reduction of the fuel temperature when a material with a good thermal conductivity is used.

TABLE I. Comparison of the Elastic Constants with the calculation obtained by different authors. Young's modulus (Y), Shear modulus (G) and Bulk modulus (B) are expressed in units of GPa.

Poisson is a dimensionless coefficient (ν) –see Ref. [36]–

	C_{11}	C_{12}	C_{44}	B	Y	G	ν
Present work	376.35	121.38	257.65	206.37	317.15	194.26	0.142
Hill et al.	390.1	142.7	191.0	225.1	313.6	123.7	0.268
Iuga et al.	420	132	267	228		208	
Priya et al. (FP-LMTO)	420	126	287	223			0.231
Rappe et al. (Exp.)	390	142	256				
Madelung et al. (Exp.)	379	141	252				

The Table I shows our calculations of elastic constants, Young's modulus, Shear modulus, Bulk modulus and Poisson coefficient by using the M^3 methods. We find an excellent agreement among our results, experimental data and the open bibliography. Thermal dependence properties as Specific heat (C_V), Entropy and Helmholtz free energy are included in the Figure 3. The Figure 4 shows the results of our calculations of the thermal expansion coefficient for SiC (one of the most promising materials proposed as claddings for the new ATFs).

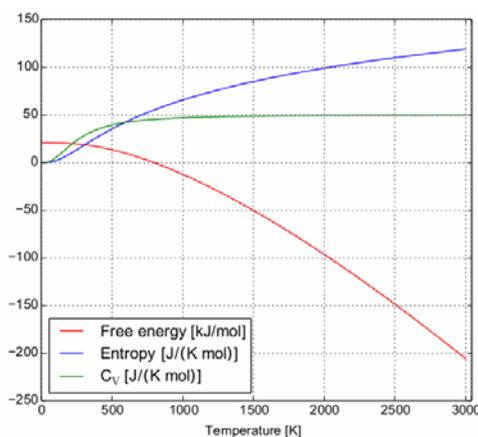


Figure 3: Thermal properties of the β -SiC phase as a function of temperature. The specific heat at constant volume (C_V), the vibrational entropy (S_V) and the vibrational Helmholtz free energy (F_V) were calculated as a function of temperature.

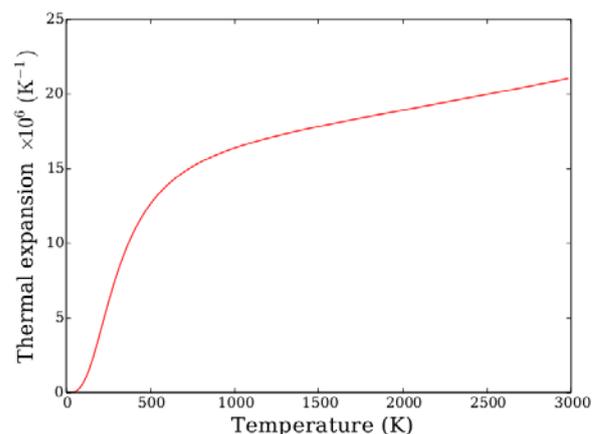


Figure 4: Temperature dependence of β -SiC phase linear thermal expansion coefficient vs. temperature.

The previous results highlight that the BaCo code is ready to be applied to these new fuels where that geometrical condition of the fuel is included for these materials or another ones under development. The calculations used for those plots were made without all the theoretical and empirical baggage needs for a good experimental agreement. In fact there are not

experiments with these types of fuel materials. We emphasize we could obtain a valid point of view by using codes at least for illustrative purposes.

VII. CRP FUMEX I (1993-1996)

The first edition of the CRP FUMEX (“Coordinate Research Project on Fuel Modelling at Extended Burnup”) of the IAEA (“International Atomic Energy Agency”) was devoted to several blind tests by using experimental data provided for the OECD HRP (“Halden Reactor Project”) (6). This CRP was originally focussed on thermal and mechanical calculations; finally the thermal affairs were mainly assessed. A set of instrumented fuels allowed following the evolution of some parameters (pellet centre temperature, inner pressure of the rod, cladding elongation, fission gas release and cladding diameter). The experiences include PIE analysis. The final burnup reached for the fuels were intermediate (25 MWd/kgU) and high (50 MWd/kgU). The main features of these exercises were the strong details of the experimental data of the HPR (see the Figure 3 where a simplified power history of the case 1 is included). The comparisons among the calculations of the participants and the experimental results were focused in the thermal issues of the fuel behaviour. Case 1 looks similar than the expected behaviour of the CAREM fuel (4), a new reactor at present designed by CNEA.

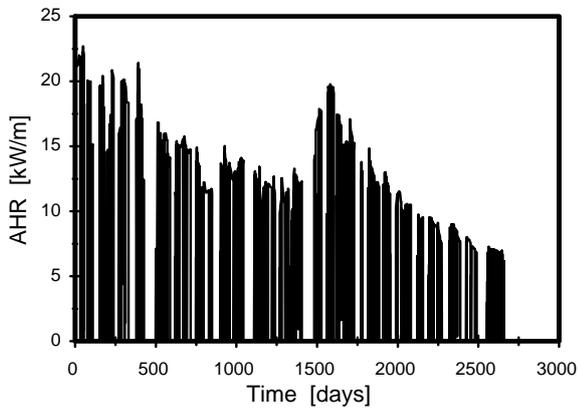


Figure 5: Power history corresponding to the Case 1 of the CRP FUMEX I.

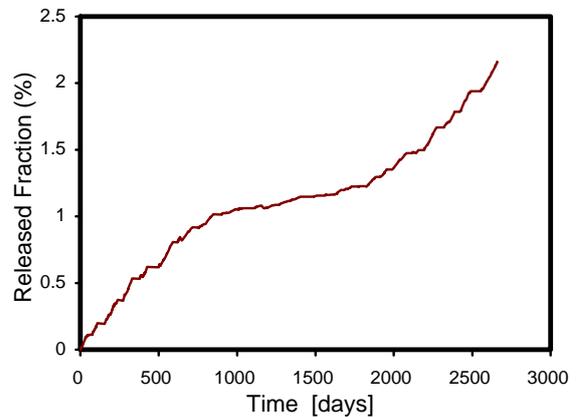


Figure 6: BaCo calculation for Fraction of Fission Gas Release, case 1 of CRP FUMEX I. The experimental result at EOL (End of Life) was FGR = 1.8 %

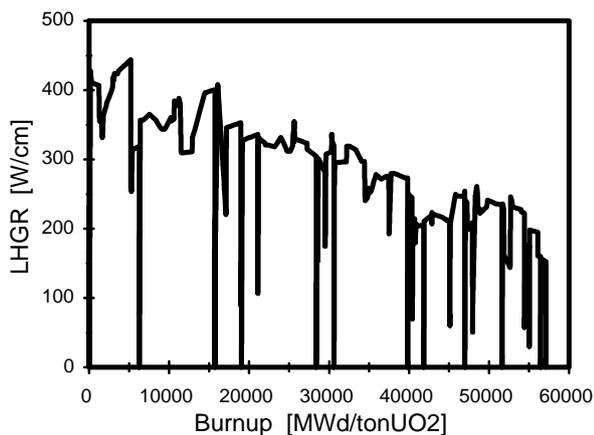


Fig. 7: Power history corresponding to the Case 2 of CRP FUMEX I.

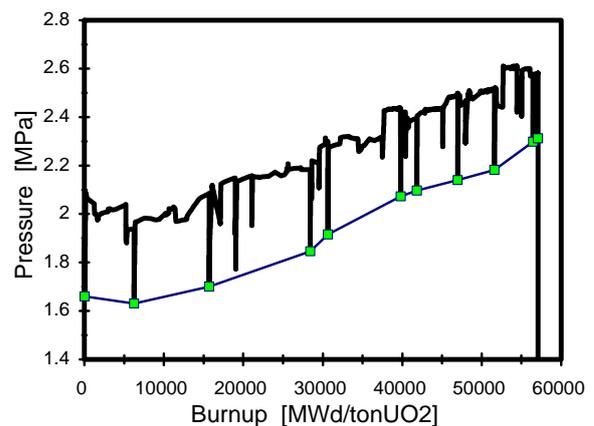


Fig. 8: Pressure in the rod, Case 2 of CRP FUMEX I. The experimental data are the squared dots corresponding to the pressure at specific shutdowns.

The first step in the resolution of the exercises was the treatment of the experimental data due to its extreme length. The second step was the detection and fixing of bugs in the codes and in the analysis of the HPR data.

We found a good agreement between the experimental data and the experimental data. As an example of the BaCo code performance see the Figure 6 showing our answer for the fission gas release. The Figure 7 includes the power history for the FUMEX case 2 and the Figure 8 shows the BaCo output for inner pressure in the rod in the same case. This results emphasized the performance of BaCo due to the calculation of the inner gas pressure inside the fuel rod are taking into account the thermal calculation, the fission gas release and the evaluation of the free volume. The complete evaluation of the CRP FUMEX I was published in the final report of the IAEA (6).

VII.A. A Fuel Failure in the CRP FUMEX I

Case number 4 of the first edition of the CRP FUMEX was a demanding exercise. It was a blind test as all the cases of FUMEX I. Two experimental fuel rods were instrumented and they were assembled in an “unknown” IFA of the HRP. One of them was filled with 3 bar He (rod A) and the second one with 1 bar He (92%) and Xe (8%) (rod B). The Figure 9 shows the power history of these fuel rods and the Figure 10 shows the gas pressure of the rod A.

A failure was attained in the fuel rod at the middle of the expected full irradiation. The event is not mentioned in the final TECDOC of IAEA (6) but it was commented by Dr. W. Wiesenack during the first RCM (“Research Coordinated Meeting”) in Halden, July 1993. The on-line measurement of the gas pressure was stopped due to a failure in the rod at the top of a power ramp. Nevertheless it was possible to continue the experiment. The calculations with the BaCo code were in good agreement with the experimental data (see Figure 10). The coolant pressure was ~33.6 bar. The codes can continue after the event and it was calculated an overpressure into the fuel rod.

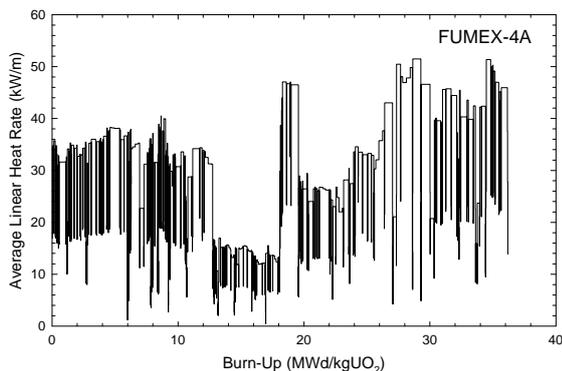


Figure 9: Power history corresponding to the Case 4-A of CRP FUMEX I.

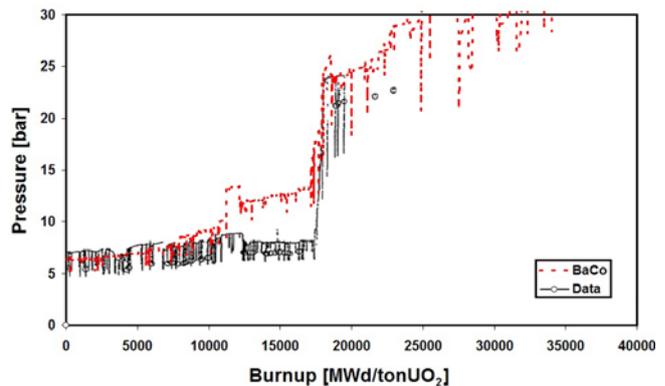


Figure 10: Gas pressure inside the fuel rod 4-A. Experimental data and BaCo calculations.

VIII. CRP FUMEX II (2001-2006)

The CRP FUMEX II was covered for 27 fuel performance database cases containing important fuel performance information such as fission gas release, fuel centreline temperature, rod internal pressure, clad creep and radial FP distribution measurement data. Those cases were included in the IFPE (7). The second edition of the CRP FUMEX was not a blind test. The data of the cases included the results of the exercises. The major objective of the program was to improve the high burnup fuel performance code prediction capabilities. We selected the PWR Cases 15 and 16 of the program in order to illustrate the accuracy of the BaCo predictions and detailed information of these cases in order to assess the performance of our code.

This CRP included ideal power histories of CANDU fuels at very high power levels. It was found a high probability of failures at those levels of irradiation due to that the calculated gas pressure in the fuel rods were over the coolant pressure as it is explained in reference (27).

VIII.A. CRP FUMEX II -Case 15, RISØ Test-

The Risø National Laboratory in Denmark have carried out three irradiation programs of slow ramp and hold tests, so called 'bump tests' to investigate fission gas release and fuel micro structural changes. The third and final project, which took place between 1986 and 1990, bump tested fuel re-instrumented with both pressure transducers and fuel centreline thermocouples. The data from the project were particularly valuable due to the in-pile data on fuel temperatures and pressures as well as extensive PIE (21). This bump irradiation test, case 14 of the CRP FUMEX II, was carried out on 1988 in the test reactor DR3 at Risø under PWR conditions. A fuel rod was refabricated from a segment supplied by Advanced Fuels Corporation (ANC) and instrumented with pressure transducer and fuel centreline thermocouple. The fill gas was 14.66 bar helium. Figure 11 shows the pellet centre temperature calculated with BaCo and the experimental measurement.

Bump testing of AN4, case 15 of the CRP FUMEX II, was carried out in December 1987. The fuel rod was refilled with Xe during refabrication. This case is valuable for the comparison with the previous cases of fuel pins filled with He. Likewise the use of the Xe as filling gas reproduces the worst case of thermal conductivity in the gap pellet-cladding. Figure 12 shows the inner gas pressure calculation and data. The difference between data and BaCo at the first part of the experiment is done due to the position of the pressure transducer (at the top of the fuel), the shutdown after the first ramp and the axial power profile. The inner pressure at the bottom is higher than at the top of the fuel due to the power profile and PCI at the middle of the rod. As BaCo calculates an average gas pressure then we have that difference. Nevertheless we have a very good agreement between these experiments and the BaCo code results.

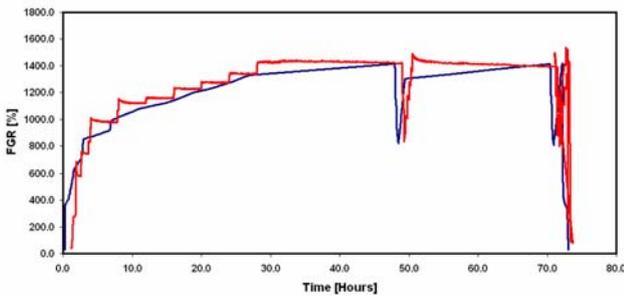


Figure 11: Pellet centreline data and calculation during the bump test. Case 15 of CRP FUMEX II.

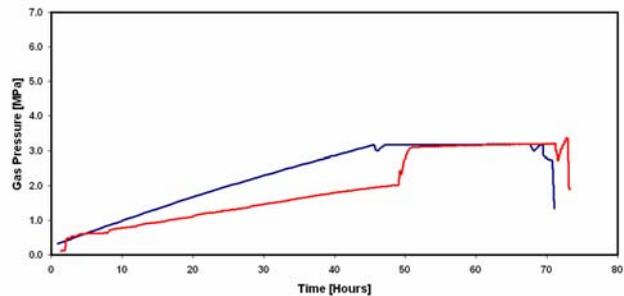


Figure 12: Experimental data and calculation of the inner gas pressure during the bump test at EOL.

TABLE II: Comparison Between the BaCo code Calculations and the Experimental Data for the Case 16 –HBEP test– of the CRP FUMEX II.

Case 16 (rod 363)	Data	BaCo
Average Burnup at EOL [MWd/kgU]	66.7	69.0
FGR [%]	3.80	3.25
Hot Pressure [MPa]		3.29
Pressure STP [MPa]	2.06	2.84
Case 17 (rod 365)	Data	BaCo
Average Burnup at EOL [MWd/kgU]	69.4	65.7
FGR [%]	2.40	3.70
Hot Pressure [MPa]		6.55
Pressure STP [MPa]	3.38	5.52
Case 18 (rod 370)	Data	BaCo
Average Burnup at EOL [MWd/kgU]	50.9	52.0
FGR [%]	1.40	2.00
Hot Pressure [MPa]		6.31
Pressure STP [MPa]	3.28	4.62

VIII.B. CRP FUMEX II -Case 16, HBEP Test-

The High Burnup Effects Programme (HBEP) was an international group-sponsored program managed by BNW (Battelle Pacific Northwest Lab.). The principal objective of the HBEP was to obtain well characterized data on FGR for typical LWR fuel irradiated to high burnup levels (22). The data set produced for the code simulation contains a full irradiation history with clad temperature and local power. The selected cases include annular pellets. The data are particularly valuable for the evaluation of the FGR at EOL and the fission products radial distribution. The measurements for the code comparison were: FGR at EOL, fission products and Pu distribution with a burnup ~ 51 and $67\sim 69$ MWd/kg(UO₂). The main results are included in the Table II.

Figure 13 shows the power history of the case 16 of CRP FUMEX II. The burnup was calculated with BaCo using the time as input data. We find a good agreement between the calculated burnup and the data (see the Chart 1). The FGR (“Fission Gas Release”) calculation is included in Figure 14. The release is thermally activated due to the limitation of our FGR model where the so-called HBS is not included. Nevertheless, the empirical approach used in the FGR model includes high burnup fuel irradiation results in their parameterization (1). The FGR calculated agrees very well with the experimental result at EOL. Figure 15 shows the inner gas pressure calculated with the BaCo code. We find an acceptable correlation between our estimation and the data at EOL. The cases do not include the evaluation of pellet stack length data but we include that calculation with an illustrative purpose (see Figure 16). Here we can identify a pellet densification up to a burnup of ~ 170 days; swelling is present after that date.

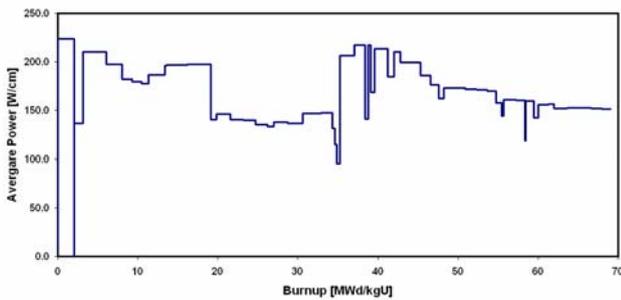


Figure 13: Average linear power of the fuel rod 363 from the HBEP experiment (Case 16 of CRP FUMEX II). Burnup calculated with the BaCo code (time was the data).

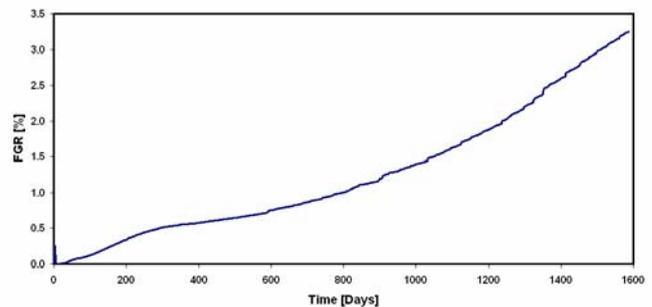


Figure 14: Fission gas release calculated with the BaCo code (Case 16 of the CRP FUMEX II). FGR data at EOL was: 3.80 %.

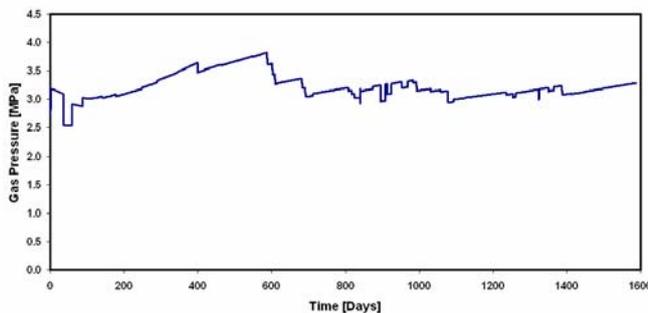


Figure 15: Inner gas pressure of the fuel rod 363 from HBEP experiment (Case 16 of CRP FUMEX II -HBEP test-). Pressure data at EOL was 2.06 (STP) and 2.84 MPa (STP) was calculated with the BaCo code.

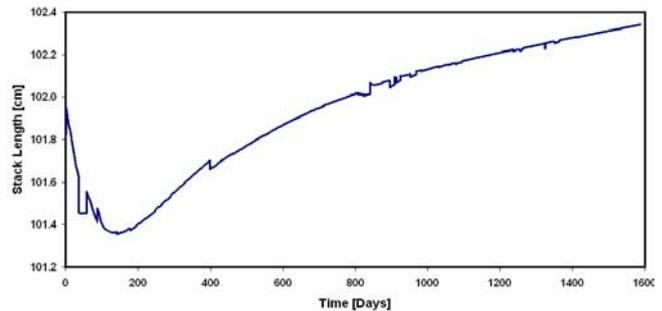


Figure 16: Pellet stack length calculated with the BaCo code for the fuel rod 363 from HBEP experiment (Case 16 of CRP FUMEX II).

IX. CRP FUMEX III (2008-2011)

The third edition of the CRP FUMEX III (24) is based on a big set of experiments of the OECD-IFPE (25). A minor set of six irradiations were selected for the organizers as mandatory cases in order to produce a comparative evaluation of the codes. The Risø cases of the CRP FUMEX II were repeated in the third edition due to its difficulties (see previous section with this case).

IX.A. CRP FUMEX III (AREVA idealized case 2)

This case is an idealized irradiation based on measurements of three fuel rods operated for 3, 4 and 7 cycles in a commercial French PWR reactor. It allows an empirical evaluation of the FGR of a single power history with a maximum burnup of about 81500 MWd/tonU and a FGR of about 9%. The Figure 17 illustrates the BaCo calculations of FGR and the given FGR “data” including the uncertainties based on the measurements and the fabrication.

The participants of the CRP FUMEX III were pushing the limits of their codes in order to simulate this case due to the extreme burnup of discharge. BaCo found good agreement in the two first points in the area of the usual extended burnup. Nevertheless we obtain an under prediction of the third point due to the fault of the modelling of the influence of Hi-Bu microstructure (in particular its influence with the FGR).

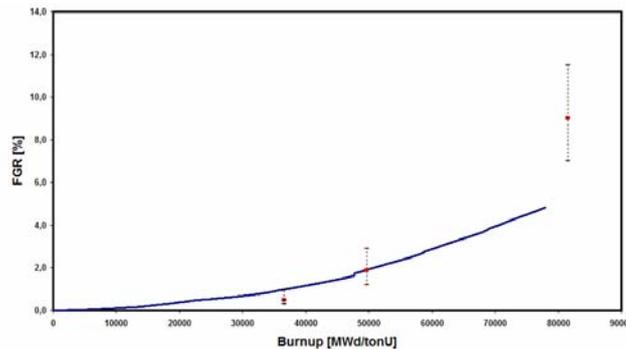


Figure 17: BaCo code calculation of the Fission Gas Release (FGR) vs. Burnup (idealized case provided by AREVA).

IX.B. CRP FUMEX III (AECL-JC-BUNDLE)

A Prototype CANDU Fuel bundle for the Bruce reactor was irradiated in the NRU experimental reactor at Chalk River Laboratories in experimental loop facilities under typical CANDU reactor conditions. The bundle was a 37-element fuel assembly prototype, it was coated with graphite and it was not instrumented. Coolant for the test was pressurized light water under typical PHWR conditions of approximately 9 to 10.5 MPa and 300°C. The bundle was subjected to extensive post-irradiation examination (26). The outer element burnup averaged was approximately 640 MWh/kgU at EOL (End of Life”). An outer element power was varied between 57 kW/m near the beginning of life (BOL) and 23 kW/m at EOL.

The Figure 18 shows the BaCo calculations of the fuel pellet centre temperature at three axial positions of the fuel. It was included the Vitanza threshold in order to take a first approach to the fission gas release (FGR). We find that the curves of temperature for the three axial segments are over the Vitanza threshold. The Figure 19 includes the evolution of the central hole, the radius of the columnar grains, the equiaxed grains and the zone without restructuring. The heat transference during irradiation is not optimized due to the use of a 90% of Ar as filling gas. The Figure 20 shows the inner gas pressure of the fuel rod of the CANDU fuel rod under study and the coolant pressure included as a reference line. The pressure is under the coolant pressure during the entire irradiation as we expect from a conservative point of view.

The Figure 21 shows the curves of the inner radius of the cladding and the radius of the pellet. We includes the lines of the as fabricated pellet radius and the as fabricated inner cladding radius as a reference. We do not obtain the closure of the gap at BOL like we expect for the CANDU fuels due to the extreme conditions of this experiments.

An example of the 3D tools used for the improvements of the normal BaCo output is included in the Figure 22. The plots are: the 3D mesh used for the finite element post-processing, 3D radial displacement where the ridges are clearly shown, the

hoop stress, the von Mises equivalent stress and the radial profile at the most demanding pellet during the irradiation of the bundle AECL-JC.

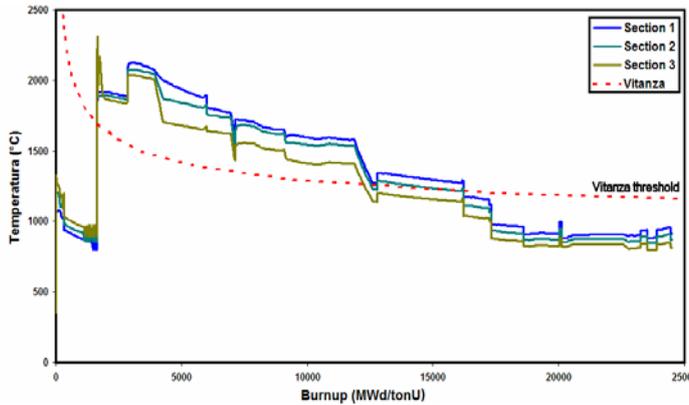


Figure 18: Fuel pellet centre temperature calculated with the BaCo code. Outer fuel rod of the Bundle AECL-JC.

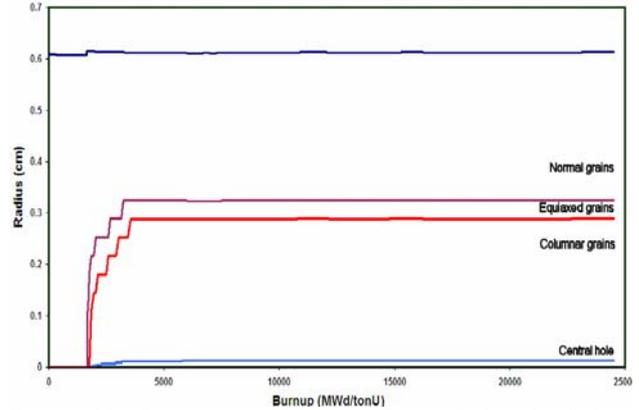


Figure 19: Grain size evolution. Outer fuel rod of the Bundle AECL-JC.

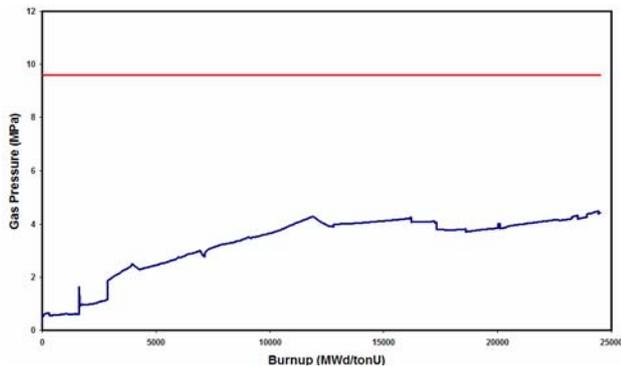


Figure 20: Inner gas pressure of the fuel rod. Outer fuel rod of the Bundle AECL-JC. Coolant pressure included as a reference line.

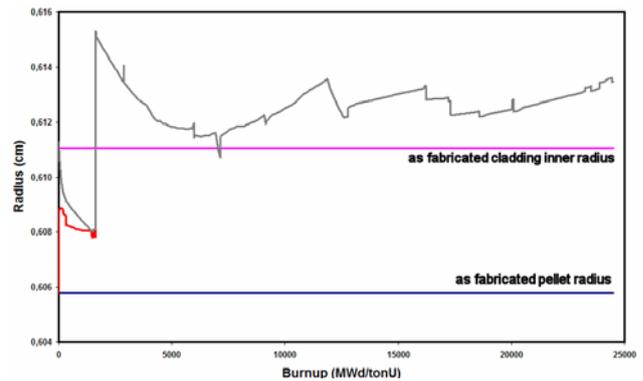


Figure 21: Pellet and inner cladding radius evolution. Outer fuel rod of the Bundle AECL-JC.

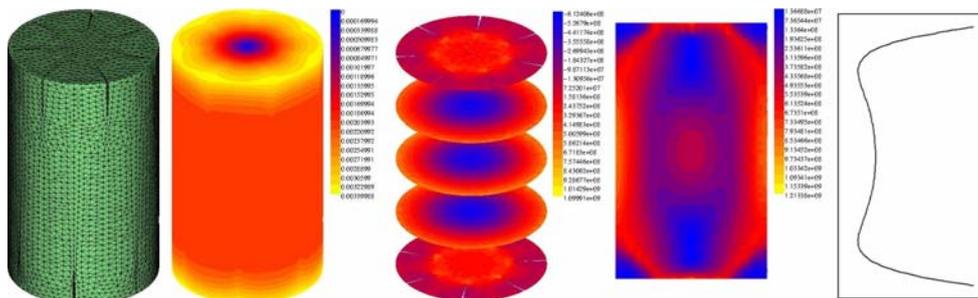


Figure 22: 3D mesh for finite elements calculation, 3D radial displacement, hoop stress, von Mises equivalent stress and radial profile of the most demanding pellet during the irradiation of the bundle AECL-JC.

IX.C. AECL-JC-BUNDLE AT DRY STORAGE CONDITIONS

The fuel element must not fail during the operation of the power plant. It is emphasized in this section that the fuel integrity must also be kept during the intermediate storage at pools or silos.

The simulation of the fuel behaviour under dry storage conditions can be calculated by using the BaCo code as an extension of the normal application of the analysis of nuclear fuel elements under irradiation. The safe conditions of storage, in particular the temperature of the dry storage system, were analyzed and the results are presented in Figures 23 to 26.

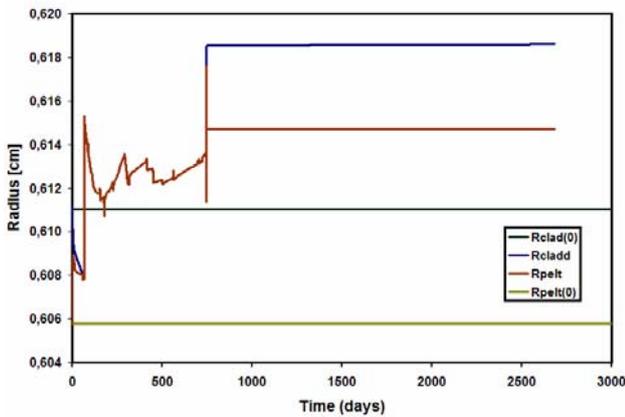


Figure 23: Pellet and clad inner radius evolution during irradiation and at dry storage conditions. Bundle AECL-JC.

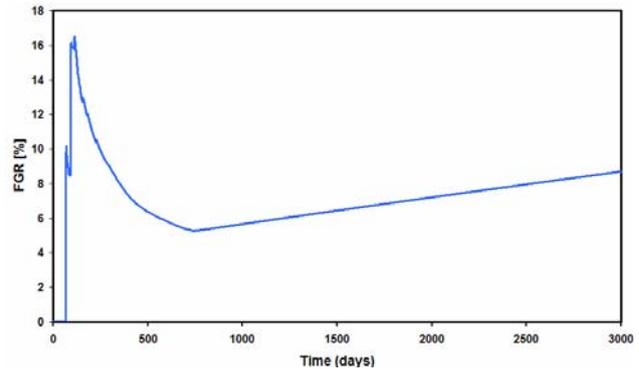


Figure 24: Fission gas release during irradiation and at dry storage conditions. Bundle AECL-JC.

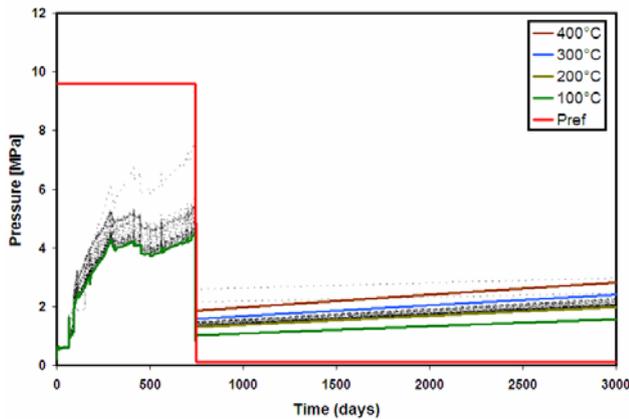


Figure 25: Fuel rod inner gas pressure during irradiation and at dry storage conditions. Bundle AECL-JC.

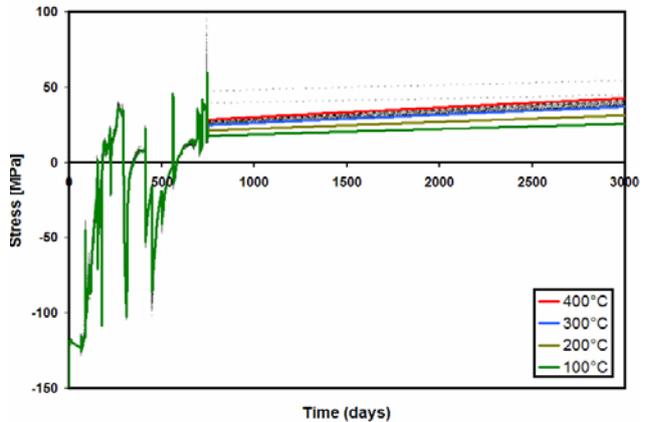


Figure 26: Hoop stress during irradiation and at dry storage conditions. Bundle AECL-JC.

The Figure 23 shows the evolution of the pellet and cladding radius during irradiation and at the dry storage. We observed the opening of the pellet-cladding gap due to the change of the boundary conditions at EOL; the coolant pressure is present during irradiation and the ambient pressure during storage (approx. 3000 days).

We found that there is a small increment of stresses and gas pressure into the fuel rod due to a small fission gas release in the presence of the corrosive elements or compounds as I, Cs, CsI, etc. A Stress Corrosion Cracking (SCC) failure could be achieved in the fuel due to the accumulated damage of the cladding during irradiation and the small but constant increment of FGR.

The Figure 24 shows the FGR at the same time of the previous plot; it is observed a small release of fission gasses thermally activated. The Figure 25 shows a parametric analysis of the inner gas pressure at four different values of the

temperature of the storage device; a statistical analysis is included. The Figure 26 includes the same analysis for the hoop stress of the cladding of the Bundle AECL-JC.

IX.D. A FUEL FAILURE IN THE CRP FUMEX III

The irradiation of the first MOX nuclear fuel rods made in Argentina began in 1986. These experiences were made in the HFR Petten (“High Flux Reactor”), Holland. Six MOX fuel rods were fabricated in the α Facility (GCCN-CNEA-Argentina). The modelling support of the experiment was conducted with the BaCo code (10).

The power histories were defined from calculations performed with the BaCo code in 1986 in order to obtain a high burnup compatible with the 80’s PHWR technology, to produce mechanical demanding conditions at the cladding and to define a high power ramp at EOL up to a value enough to induce a failure due to PCI-SCC. The final burnup of the most demanding fuel rod was 15000 MWd/ton(M). Ramping of that fuel rod was interrupted when an increase of coolant activity was detected. After discharge, a visual inspection of the rod showed the presence of a small circular hole in the cladding. Additional PIE showed that the hole was due to a SCC failure as it was predicted with BaCo.

These irradiations were included in the IFPE in 2000 and they were cases of the CRP FUMEX III. The name of the experiment is: IFPE/CNEA-MOX-RAMP.

The Figure 27 shows the BaCo calculations of the hoop stress at the cladding of the BU15 experiment. The Figure 28 is the PIE of a part of the defective fuel rod showing a crack due to SCC. The calculated hoop stress at the cladding is over the PCI-SCC threshold of $\sigma_{SCC} = 170$ MPa for PHWR fuels.

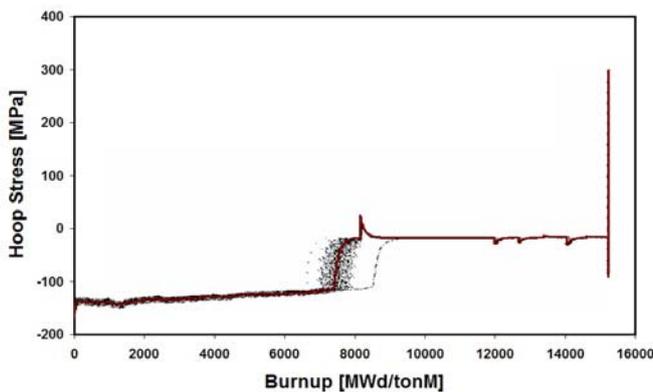


Fig. 27: Hoop stress (including a sensibility analysis) of the CNEA-MOX-RAMP case (CRP FUMEX III).

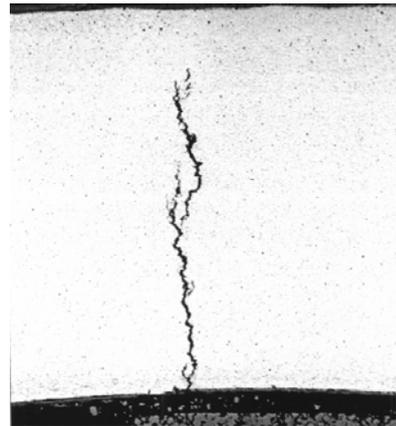


Fig. 28: SCC failure at the CNEA-MOX-RAMP case (10).

X. OLD JEWELS FOR PRESENT DEVELOPMENTS

We will illustrate the use of “ancient” experimental irradiations in the frame of new fuel improvements. The first is the proposal for some changes in the design of WWER fuel pellet (28) and we continue with a simulation of the behaviour of the CAREM fuel (4).

X.A. WWER fuel pellet improvements

At present some improvements of WWER fuel pellets are analyzed in order to determine the replacement of a flat and hollowed pellet with a solid and dashed one among other changes (28).

The extensive collection of fuel irradiation collected at the “International Fuel Performance Experiments (IFPE) database” (29) of the NEA-OECD are not fully analyzed due to data volume. Something similar happens with the powerful collection of irradiations performed at the international facilities as the Halden Reactor Project, the Studsvik Research Reactor, the HFR Petten reactor, etc.

An analysis of the WWER fuel behaviour with the BaCo code can be found in Ref. (30) and at present we are studying a complete 3D analysis of those improvements in the geometry of the pellets (31). In order to validate the calculations we are using irradiations of WWER fuel rods included in the CRPs FUMEX II and III (7) and experimental irradiations of the Halden Reactor Project.

As a 3D exercise of validation of our calculation we show in the Figure 29 the radial profile of two experimental fuel rods irradiated at the Halden reactor (32). Those rods have some hollowed pellets at the top of the fuel with the purpose to include a thermocouple. The figure includes the power profile of the rods. We see that the power is slightly greater than in the rest of the rod. Nevertheless we observe a reduction of radial deformation of the fuel diameter and a reduction of the ridges height as we calculate with BaCo. It is interesting to mention that this validation test is obtained by using a non-specific experiment. We observe the same behaviour at the Figure 30 where an experimental comparison of hollow and solid pellets is included. Here PCMI is much reduced in the hollow pellet rod and, unlike the solid pellet rod, results in no plastic permanent deformation of the clad (33, 34).

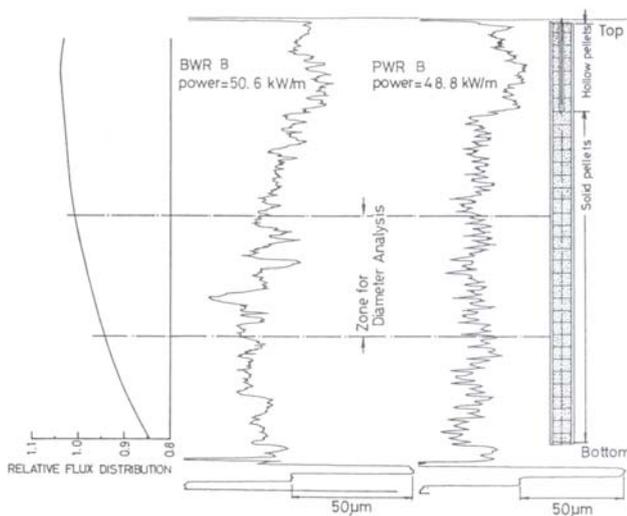


Figure 29: Rod profile of an experimental fuel at the Halden Reactor. At the top hollowed thermocoupled pellets are present (32).

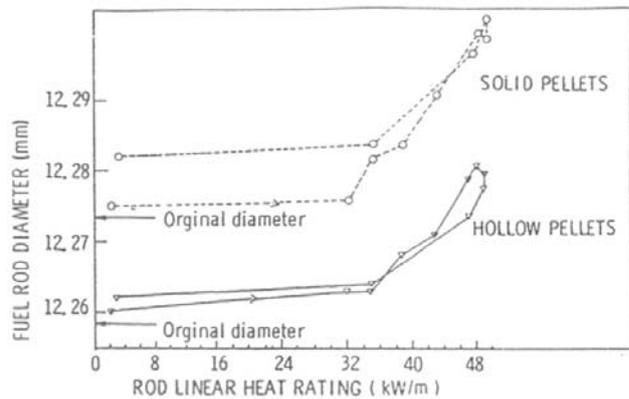


Figure 30: Clad average diameter versus linear heat rate for hollow and solid pellet rods in IFA-509 during a ramp at 3.0 MWd/kgUO₂ (33, 34).

X.B. The CAREM fuel and the CRP FUMEX

The CAREM Reactor Project is a present development of CNEA, Argentina. This project consists of the development, design, and construction of an advanced small integral type PWR, CAREM 25 is the prototype of the concept (4).

The development of the fuel for the CAREM reactor is sustained at CNEA. The simulation of the CAREM fuel behaviour and the definition of geometrical fuel parameters were started with the BaCo code. One of the tests for the validation of the fuel design and the previous calculations is experimentally supported for a set of instrumented irradiations of individual fuel rods at the Halden Reactor. The use of the codes was essential in order to reduce the number of these expensive experiments and to define a frame to analyse the experimental results (35).

The code simulations start with the search and study of equivalent experiments of irradiation; the Case 1 of the CRP FUMEX I of the IAEA presents a similar power history as the expected for CAREM and this experiment is using similar fuel rods than the CAREM ones (see Figure 5). This was one of the experiments used in order to validate the BaCo code results and to reduce the cost of the tests.

We found a deep feedback between the usage of the computer codes and the analysis of real experiments as it is happening in the set of simulation and experiments of the CAREM fuel rods.

XI. CONCLUSIONS

An extensive field of simulations by using a wide field of fuel rods could be not enough to validate this kind of fuel developments. Specific simulations are needed when we are designing an innovative fuel into an innovative reactor as in the case of the fuel of the CAREM and Generation-IV reactors and the new ATF fuel concepts. Those simulations require a set of experiments in order to validate the results of the computer codes. Nevertheless we emphasize the use of BaCo as a framework for the analysis of experimental irradiations including the PIE and/or the preparation of the actual experiment through a first step of simulations in order to reduce the number of expensive set of irradiation tests.

The structure and modularity of BaCo allow us to include new models of material behaviour under irradiation. That was sketched in Section VI at least for illustrative and academic purposes. Those capacities can be enhanced by using the Multiscale Modelling of Materials (M³). In fact the M³ methodology enhances and sinergetically supports the experimental results.

It was extensively presented the performance of the BaCo code in the CRP FUMEX I, II and III and, at present, in the CRP ACTOF, due to the relevance of the exercises of intercomparison of the IAEA and the usage of those open information. In the same way we show an easy way to interpret old experiments for present applications. Those experiments are particularly valuable when we have PHWR fuels and we are designing our first PWR (as the CAREM NPP) with low burnup as the case of Argentina. It was remarked in the paper the valuable experimental data available and not sufficiently exploited. In the same way it was clearly shown the high relevance of the international projects of fuel codes benchmarking and intercomparison.

Finally, the BaCo code shows itself as a powerful tool for analysis of the behaviour of nuclear fuel, modelling of present and new materials, fuel design, assistance in the analyses of the NPPs performance and analysis of ancient and present experiments of irradiation and its proposals by taking into account the economy and the safety of the nuclear fuel cycle.

ACKNOWLEDGMENTS

Halden Reactor Project who kindly made available for us its valuable experimental data, CNEA, CONUAR and IAEA for the continuous support.

REFERENCES

1. A. C. MARINO et al., "BaCo (BArro COmbustible) Code Version 2.20: a thermo-mechanical description of a nuclear fuel rod", *Journal of Nuclear Materials*, **volume 229**, April II, p155-168 (1996).
2. A. C. MARINO, "Starting Point, Keys and Milestones of a Computer Code for the Simulation of the Behaviour of a Nuclear Fuel Rod", *Science and Technology of Nuclear Installations*, **volume 2011**, Article ID 326948 (2011).
3. D. O. BRASNAROF et al, "A New Fuel Design for Two Different HW Type Reactors", *Science and Technology of Nuclear Installations*, **volume 2011**, Article ID 194650 (2011).
4. H. BOADO MAGAN et al, "CAREM Projects Status", *Science and Technology of Nuclear Installations*, **volume 2011**, Article ID 140373 (2011).
5. I. MISFELD, *The D-COM blind problem on fission gas release*, IAEA, International Working Group on Fuel Performance and Technology for Water Reactors, OECD-NEA-CSNI/IAEA Specialist's Meeting on Water Reactor Fuel Safety and Fission Products Release in Off-Normal and Accident Conditions, RISØ National Laboratory, IWGFTP/16 (1983).
6. "Fuel modelling at extended burnup", Report of the Co-ordinated Research Programme on Fuel Modelling at Extended Burnup-FUMEX-, 1993-1996, IAEA-TECDOC-998.
7. J. KILLEEN et al, "Fuel modelling at extended burnup: IAEA coordinated research project FUMEX-II", *Proc. of the International LWR Fuel Performance Meeting (Top Fuel '06)*, Salamanca, Spain, October 2006.
8. A. C. MARINO, "Computer simulation of the behaviour and performance of a CANDU fuel rod", *Proc. of the 5th International Conference on CANDU Fuel*, Toronto, Canada, September 1997.
9. A. C. MARINO, "An approach to WWER fuels with BaCo", *Proc. of the 7th International Conference on WWER Fuel Performance, Modelling and Experimental Support*, Albena, Bulgaria, September 17-21, 2007.
10. A. C. MARINO, P. ADELFRANG & E. E. PÉREZ, "Irradiation of Argentine MOX fuels. Post-irradiation results and experimental analysis with the BaCo code", *Journal of Nuclear Materials*, **volume 229**, April II, p169-186 (1996).

11. G. L. DEMARCO & A. C. MARINO, “3D Finite Elements Modelling for Design and Performance Analysis of UO₂ Pellets”, *Science and Technology of Nuclear Installations*, **volume 2011** (2011), Article ID 843491
12. A. C. MARINO et al, “Sensitivity analysis applied to nuclear fuel performance related to fabrication parameters and experiments”, *Proc. of the 14th International Conference on Structural Mechanics in Reactor Technology*, Lyon, France, August 1997.
13. A. C. MARINO et al, “High power ramping in commercial PHWR fuel at extended burnup”, *Nuclear Engineering & Design*, **volume 236**, no. 13, pp. 1371–1383 (2006).
14. J. A. TURNBULL et al, “Experimental data on PCI and PCMI within the IFPE database”, *Proc. of the International Seminar on Pellet-Clad Interaction in Water Reactor Fuels (PCI '04)*, Aix-en-Provence, France, March 2004.
15. A. C. MARINO et al, “Present and Future Trends in PHWR Fuel Material Modelling with the BaCo code”, *Proc. of the 21st International Conference on Structural Mechanics in Reactor Technology, (SMiRT 21)*, November 6-11, 2011, New Delhi, India.
16. A. C. MARINO et al, “Simulation of Nuclear Materials and Fuels by using the BaCo code and Multiscale Modelling of Materials (M³)”, *Water Reactor Fuel Performance Conference (TopFuel 2012)*, September 2-6, 2012, Manchester, United Kingdom.
17. A. C. MARINO, “PHWR fuel rod behaviour during dry storage”, No. 2022, *Proc. of the Water Reactor Fuel Performance Meeting (WRFPM 2009/Top Fuel)*, September 6-10, 2009, Paris, France.
18. A. C. MARINO, “CANDU Fuel Rod Behaviour during Dry Storage”, *Proc. of the 11th International Conference on CANDU Fuel*, Niagara Falls, Ontario, Canada, October 17-20, 2010.
19. A. C. MARINO, “An overview of the dry storage of nuclear fuels with the BaCo code”, *Proc. of the 8th International Conference on WWER Fuel Performance, Modelling and Experimental Support*, Helena Resort near Burgas, Bulgaria, September 26-October 4, 2009.
20. A. C. MARINO, “Crack and dishing evolution models and PCI-SCC considerations for fuel pellets in a quasi-bidimensional environment”, *Proc. of the “Les Journées de Cadarache 2004, International Seminar on Pellet-Clad Interaction in Water Reactor Fuels”*, Aix en Provence, France, March 9-11, 2004.
21. P. KNUDSEN et al., *Final Report on the Risø Fission Gas Project*, RISOE-FGP-R17rev. (June 1983) NEA -1634/01 (<http://www.nea.fr/abs/html/nea-1634.html>)
22. *High Burnup Effects Programme Final Report*, DOE/NE/34046-1 [HBEP-61(3P27)] NEA-1510/03 (<http://www.nea.fr/abs/html/nea-1510.html>)
23. OECD-NEA International Fuel Performance Experiments (IFPE) database (<http://www.oecd-nea.org/science/wprs/fuel/ifpelst.html>)
24. Report of the CRP on “Improvement of computer codes used for fuel behaviour simulation” (FUMEX-III, 2008-2011), to be published for IAEA.
25. OECD-NEA International Fuel Performance Experiments (IFPE) database (<http://www.oecd-nea.org/science/wprs/fuel/ifpelst.html>)
26. OECD-NEA International Fuel Performance Experiments (IFPE) database (<http://www.oecd-nea.org/tools/abstract/detail/nea-1596>)
27. A. C. MARINO, “CRP FUMEX PHWR cases a BaCo Code Point of View and Its Results”, *Proc. of the International IAEA Technical Meeting on “Fuel Integrity During Normal Operating and Accident Conditions in Pressurized Heavy Water Reactor (PHWRs)”*, September 24-27, 2012, Bucharest, Rumania.
28. V. MOLCHANOV, “Nuclear Fuel for VVER Reactors. Actual State and Trends”, *Proc. of the 8th International Conference on WWER Fuel Performance, Modelling and Experimental Support*, September 27-October 02, 2009, Helena Resort near Burgas, Bulgaria.
29. J.C. KILLEEN, E. SARTORI, J.A. TURNBULL, “The Relevance of the IFPE Database to the Modelling of VVER-Type Fuel Behaviour”, *Proc. of the 6th International Conference on WWER Fuel Performance, Modelling and Experimental Support*, September 19-23, 2005, Albena, Bulgaria.
30. A.C. MARINO & G.L. DEMARCO, “An Approach to WWER fuels with BaCo”, *Proc. of the 7th International Conference on WWER Fuel Performance, Modelling and Experimental Support*, September 17-21, 2007, Albena near Varna, Bulgaria.
31. A.C. MARINO, G.L. DEMARCO & L. FURLANO, “A 3D Analysis of the Geometry of a WWER Fuel Pellet”, to be published in the *Proc. of the 11th International Conference on WWER Fuel Performance, Modelling and Experimental Support*, September 26-October 03, 2015, Varna, Bulgaria.

32. M. ICHIKAWA et al., “Preliminary results from power ramping experiments by LWR Rigs”, *Proc. of the Enlarged Halden Programme Group Meeting*, Løen, Norway, HRP-305/8, 1985.
33. H. U. STALL, “Radial and Axial Deformation Behaviour of Solid and Hollow Fuel Rods during Base Irradiation and Power Ramp in IFA-509.2”, *HWR-49 May 1982*.
34. OECD Documents, Review of Nuclear Fuel Experimental Data prepared by J. A. TURNBULL, January 1995 (<http://www.oecdnea.org/html/science/docs/pubs/nea0197-fuel.pdf>).
35. A. C. MARINO, M. MARKIEWICZ & E. ESTEVEZ, “Verificación del Comportamiento de las Barras Combustibles para el Reactor CAREM vía Código de Cálculo para el Núcleo de Equilibrio”, *Proc. of the XXXVII Reunión Anual de la Asociación Argentina de Tecnología Nuclear (AATN XXXVII)*, paper #120, November 22-26, 2010, Buenos Aires, Argentina.
36. A. C. MARINO, A. BARUJ, L. FURLANO and E. L. LOSADA, “Combustibles tolerantes a accidentes (ATF, “Accident Tolerant Fuels”)", *Proc. of the XLII Reunión Anual de la Asociación Argentina de Tecnología Nuclear (AATN XLII)*, paper #095, november 21-25, 2015, Buenos Aires, Argentina.