COMPUTER SIMULATION OF THE BEHAVIOUR AND PERFORMANCE OF A CANDU FUEL ROD

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ABSTRACT

At the Argentine Atomic Energy Commission (Comisión Nacional de Energía Atómica, CNEA) the BACO code (for "BArra COmbustible", fuel rod) was developed. It allows the simulation of the thermo-mechanical performance of a cylindrical fuel rod in a Pressurized Heavy Water Reactor (PHWR). The standard present version of the code (2.30), is a powerful tool for a relatively easy and complete evaluation of fuel behaviour predictions. Input parameters and, therefore, output ones may include statistical dispersion. As a demonstration of BACO capabilities we include a review of CANDU fuel applications, and the calculation and a parametric analysis of a characteristic CANDU fuel.

1. INTRODUCTION

In a nuclear reactor, fuel rod materials support relatively large temperatures and suffer the effects of an aggressive chemical and radiation environment. Therefore, mechanical solicitation might sometimes be near the limits of materials endurance even in normal operating conditions. The economics of energy production might be greatly improved by quite minor corrections in design and fuel processing and operating conditions. Any of these requires a careful checking of fuel design. This has to consider parts performance as well as their in service thermo-mechanical coupling. This coupling requires of computer codes to obtain results quantitatively and even qualitatively valid. Numerical predictions depend heavily on realistic modelling. Therefore, computer codes should include models of the main mechanical and chemical phenomena taking place in the fuel, the cladding, the interfaces, and gap spaces and their coupling, as well as an accurate evaluation of temperature evolution; i.e., it should synergistically model thermal and mechanical behaviour of the fuel.

Argentina has two nuclear power stations in operation: Atucha-I (a Pressure Vessel PHWR) and Embalse (CANDU 600 type). Although both are PHWRs, reactor and fuel design are different in the two cases. Atucha fuel rods are nearly five meters long against the half a meter of CANDU fuels. The cladding is self standing in the first case and collapsible in the second. The decision on code development taken in the late seventies at CNEA was to simulate cylindrical fuel rods containing UO_2 pellets and supported by a Zry cladding, where reasonably general material models were used; that approach could at the same time cover both types of fuels. The first attempt in that respect was the thermal code PIZZA (*Ref. 1*); after that, the PELT (*Ref. 2*) and BACO (*Ref. 3* and

4) codes were developed. The numerical structure of the BACO code was an improved version of that of FRUMP, the code developed by then at Harwell (*Ref. 5*). BACO was for a time probably one of the more complete fuel performance simulation codes which included both pellet cracking, restructuring, anisotropic cladding, etc. The code was tested by comparison with other ones of similar potentiality, like URANUS (*Ref. 6*) and, more recently, in a co-ordinated round robin comparison of fuel code predictions, with experimental results (*Ref. 7*).

BACO (BArra COmbustible) is a code for the simulation of the thermo-mechanical and fission gas behaviour of a cylindrical fuel rod under operation. The BACO code in its version 2.20 was recently described by Marino et al. (*Ref. 8* and *9*). The present 2.30 version is as user friendly as the 2.20 but allows for a more detailed graphic output.

Predicting the thermal and mechanical performance of the CANDU fuel is challenging for computer codes not designed "ad hoc". One must remember the characteristics of fuel performance (collapsible cladding, filling gas pressure, cladding creep down during irradiation, etc.). Here, except for the example of our experiments on MOX fuels, we shall concentrate on results for CANDU fuels.

2. BACO CODE DESCRIPTION

The BACO code structure and models in its present versions are described in *References 8* and *9*, including steady state and transient thermal analysis. The number of instructions is at present (version 2.30) of approximately 9000 Fortran 77 sentences. Data post-processing improves the code's performance and analysis of results.

On modelling the UO_2 pellet, elastic deformation, thermal expansion, creep, swelling, densification, restructuring, cracks and fission gas release are included. While 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 the incorporation of different material properties. It can be used for any geometrical dimensions of cylindrical fuel rods with UO_2 pellets (either compact or hollow and with or without dishing) and Zry cladding.

Fuel rod power history and either cladding or coolant external temperature are inputs to the program. Rod performance is numerically simulated using finite time steps. The code automatically selects time steps according to physical criteria. Temperature distribution in the 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 UO_2 grain boundary, internal gas pressure and current composition of the internal gas, are calculated. The output contains the distribution along the rod axis of these variables.

3. BACO CODE VALIDITY TESTS

3.1. EXPERIMENTAL IRRADIATIONS AT THE NRX REACTOR

The work reported by Notley (*Ref. 10*) was used for testing the BACO code and results reported in *References 8* and *9*. In Notley's work, six Zircaloy-sheathed UO_2 fuel elements were irradiated at power outputs between 760 and 600 W/cm to a burnup of about 5500 MWd/tonU. Then two of them and another two new rods were irradiated at lower powers for a further 1250-

1700 MWd/tonU. The experiment was irradiated in the X-2 loop of NRX reactor. All elements were destructively examined and some of them were measured during the irradiation. The predicted and measured rod radius change $\Delta R/R$, fission gas released, columnar and equiaxed grains and central hole are provided in *Reference 10* and calculated with BACO (*Ref. 8* and *9*).

We find that, although the predictions of $\Delta R/R$ and the gas released are approximately correct, the measured rod dimension changes are somewhat larger than predicted at low power and low burnup and are overpredicted by the code at high power and burnup. We discussed in *Ref. 9* that this might be related to burnup and power ranges to which the code parameters have been fitted.

3.2. FUELOGRAMS

In CANDU reactors, fuel reshuffling is done under reactor operation. During reshuffling, the fuel undergoes a power ramp due to the power distribution along the fuel channel. For this reason, it is interesting to study the behaviour of a CANDU fuel under fast (10-20 min long) power ramps. The linear heat generation rate (LHGR) before the ramp, the burnup at which the ramps occurs, and the ramp height, cover a wide range. AECL has published bounds for safe operation, based on actual experience of power ramping due to fuel reshuffling in nuclear power stations. Usually (*Ref. 11*), the maximum power increase and maximum power such that fuel operation below those values present no failures, are given as a function of burnup.

The experimental bounds for power increase and maximum power corresponding to the Pickering Stations are plotted in *Ref. 13*. Power histories simulating reshuffling were simulated with the BACO code. In the Code, the criterion for safe operation was based on the maximum hoop stress at the cladding inner surface; this is related to susceptibility to stress corrosion cracking. BACO results are in good agreement with AECL data; even the mispredictions can be explained on a physical basis (*Ref. 14*).

3.3. MOX FUELS RODS IRRADIATION

The irradiation of the first Argentine prototypes of PHWR MOX fuels began in 1986. The six rods were fabricated at the α Facility (GAID-CNEA-Argentina) (*Ref. 15*). These experiences were made in the HFR-Petten reactor, Holland. The rods were prepared and controlled at CNEA's Facility. The postirradiation examinations were performed at the Kernforschungszentrum Karlsruhe, Germany, and at the JRC, Petten. The parameters of the irradiation, the preparation of the experiments and post-irradiation analysis were sustained by the BACO code predictions.

Two rods included iodine doped pellets (CsI and the second one, elemental iodine). The concentration of iodine was calculated to simulate a burnup of 15000 MWd/ton(M). The power histories were defined with the BACO code including power cycling and a final ramp. The presence of microcracks in the cladding inner surface was observed in the iodine CsI doping test. The experience named BU15, was performed with those rods. The goal of this experience was to verify the fabrication processes and study the fuel behaviour with respect to PCI-SCC (pellet cladding interaction - stress corrosion cracking). The results and code predictions are reported in *Reference 15*. It was interesting to find a fuel failure which could be possibly related to a PCI-SCC mechanism.

4. A CANDU FUEL ROD ANALYSIS

We simulate hereafter a CANDU fuel rod performance under an hypothetical, however realistic, power history. With the purpose of illustrating some of BACO's code capabilities, relatively highly demanding in power conditions are considered.

4.1 NORMAL OPERATION CONDITIONS

The reactor's assumed power history used here for the fuel rod performance analysis, is sketched in *Figure 1*. Reactor operation is considered to be at a relatively high power level during all the irradiation and, at the beginning of the third stage, after the second shutdown, the start-up is a step-by-step one.

The maximum temperature calculated at the pellet centre was 1970 °C (See *Figure 8* afterwards). In *Figure 2* we plot the fission gas produced at the fuel, the one released, the one trapped into the matrix of UO_2 and, finally, that retained at the grain boundary. The fraction of fission gas released at EOL (End Of Life) is 7.2 % (thin curve in *Figure 2*). The increase of the fraction released during the stages of high power (more than 500 W/cm), at the power ramps of 1000 MWd/tonUO_2, at the first reshuffling and during the peak power at 3300 MWd/tonUO_2 can also be identified the figure.

In *Figure 3*, the pellet and inner cladding radius evolution are plotted. Pellet and cladding come in contact after a brief period of BOL (Beginning Of Life) and that contact is broken during shutdowns. Radius variations are related to power changes by the coupling of cladding creep-down and pellet densification and swelling. The densification takes place before the 1000 MWd/tonUO_2 and swelling after the middle of the irradiation. The pellet stack and its associated cladding length evolution are plotted in *Figure 4*. There is a thermal expansion at BOL, until pellet-cladding contact occurs, at very low burnup. Thereafter, the radial coupling between pellet and cladding imposes both curves to be parallel except at reactor shutdowns, where pellet-cladding contact is predicted to be broken by effect of the fuel thermal contraction.

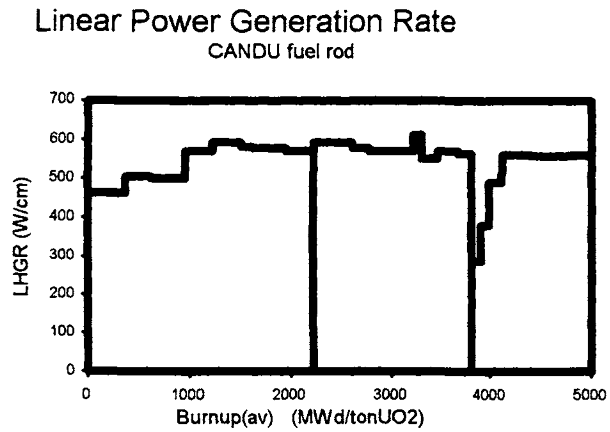

Figure 1: CANDU fuel rod: linear heat generation rate as a function of averaged burnup.

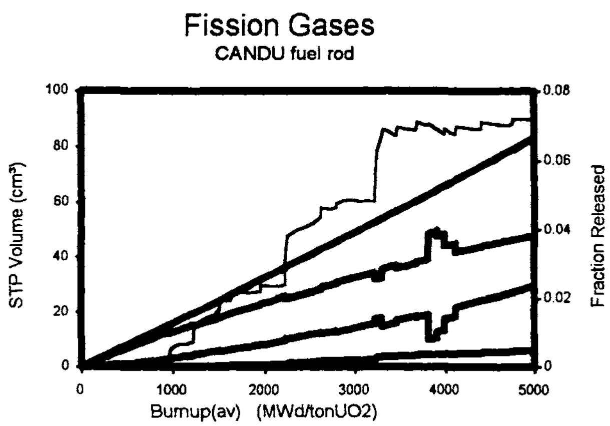

Figure 2: Predicted fission gas evolution (thick curves). The unit is the volume of gases at STP conditions (Standard Temperature and Pressure). The upper curve represents produced fission gases, the lower curve are released gases, the upper-centre curve is the trapped gases and the lower-centre curve is the fission gases at the grain boundary. The thin line shows the fraction of predicted fission gas released.

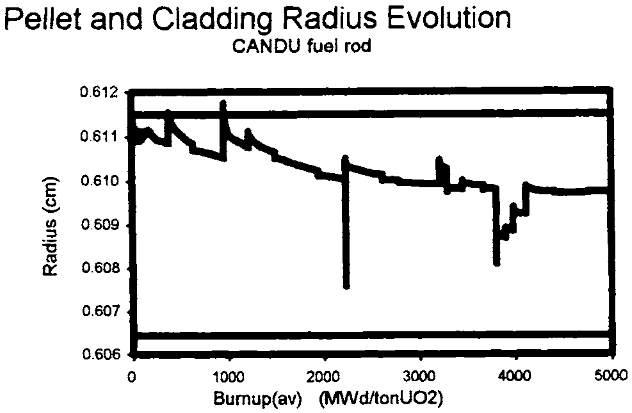

Figure 3: Predicted pellet and inner cladding radius evolution. Pellet and cladding are in contact. Upper and lower lines represent the pellet and inner cladding radius at the as-fabricated values.

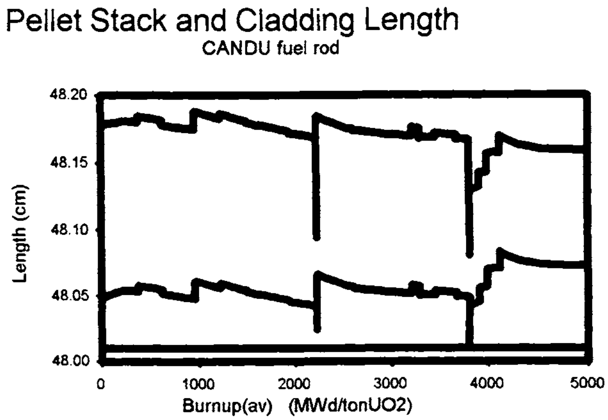

Figure 4: Pellet stack and cladding length evolution. The straight line is the pellet stack at the as-fabricated value.

Compression is generally predicted for the "hoop stress" calculated at the cladding (i.e., tangential stress at the inner surface of the cladding). However, stress reversal happens due to local power increment followed by stress relaxation, i.e., creep of the cladding. The maximum calculated hoop stress was 96 MP. Radial contact pressure has a direct correspondence with the previous figure. The maximum calculated contact pressure is 16 MPa. (See *Figure 9* afterwards.)

In *Figure 5* we plot the thermal gap conductance of the fuel rod. The overall degradation of the conductance during fuel life is due to fission gas release, and local variations are induced to power changes.

There is an increment of pressure of the free gases (He, Xe, Kr) in the rod due to the fission gas release, and local variations are induced by power changes. The calculated gas pressure at EOL (2.8 MPa) is smaller than the pressure of the coolant assumed for the calculation (10.6 MPa). (See *Figure 10* afterwards).

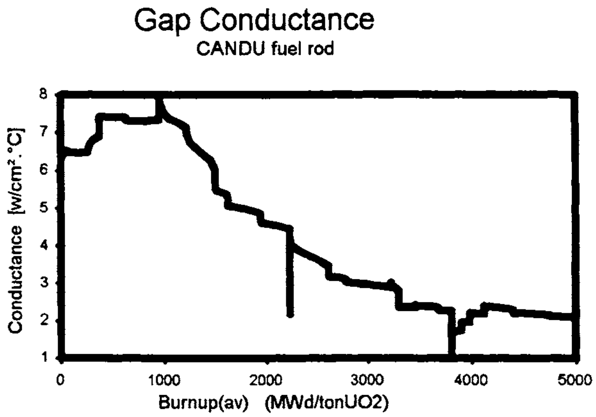

Figure 5: Thermal conductance of the pellet-cladding gap.

Figure 6 shows the evolution of crack opening induced by the tangential stresses in the pellet. We identify two kinds of cracks: those opening from the surface of the pellet ("cracks-out") and those from the centre of the pellet ("cracks-in"). In operation, cracks-out commonly open. The cracks-in open during power-downs ramps, specially at shutdowns, and they remain open only if operation continues at low power (low temperature) do they remain open. The cracks-in are closed by restructuring.

Figure 7 represents the BACO code evaluation of the pellet grain size. We identify an external zone without restructuring, a central hole which opens due to pore migration, an internal zone with columnar grains and a ring with equiaxed grains. The predictions of the above two plots (*6* and *7*) can be easily checked with pellet ceramography.

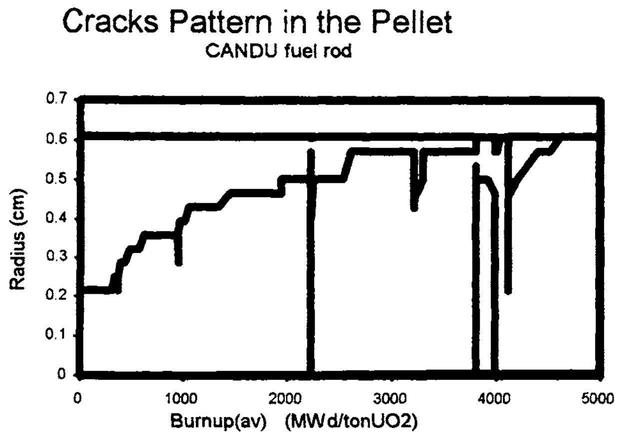

Figure 6: Pellet cracks evolution. The upper line represents the as-fabricated pellet radius. The lower curve (which nearly agrees with the x-axe) is the predicted central hole. The upper curve shows the cracks opening from the surface. The lower curve, among the 3800-4000 MWd/tonUO_2, shows cracks opening from the pellet centre.

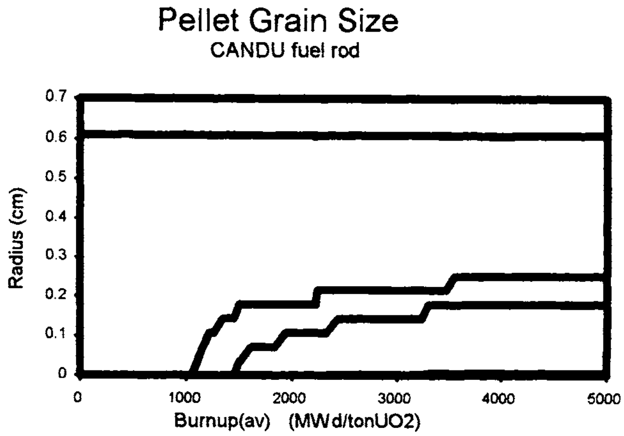

Figure 7: Pellet grain size evolution. The upper line represents the as-fabricated pellet radius. The lower curve (near the x-axe) is the central hole; the next ones, from the bottom are the columnar grains, and the ring with equiaxed grains should be located in the space from the columnar grains to the next curve.

4.2 EXTREME CONDITIONS IN ROD FUEL PARAMETERS

The purpose of this exercise is to consider how the combination of assumed extreme rod dimension conditions, but within reasonable tolerance for its fabrication, can affect performance. We define two extreme situations:

1) A rod with the largest gap between pellet and cladding compatible with the as-fabricated tolerances, and
2) A rod with the smallest gap.

The first situation should give rise to the maximum temperature in the fuel, and the second to maximum stress between pellet and cladding.

For the same power history of *Figure 1*, *Figure 8* includes the pellet centre temperature at the maximum gap situation. The largest temperature attained in this case is 2070 °C (while it is of 1920 °C for the minimum gap situation). *Figure 9* includes the BACO calculation of hoop stress with a minimum gap situation. Here, the stress reverses several times from the normal compression into expansion with peaks at the same burnups. The behaviour until the 1000 MWd/tonUO_2, decrement in the stress value is due to pellet-cladding contact at BOL.

We obtain a stable solution which proves that the BACO code is a good tool to be used for fuel rod design.

4.3 STATYSTICAL ANALISYS

As said in the Introduction, the flexibility of the BACO code and its speed in computer time allow to perform systematic statistical analysis; using allowed fabrication dimensional limits and a statistical distribution of values within those. Several runs (a minimum of 300) are performed with different sets of initial values for the rod dimensions. We study the predicted variations in:

1) Pellet centre temperature,
2) Cladding hoop stress, and
3) Gas pressure predictions.

The rod input data were randomly selected within assumed fabrication tolerance for pellet diameter and height, inner and outer diameter of the cladding and pellet density. The random selection of input values was done assuming a uniform distribution of values between limits.

Figures 8, 9 and *10* represent the BACO code parametric analysis of some performance parameters in a CANDU fuel rod. In the curves we plot:

1) Standard parameters of input data of the rod,
2) The parameters of the maximum gap situation,
3) The parameters of the minimum gap situation, and
4) The points of the random selection.

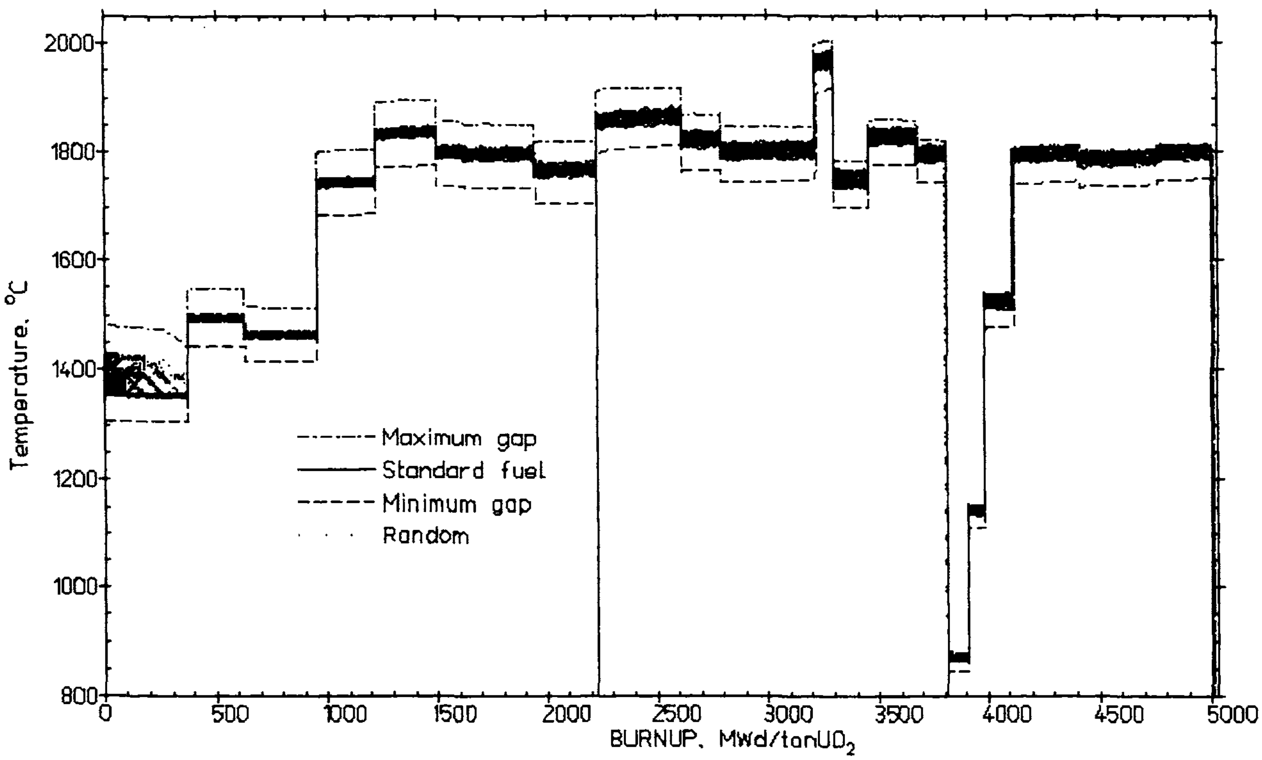

Figure 8: Statistical analysis of a CANDU fuel rod. Pellet centre temperature vs. averaged burnup.

Figure 8 is the BACO code calculation of the pellet centre temperature for the same viewer history of *Figure 1*. All the calculated random points are between the extreme values in as-fabricated tolerances; taken at approximate realistic values. At BOL, and depending of the combination of dimensional parameters, pellet-cladding contact may or may not happen; however it converges around the 500 MWd/tonUO$_2$ where all the random calculations present pellet-cladding contact

Figure 9 shows the dispersion in the cladding hoop stress with the same inputs as the previous plot. The points show a great dispersion at BOL due to the pellet-cladding contact situation. Calculations show that the hoop stresses converge during the irradiation; that is clearly demonstrated by the small dispersion at EOL.

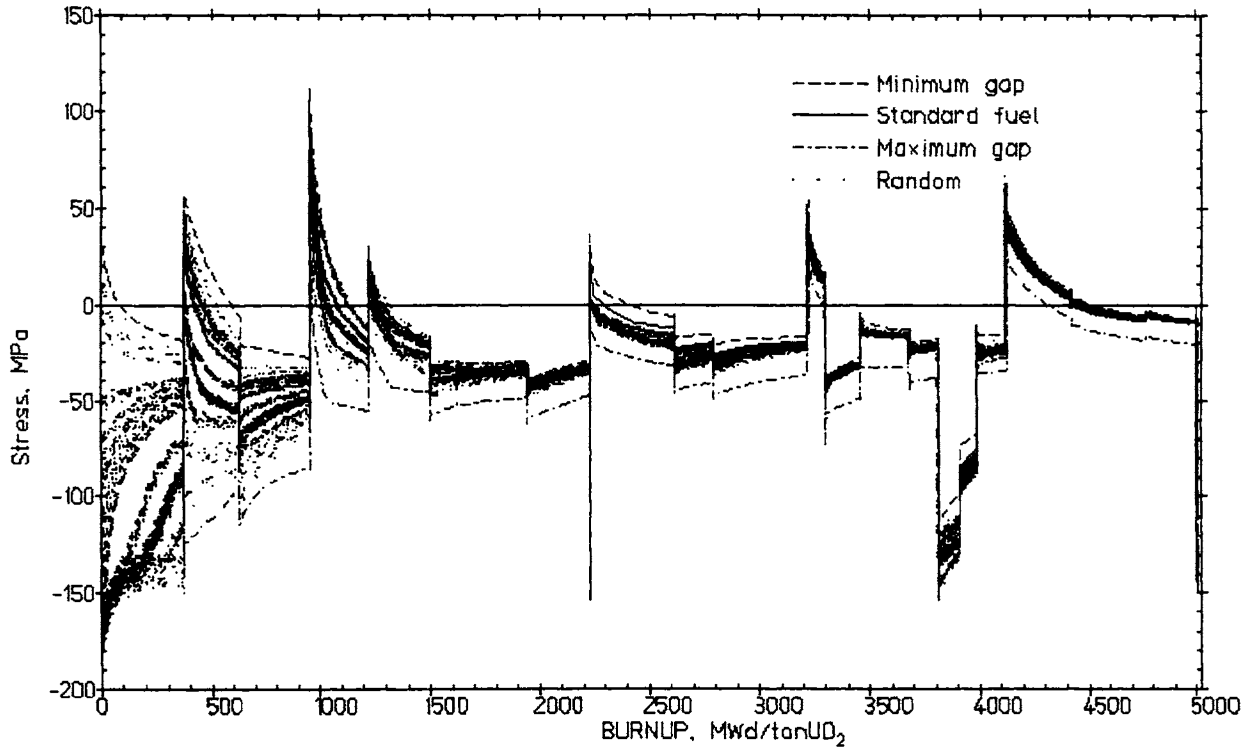

Figure 9: Statistical analysis applied to a CANDU fuel rod. Hoop stress at the cladding.

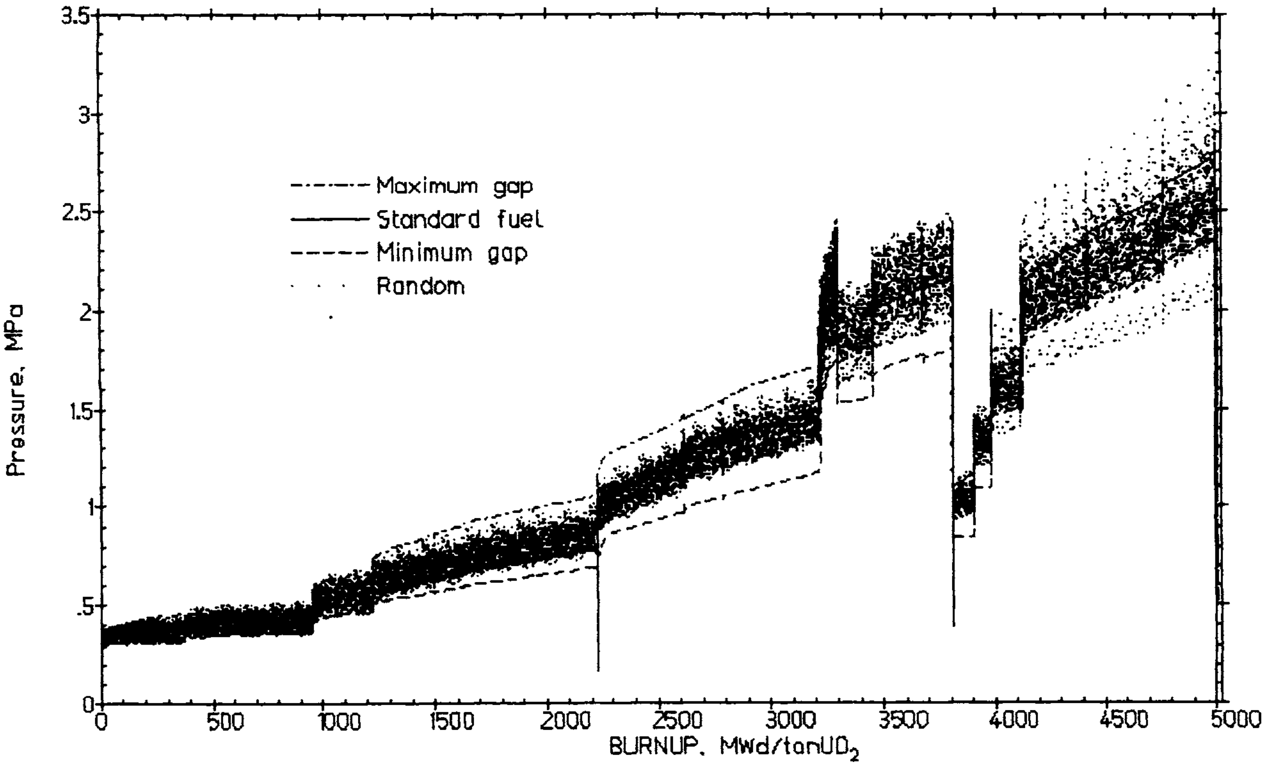

Figure 10: Statistical analysis of a CANDU fuel rod. Gas pressure of the free gases in the rod vs. averaged burnup.

Figure 10 shows pressure from the free gases pressure at the fuel rod. The gas pressure calculation takes into account the thermal calculation, dimensional calculation (stresses), fission gas release, etc. That is the coupling of all the fuel rod parameters (input data and behaviour modelling). There is a small dispersion at BOL. The calculated values of pressure diverge during irradiation. Finally, after 3500 MWd/tonUO_2, there are values both smaller and larger than those predicted at the extreme conditions of the "gap" size situation. *Figure 11* is a histogram of the rod gas pressure of the free gases at EOL. The main value agrees with the one calculated for the standard fuel parameters.

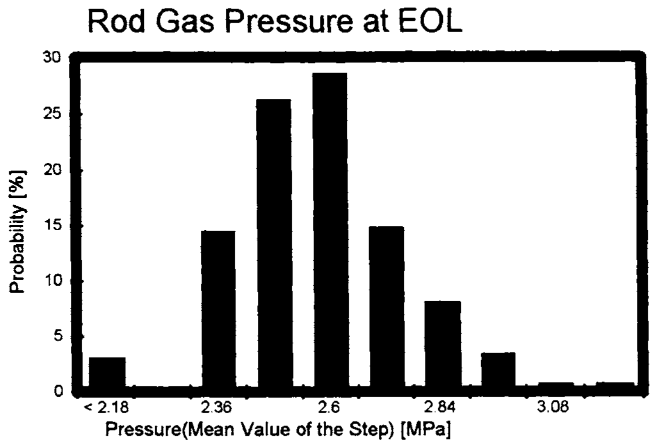

Figure 11: Histogram of the gas pressure of the free gases in the rod at EOL.

5. CONCLUSIONS

As said in the Introduction, BACO (BArra COmbustible) is a code for the simulation of the thermo-mechanical and fission gas behaviour of a cylindrical fuel rod under operation. Its modular structure, where each mechanical model is contained within a separate subroutine, and the detailed coupling of thermo-mechanical and irradiation induced phenomena makes it a powerful tool for studying the influence on fuel performance of material properties, parts dimensions, etc. It also allows to run detailed computer experiments. These characteristics were emphasised in the examples.

The sensibility analysis (section 4) shows the importance of considering all the as-fabricated fuel rod parameters in the fuel performance. For example, a complete fuel element design must consider the dispersion in rod dimensions due to fabrication. The analysis sketched in 4 shows that the study of those cases considered *a priori* as extreme ones is not enough, and that a statistical analysis must be performed.

Changes in the design of rod in fabrication parameters can be tested. This exercise shows, on one hand, the sensitivity of the predictions concerning such parameters and, on the other, the potentiality of the BACO code for a probability study. The latter is due to the fast running of the code and to the modular character of data input and the numerical and graphical output. The results shown here have only a qualitative purpose and are not representative of the variations in the fuel rod fabrication, where the dimensional variations are kept to a narrow band within tolerance.

6. ACKNOWLEDGEMENTS

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