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DIONISIO 2.0: A CODE TO SIMULATE THE BEHAVIOUR OF A NUCLEAR FUEL ROD UNDER IRRADIATION IN NORMAL AND ACCIDENT CONDITION

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Abstract. In this paper we present a brief description of the last version of the nuclear fuel performance code DIONISIO. Designed to describe most of the main phenomena occurring in a fuel rod during operation of the power reactor, the code is under continued development in the Code and Models Section of the Nuclear Fuel Cycle Management of CNEA. The new version of the code was improved with the incorporation of calculation tools designed to extend the application range of the code to high burnup and accident condition across the participation of two international projects sponsored by IAEA.

1 INTRODUCTION

The fuel performance code DIONISIO is designed to describe most of the main phenomena occurring in a fuel rod during operation of the power reactor. The rod is divided into a user defined number of axial segments. Preliminary calculations give the coolant temperature and linear power distributions in terms of input parameters and axial coordinate, z. These functions provide the boundary conditions and the linear power for the whole rod. In each segment, with the boundary conditions assumed uniform and equal to the mean value in the segment, the program simulates the system formed by a pellet and the corresponding gap and cladding portions, as described above, and solves the numerous phenomena that take place under the local boundary conditions. The finite element method is used to integrate the non-linear thermal and mechanical differential equations (Soba and Denis, 2008). Starting from a given (condensed) power history under normal operation conditions, the code predicts the temperature distribution in the domain, elastic and plastic stress and strain, creep, swelling and densification, release of noble gases, neodymium, caesium and iodine to the internal volume of the rod, gas mixing, pressure increase, irradiation growth of the Zircaloy cladding, development of an oxide layer on its surface and hydrogen uptake, restructuring and grain growth in the pellet. The effects of a corrosive atmosphere (SCC) either on the internal or external cladding wall as well as the possibility of pellet-cladding interaction (PCI) are also considered (Denis and Piotrkowski 1996: Denis and Piotrkowski, 1997; Soba, 2007; Denis and Soba, 2003; Soba and Denis, 2006; Soba and Denis, 2008). The results obtained for this representative system are assumed to hold for the entire rod segment. Thus, in each segment the program produces as outputs the values of the temperature, stress, strain, gas release, among others, as functions of the local coordinates r and z. Then, the general rod parameters (internal rod pressure, gas inventory within the rod, pellet stack elongation, etc.) are evaluated at the end of every time step, combining the results of all the axial segments. This new code architecture, which constitutes one of the recent developments incorporated to the 2.0 version of DIONISIO, allows taking into account the axial variation of the linear power and coolant temperature and, consequently, evaluating the dependence of all the significant rod parameters with the longitudinal coordinate.

The new version of the code was also improved with the incorporation of calculation tools designed to extend the application range of the code to high burnup. On the one hand, a group of subroutines, which are tuned for UO2 fuels in LWR conditions, predict the evolution of the radial distribution of 235U, 236U, 238U, 239Pu, 240Pu, 241Pu and 242Pu (Soba et al., 2013). On the other hand, a set of subroutines has been included to simulate the microstructural modifications that the pellet suffers at its external edge under high and very high burnup conditions (Lemes, 2013). Furthermore, subroutines designed to predict the distribution of Caesium, Iodine, Neodymium and Xenon in the pellet solid lattice were also integrated to DIONISIO 2.0 (Soba, et al. 2014), on the basis of experimental information reported in (Lassmann, et. al, 1995; Lassmann et al. 2003).

This paper is structured as follows: section 2 is dedicated to describing the new features introduced in the code version 2.0; in section 3 the more representative results obtained from the battery of experiments used in this work to test the code are described and analyzed; in section 4 general conclusions are summarized.

2 GENERAL DESCRIPTION OF THE CODE

2.1 Domain of resolution

Figure 1.a) shows a portion of a fuel rod consisting of several axial segments. The number of rod segments, and hence the number of pellets per segment, is defined by the user. All the pellets in a given segment are assumed to behave identically (subjected to identical boundary conditions) hence only one pellet, and the corresponding gap and cladding portions, need to be simulated in each segment. In every time step, a complete description of the local system variables is obtained by solving the tightly coupled non linear differential equations (heat, stress-strain, etc.) in such representative system, using the finite elements method. (In particular, the number of segments can be chosen equal to the number of pellets, in which case each pellet is individually described). Axial symmetry and also symmetry with respect to the transversal mid-plane of the pellet are assumed, as schematically shown in Figure 1.b). A typical finite elements discretization of the *r-z* domain is presented in Figure 1.c).

A simple model has been chosen in DIONISIO to compute the coolant temperature axial profile, which input data are provided in the irradiation tests to be simulated. The linear power profile is also given in these tests (although in a variety of formats) or can be simply obtained from the experimental data. For the 2.0 code version, both profiles are discretized according to the user defined rod segmentation, to serve as input data for the separate simulations of the rod segments.

In the calculation scheme of DIONISIO 2.0, the local system is solved as many times as the number of segments in the rod. Then, the temperature and stress-strain distributions in the complete rod are obtained as step-like functions. With respect to the gas inventory, after calculating the amount of gas released by each rod segment (the release of one pellet times the number of pellets in the segment) the code evaluates the release of the whole rod. The composition of the gas mixture in the gap and its thermal conductivity (MATPRO, 2011) are recalculated in every time step. The internal rod pressure is evaluated with the ideal gas law using the total number of gas atoms in the free volume within the rod and the average temperature in the total void volume in the rod (gap and dishings in all the segments, and plenum). The elongations of every individual pellet and the corresponding cladding are added up to obtain the total elongation of the pellet stack and the rod.

The code has a parallel treatment of the linear solver using openMP (www.openmp.org).

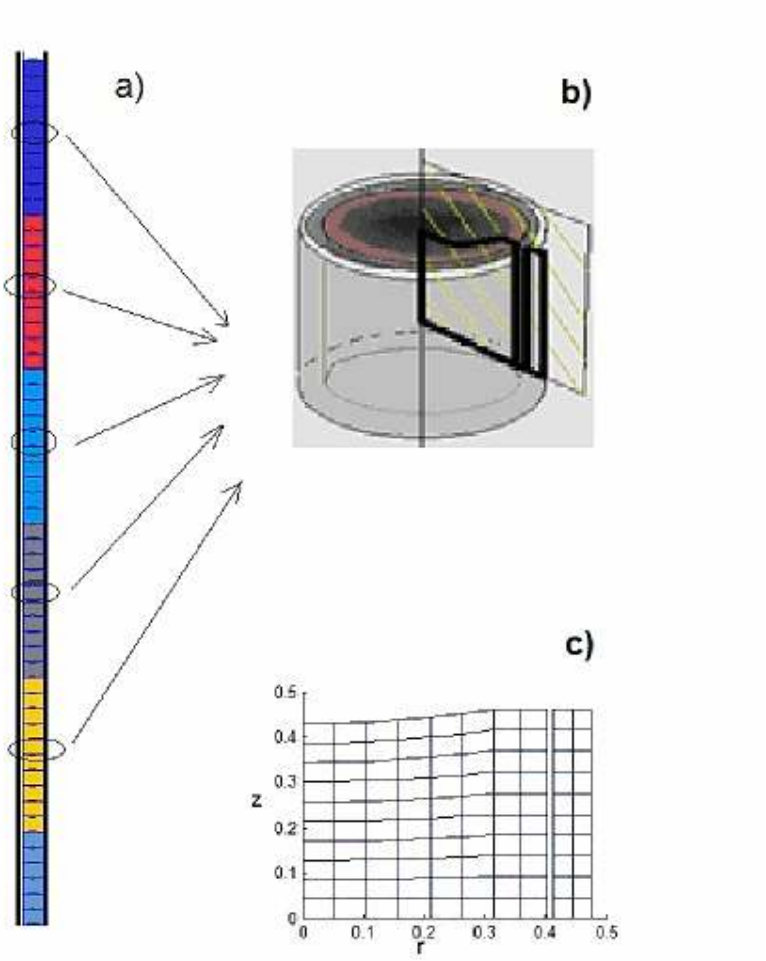


Figure 1: a) Portion of the rod formed by several segments, each one containing a number of pellets. b) One pellet and the corresponding portions of gap and cladding; superimposed is the calculation domain. c) Finite elements discretization of the domain

2.2 High burnup considerations

When the residence time of nuclear fuel rods of uranium oxide is increased beyond a given threshold value, several properties of the pellet material suffer changes and hence the subsequent behaviour of the rod is significantly altered. Due to the absorption of epithermal neutrons by ^{238}U (its absorption cross section exhibits resonant peaks in the energy range comprised between 5 and 2000 eV) and to the chains of nuclear reactions that take place thereafter, several Pu isotopes are born especially at the pellet periphery. In particular, the fissile character of ^{239}Pu and ^{241}Pu is the cause of the increased number of fission events that occur in that ring. For this reason, the radial dependence of the power generation rate and the burnup accumulation need to be considered. These parameters, which at low and intermediate burnup levels can be considered with a reasonably good approximation as uniformly

distributed, reach values two or three times higher at the pellet edge than at the rest of the pellet when the average burnup exceeds a certain magnitude. The numerical codes designed to simulate fuel behaviour under irradiation must include the radial distribution of power density, burnup and concentration of diverse nuclides to produce predictions valid in the high burnup range.

The complete treatment of all the isotopes involved in the nuclear reactions within the pellet encompassing the whole energy spectrum is the task of the codes specialized in reactor physics. A simplified treatment consisting in reducing the energy spectrum to a single group was proposed in the past (Palmer et.al., 1983). The calculation scheme chosen for DIONISIO consists in adopting this simplification and restricting the balance equations to the more abundant isotopes: ^{235}U, ^{236}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{242}Pu. Starting from reliable values of the isotopes concentrations obtained with the neutronic codes CONDOR (Villarino, 2002) and HUEMUL (Grant, in preparation) in a range of irradiation conditions, empirical expressions were fitted to represent, with the higher possible accuracy, the absorption, capture and fission cross sections of these isotopes as functions of the initial enrichment in ^{235}U, the average burnup and the radial coordinate, within the approximation of one neutron energy group.

The general trend to extending the time of residence of the fuel in the reactor is generally accomplished by increasing the initial loading of fissile elements in the fuel via enrichment. This originates the need of introducing some neutron absorber material in the core to compensate the reactivity in excess in the fresh fuel. One of the usual strategies consists in including Gd_2O_3 as burnable absorber in the UO_2 matrix. Its presence has significant effects on the fuel performance: radial modification of the power profile, degradation of the thermal conductivity of the fuel and reduction of the fuel melting point. DIONISIO 2.0 is capable of simulating UO_2 fuels doped with Gd_2O_3 as a burnable poison. The system of equations described above is enlarged to include the Gd 155 and 157 isotopes that play a role in the burnup process, particularly at the beginning of fuel irradiation.

The inhomogeneous distribution of fissile Pu isotopes that builds up for extended irradiation periods and the consequent increase of local burnup in the pellet periphery (rim zone) originate the gradual development of a new microstructure characterized by small grains and large pores as compared with those of the original material. In this region Xe is absent from the solid lattice (although it continues to be dissolved in the rest of the pellet). The porous microstructure in the pellet edge causes local changes in the mechanical and thermal properties, thus affecting the overall fuel behaviour.

A model was developed to describe the behaviour and progress of porosity at local burnup values ranging from 60 to 300 MWd/kgU. The analysis includes the interactions of different orders between open and closed pores (Blair et.at., 2008; Khvostov et.al., 2011), the growth of the pore radius by capturing vacancies, the evolution of the number density of pores, the overpressure within the closed pores and the inventory of fission gas dissolved in the matrix, retained in the closed pores and released to the free volume of the rod. The local burnup, obtained as the result of the contributions of all the fissile isotopes, is plotted in Figure 2 as a function of the radius. Each curve has been drawn for a given value of the average burnup. In this example, the results of DIONISIO are compared with those of CONDOR.

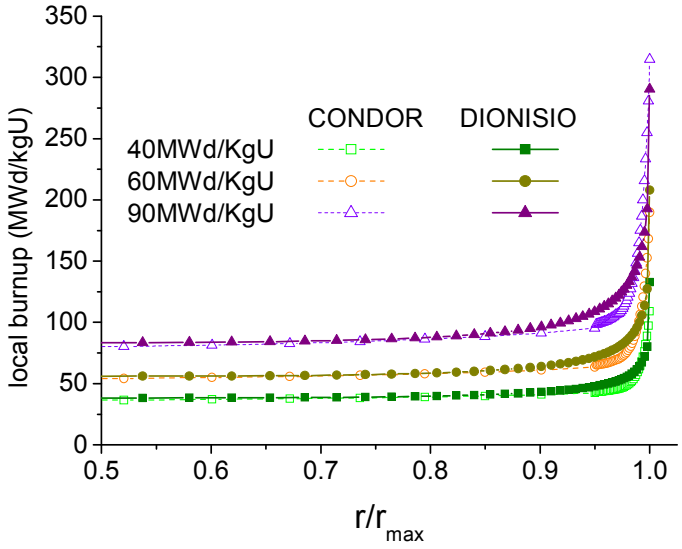


Figure 2: Comparison between the distribution of burnup obtained with the fitting laws developed in DIONISIO and the results given by CONDOR, for different levels of average burnup

2.3 Accident Models

The need of expanding the application range of the DIONISIO code to conditions typical of Loss of Coolant Accidents has prompted the development of a new module able to simulate the thermal-hydraulic conditions in the coolant. This module, which is presently under construction and testing, is intended to give account of the numerous parameters that govern the heat exchange between the fuel rod and the coolant in accidental situations. Different scenarios are taken into consideration: high heat flux with departure from nucleate boiling (DNB) or low heat flux in dry-out conditions. The model adopted analyzes and quantifies the coolant behavior in terms of the system pressure and coolant flow.

Different possible heat transfer conditions and coolant flow patterns that can be axially encountered in a PWR channel in a large and intermediate break LOCA are schematically shown in Figure 33 (NRC, 1986; Mochizuki et.al, 2009; Odar, 2001). An experimental image corresponding to an electrically heated rod is also shown in this figure where the different coolant flow regimes can be appreciated (Tondreas, 1990).

The results of these calculations are expected to provide the adequate boundary conditions for the simulation of the fuel rod behavior, particularly in a so determinant aspect as the thermal behavior. In this sense, the general code is expected to improve its predictive ability with the introduction of the heat transfer coefficients corresponding to the different flow patterns that can be encountered in the vertical current coolant flow.

The degree of development presently achieved with the thermal-hydraulic model developed for the cladding-coolant system allows analyzing and quantifying a considerable number of parameters involved in the rod evolution. Heat accumulated and released, temperature distribution in the rod, particularly on its external surface, temperature of the fluid in the cooling channel, vapor mass and volume fraction in the coolant, pressure and coolant flow drop, among others are evaluated not only in normal operation conditions but also in accidental conditions, in particular those described as LOCA events.

The fast variations and the extreme conditions the fuel rod experiences in this type of accident may cause severe rod damage. Safety reasons indicate the importance of building accurate simulation tools. But, these rapid transients are precisely the cause of some of the more challenging difficulties encountered in the simulations since the system general conditions are definitely far from equilibrium[1].

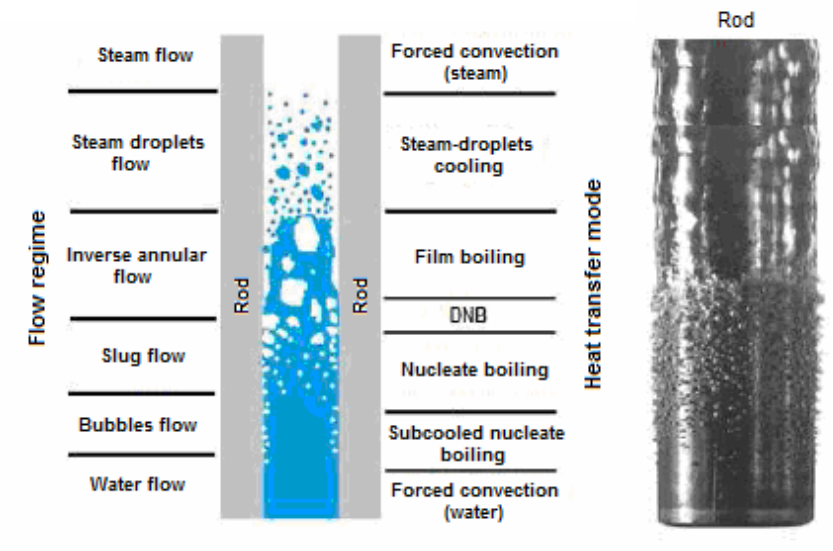


Figure 3: Heat transfer an flow configurations with high heat flux; (In the right) An image of the distribution of convective boiling around a heated rod

3 VALIDATION

In order to validate the code several experimental data reported in the IAEA and IFPE data basis were simulated with the recent version 2.0 of DIONISIO. The results presented below show the comparisons with some of the items reported in the experimental data basis. Also comparisons with available results of simulations of other codes, for instance those (some 15 codes developed in different countries) which participated in international exercises of codes comparison (those of the FUMEX series FUMEX-II, 2012; FUMEX-III, 2013) among others (van Uffelen, 2002; Sah et al., 2008) were used.

Here we present just some selected results to shows general capabilities of the code.

The CONTACT series of experiments use short rods of Zry-4 clad - UO2 pellets of typical PWR fuels irradiated in a pressurized water loop at a nearly constant power (Turnbull, 1998; Bruet et.al. 1980). In CONTACT 1 the rod was irradiated at a power level close to 40 kW/m to a discharge burnup of ~22 MWd/kgU. In CONTACT 2 the irradiation was performed at a power of 25 kW/m and an internal helium pressure between 0.1-0.2 MPa. The rod was discharged early because of a failure at a burnup of ~5.5 MWd/kgU and replaced with the identical design rod CONTACT 2bis that reached a burnup of 12.4 MWd/kgU.

Figure 4 shows the center temperature for CONTACT 1 and CONTACT 2bis and the respective prediction with DIONISIO. The more exigent thermal conditions of experiment CONTACT 1 lead to a larger final clad strain due to PCMI as compared with CONTACT 2bis.

[1] The LOCA group of subroutines were presented in a separate paper in the same section of ENIEF 2016.

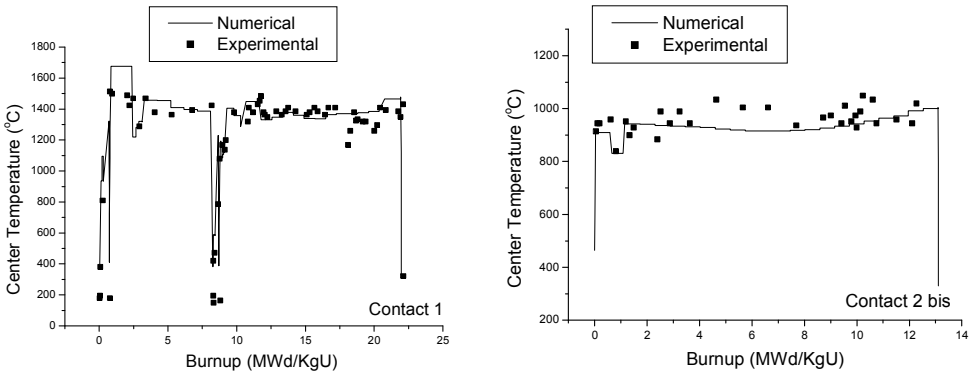


Figure 4: Center temperature for CONTACT 1 and 2bis experiments

Figure 5 shows the comparison between the experiments and the predictions of DIONISIO for the cladding strain for both cases.

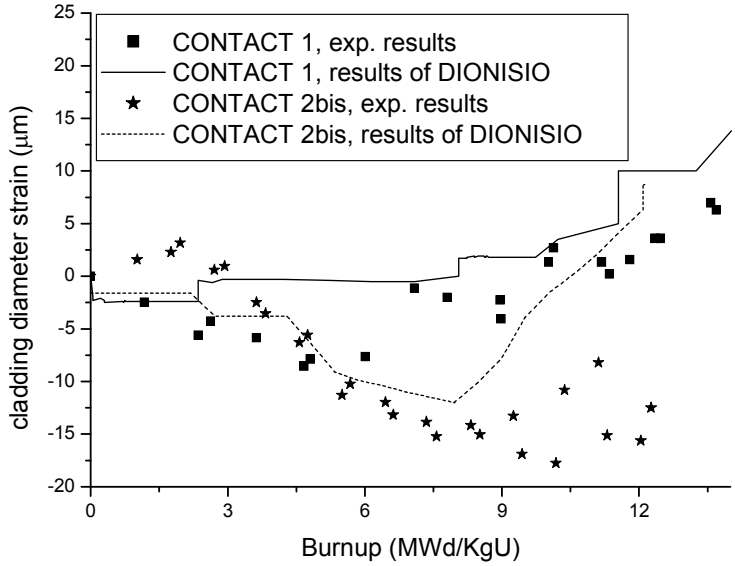
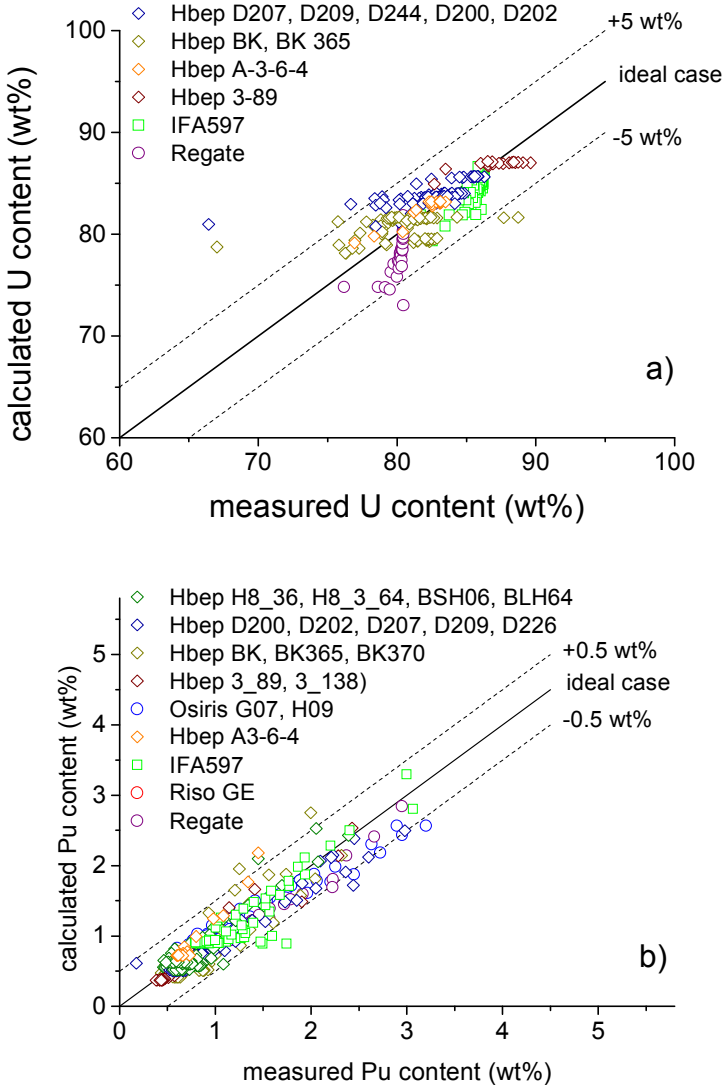
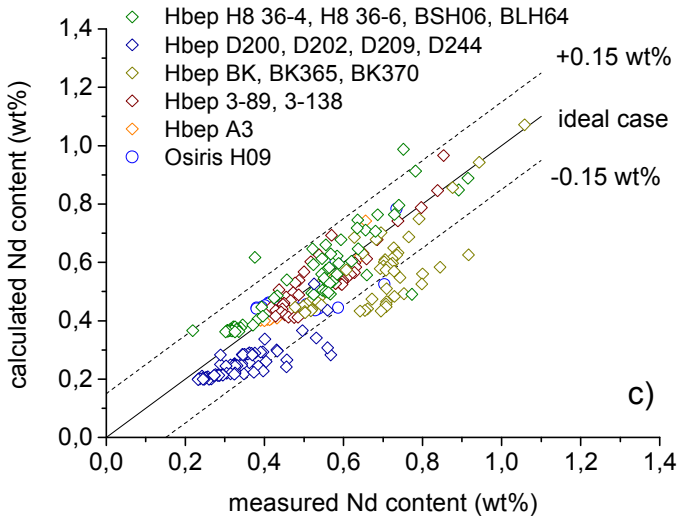


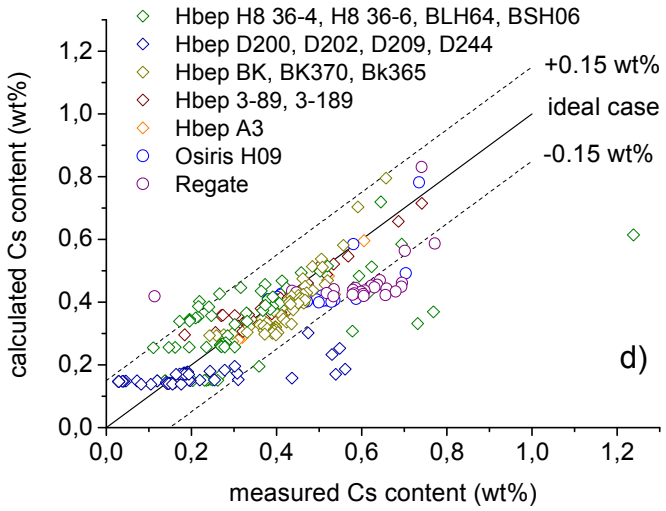
Figure 5: Cladding strain for CONTACT 1 and 2bis

In the group of graphics that form Figure 6, experimental data of total Uranium, Plutonium, Neodymium, Caesium and Xenon content (involving the stable isotopes) available in the experimental tests mentioned above are compared with the results of simulations performed with DIONISIO. In the five plots dotted parallel lines are drawn at both sides of the line of perfect agreement to underline the agreement between calculations and measurements. In particular for Pu (Figure 6 b)), 97% of the nearly 270 plotted points fall within the band ± 0.5 wt% at both sides of the bisector of the first quadrant. Equivalently, the mean value of the absolute difference between calculated and measured values represents 19% of the mean value

of the measured data, expressing also the good quality of the approximation reached with the simulations. A similar analysis applies for the plot of the total U, Nd, Cs and Xe content where the bands are limited by lines drawn at ± 5 wt% for U and at ± 0.15 wt% for Nd, Cs and Xe.







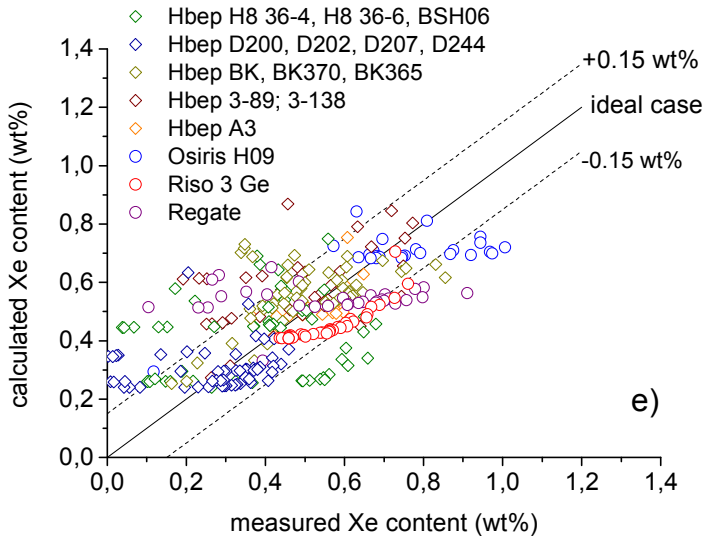


Figure 6: Calculated vs. measured values of local concentration of a) U, b) Pu, c) Nd, d) Cs, e) Xe

In Figure 7 present calculated and measured values of average burnup, centre temperature, FGR and internal pressure corresponding to experiments taken from IAEA data base are compared. In particular, an excellent agreement is evidenced in Figure 7.a), where all the points representing the average burnup fall within a narrow strip of ±2MWd/kgU around the bisecting line. In Figure 7 .b) the oblique lines delimit the values of the centre temperature comprised between 100°C over and below the calculated-measured coincidence line. The major departure occurs for the IFA432 and IFA562 experiments, (particularly in the middle temperature range 600-1200°C). This dispersion can be attributed to the difficulties in identifying the physical location of the point where the burnup measurement is performed and hence in determining its correspondence with the temperature value reported. In Figure 7.c), an acceptable agreement between calculated and measured values of FGR is seen, especially for release below 20%. Nevertheless, a trend to underprediction is recognized particularly for the values corresponding to the HBEP rods. In these experiments, abrupt final ramps were applied which most probably provoked an important release. In this respect, the DIONISIO code contains a module that gives reasonable account of gas release in isothermal processes and also in slow transients but does not possess yet the adequate subroutine to give account of fast transients. As for Figure 77.d), although the available experimental internal pressure data are comparatively scarce, the general trend is qualitatively well reproduced by the simulations.

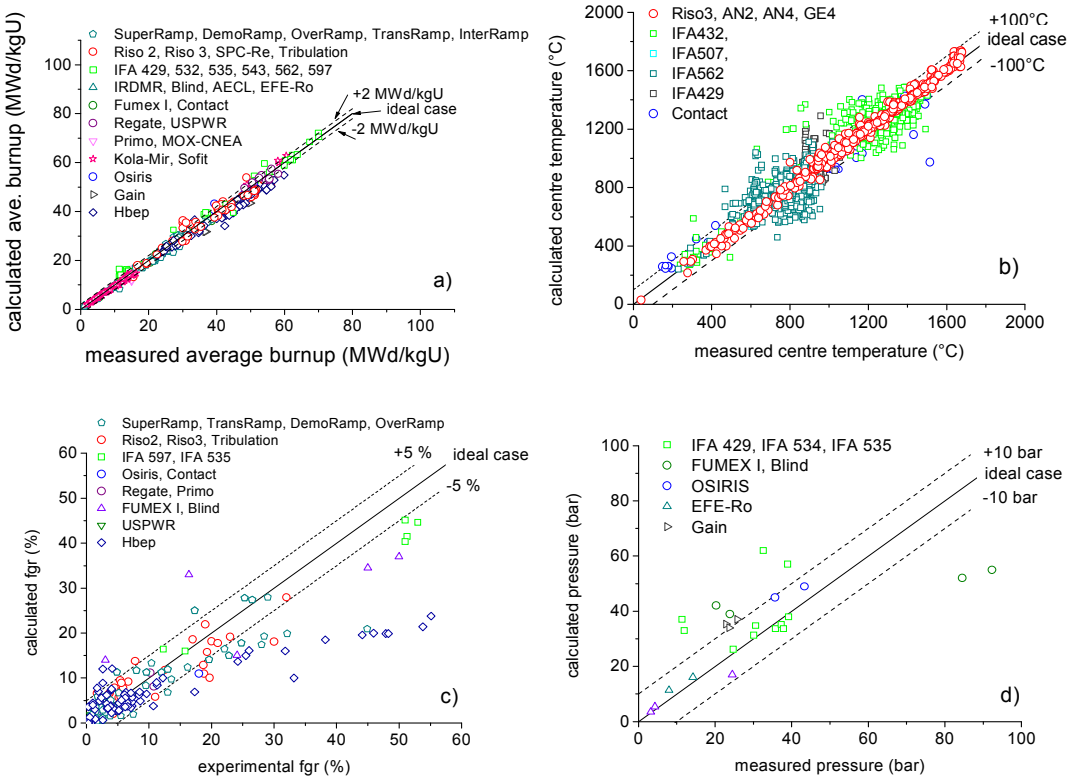


Figure 7: Calculated vs. measured data of a) average burnup, b) centre temperature, c) FGR and d) internal pressure for experiments from IAEA data base

Due to thermal expansion and mechanical restrictions, the pellet experiences a non-uniform deformation: the initially cylindrical pellet surface distorts, bending outwards, suffering a more pronounced displacement in the region of the top and bottom faces than at the central belt. If the pellet strain is sufficiently large, it may come into contact with the cladding (PMCI), particularly in regions next to the pellet-pellet contact surfaces, giving place to a bamboo type differential deformation in the cladding evidenced by the presence of equidistant circumferential ridges. The two-dimensional structure of DIONISIO along with the model of mechanical contact included in it allows an acceptable description of the bamboo effect and the radial cladding deformation. As an example a comparison between calculated and measured determinations of strain in several rods taken from IRDMR experiments are presented in Figure 8.a). About 94% of the points are distributed within the range of ±0.2% over and below the line representing the ideal case. Even though this is a significant dispersion, representing in some cases nearly 100% of the measured value, it has to be admitted that the code gives a right guess of the order of magnitude of the strain, which experimental determinations are affected by a large relative error. As an example, the evolution of the strain in the ABS rod is presented in Figure 8 .b) where the upper curve corresponds to the zone of maximum strain and the lower one to the pellet mid-plane where the strain is minimal. It is seen that the general trend is correctly represented by the numerical approach of DIONISIO although a certain discrepancy between calculated and measured points is recognized. For instance, at the beginning of irradiation, the measured mid pellet

strain shows an increase which is not accounted for by the code. Other discrepancies are also visible between 10 and 15 irradiation days. They are probably due to some averaging in the input power history that was performed in order to shorten the calculation time. In this respect further examination of the code and the input data need to be carried out in the near future.

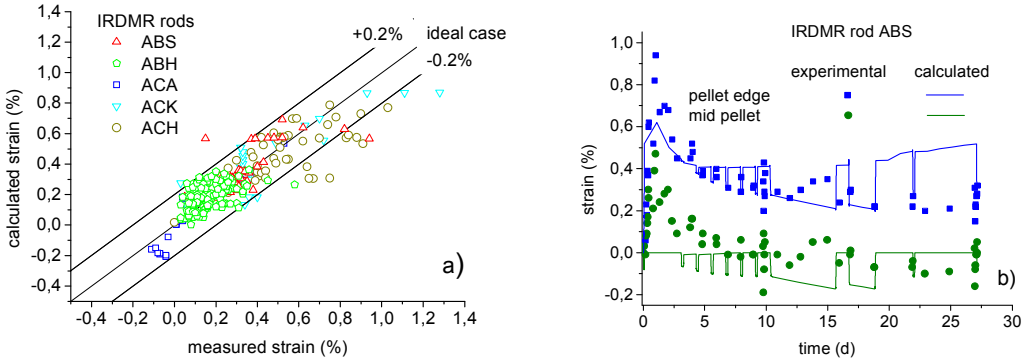


Figure 8: a) Comparison between measurements and the predictions of DIONISIO for several rods of the IRDMR experiment. b) Evolution of the strain at the pellet edge and mid-plane of the ABS rod of the IRDMR experiment

4 CONCLUSIONS

The results presented in this paper reveal that, beyond certain degree of departure between measurements and calculations, the code performance is correct, giving an adequate overall description of the relevant parameters of the fuel rod, required for the design and analysis of behavior in operation.

A wide range of data was used to make the comparisons, spanning a variety of fuel designs and operation conditions. Data obtained in experiments performed with standard fuel rods of the PWR, BWR, PHWR, CANDU and WWER types were used. The controlled experiments correspond to high, media or low burnup. Some of them were carried out on rods irradiated in commercial reactors and then instrumented to record particular behavior features.

With the improvements recently introduced, involving also subroutines for the physical and chemical properties of the fuel material in the high burnup range, the code DIONISIO in its version 2.0 evidences a good performance in the many simulations carried out. Given the complexity of the experiments and the number of physical and chemical parameters involved, the degree of dispersion between calculations and measurements does not invalidate considering the DIONISIO 2.0 code as an acceptable prediction tool even for average burnup levels as high as 60 MWd/kgU.

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