



# Inclusion of models to describe severe accident conditions in the fuel simulation code DIONISIO



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## ABSTRACT

The simulation of fuel rod behavior is a complex task that demands not only accurate models to describe the numerous phenomena occurring in the pellet, cladding and internal rod atmosphere but also an adequate interconnection between them. In the last years several models have been incorporated to the DIONISIO code with the purpose of increasing its precision and reliability. After the regrettable events at Fukushima, the need for codes capable of simulating nuclear fuels under accident conditions has come forth. Heat removal occurs in a quite different way than during normal operation and this fact determines a completely new set of conditions for the fuel materials. A detailed description of the different regimes the coolant may exhibit in such a wide variety of scenarios requires a thermal-hydraulic formulation not suitable to be included in a fuel performance code. Moreover, there exist a number of reliable and famous codes that perform this task. Nevertheless, and keeping in mind the purpose of building a code focused on the fuel behavior, a subroutine was developed for the DIONISIO code that performs a simplified analysis of the coolant in a PWR, restricted to the more representative situations and provides to the fuel simulation the boundary conditions necessary to reproduce accidental situations. In the present work this subroutine is described and the results of different comparisons with experimental data and with thermal-hydraulic codes are offered. It is verified that, in spite of its comparative simplicity, the predictions of this module of DIONISIO do not differ significantly from those of the specific, complex codes.

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## 1. Introduction

In recent years the DIONISIO code has undergone several improvements aimed at extending its application range and increasing its predicting capacity. The modifications introduced in the 2.0 version of DIONISIO have been described in detail in previous papers (Soba and Denis, 2015; Soba et al., 2013, 2015, 2014); the main characteristics are summarized here.

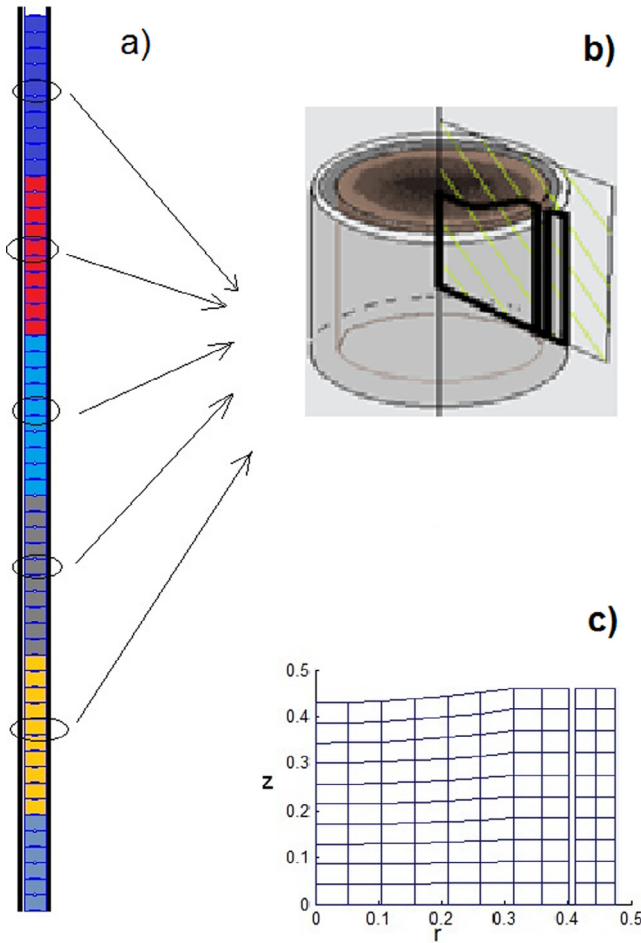
An acceptable prediction of the high burnup behavior is achieved with a simplified scheme embedded in the program, where the balance equations are restricted to the most relevant isotopes involved in the fission process and the energy spectrum is reduced to one-group. Hence, the effective cross sections of these isotopes, their concentration, the power density and burnup are obtained as functions of the radial position in the pellet, average burnup, and initial enrichment in <sup>235</sup>U. Moreover, some mathematical expressions were developed to describe the behavior and

progress of porosity and grain size at the very high local burnup values that can be reached at the pellet external ring.

To take into consideration the axial variation of reactor linear power and coolant temperature, the rod is divided into a user defined number of segments, as shown in Fig. 1a. All the pellets in a given segment are assumed to behave identically (subjected to identical boundary conditions). Therefore, only one pellet and the corresponding gap and cladding portions have to be simulated in each segment. Axial symmetry and also symmetry with respect to the transversal mid-plane of the pellet are assumed, as schematically shown in Fig. 1b. For this reason, a two-dimensional domain, as shown in Fig. 1c, involving the radial and axial coordinates needs to be considered. The finite elements method is used to solve the different aspects of the problem.

In every time step and for each axial section, a complete description of the local system variables is obtained by solving the tightly-coupled, non-linear differential equations describing the thermal and mechanical parameters. Then, the temperature and stress-strain distributions in the complete rod are obtained as step-like functions of the axial coordinate. With respect to the

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**Fig. 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.

gas inventory, the code evaluates the amount of gas released by each rod segment and then that released by the whole rod. The composition of the gas mixture in the gap and its thermal conductivity 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 elongation of every individual pellet and the corresponding cladding are added up to obtain the total elongation of the pellet stack and the rod.

This code version has been employed so far to simulate a considerable number of experiments involving fuel rods of diverse types, operating in normal conditions. Moreover, some 380 fuel rods irradiated up to average burnup levels of 40–60 MW d/kg U, which may represent local burnup levels higher than about 200 MW d/kg U in the pellet external rim were simulated with satisfactory results.

The need of expanding the application range of the code to conditions typical of Loss of Coolant Accidents (LOCA) has prompted the development of a new module able to reproduce the thermal-hydraulic conditions in the coolant. This module is intended to give account of the numerous parameters that govern the heat exchange between the fuel rod and the coolant in accident situations, thus providing the boundary conditions necessary to simulate the fuel rod behavior during a fast excursion, particularly in such a determinant aspect as the thermal behavior.

The code simulates a vertical channel containing one fuel rod. Scenarios like forced single-phase (water or vapor) convection or double-phase flow, including departure from nucleate boiling (DNB) are taken into consideration. The model adopted analyzes and quantifies the coolant behavior in terms of the system pressure and coolant velocity. Moreover, models to describe mechanical problems occurring in accidental situations, like ballooning and burst, are also included.

In the present work a separate testing plan was first followed, which consisted in comparing the predictions of the new thermal-hydraulic module with specific codes in different flow regimes. Then it was included as a subroutine of the DIONISIO code and its results were compared with available experimental data. It is seen that the predictive ability of the general code has improved with the introduction of the heat transfer coefficients corresponding to the different patterns that can be encountered in the coolant flow.

## 2. Models and parameters involved

### 2.1. Mechanical aspects

The simulation of off-normal operation conditions imposes the need of incorporating diverse mechanical models to the code, specific for these conditions. At the present time, a model to predict clad failure (burst stress) and its localization, and another of cladding creep to evaluate clad ballooning have been recently included in the code. These subroutines are turned on if accidental conditions are met.

Cladding failure is assumed to occur when the hoop stress exceeds the burst stress,  $\sigma_B$ . The empirical correlation (Rosinger, 1984; Manngard et al., 2011)

$$\sigma_B = C_1 \exp(-C_2 T) \exp\left(-(C_0 W_{fO})^2\right) \quad (1)$$

was adopted as cladding burst criterion, where  $C_0$ ,  $C_1$  and  $C_2$  are constants whose values for Zircaloy (Zry) in the single-phase domains  $\alpha$  and  $\beta$  are listed in Table 1,  $T$  is the absolute temperature and  $W_{fO}$  is the total weight fraction of oxygen picked up in high temperature metal-water reactions.

For the effective cladding creep rate the correlation (Manngard et al., 2011)

$$\frac{d\varepsilon}{dt} = C_3 \exp\left(-\frac{C_4}{T}\right) \exp(-C_5 w_{fO}) \sigma_{VM}^n \quad (2)$$

was adopted. It is valid when the cladding material is in the pure  $\alpha$  or  $\beta$  phase;  $w_{fO}$  is the excess oxygen weight fraction in the cladding metal layer and  $\sigma_{VM}$  is the von Mises stress. The constants  $C_3$ ,  $C_4$ ,  $C_5$  and  $n$  adopt the values listed in Table 1 when the Zry cladding material is in the single phase domains ( $\alpha$  or  $\beta$ ). For the two-phase ( $\alpha + \beta$ ) region, the creep rate is calculated as an average of both single-phase rates weighed with the volume fractions of both phases.

**Table 1**

Values of the constants used in correlations (1) and (2), in pure  $\alpha$  or  $\beta$  phases.

	Pure $\alpha$ -Zr	Pure $\beta$ -Zr
$C_0$	1052.63	1052.63
$C_1$ (N cm <sup>-2</sup> )	$8.3 \times 10^4$	$2.3 \times 10^5$
$C_2$ (K <sup>-1</sup> )	0.001	0.003
$C_3$ (s <sup>-1</sup> N <sup>-n</sup> cm <sup>2n</sup> )	$1.4523 \times 10^{-8}$	$2.1751 \times 10^{-7}$
$C_4$ (K)	38487.0	17079.0
$C_5$	342.0	0.0
$n$	5.89	3.78

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