Annals of Nuclear Energy 70 (2014) 147–156

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Simulation of the behaviour of nuclear fuel under high burnup conditions

Alejandro Soba [a,*], Martin Lemes [a], Martin Emilio González [a], Alicia Denis [a], Luis Romero [b]

[a] U.A. Combustibles Nucleares, Comisión Nacional de Energía Atómica, Avenida del Libertador 8250, 1429 Buenos Aires, Argentina
[b] U.A. Reactores Nucleares, Comisión Nacional de Energía Atómica, Avenida del Libertador 8250, 1429 Buenos Aires, Argentina

ARTICLE INFO

Article history:
Received 10 January 2014
Accepted 3 March 2014
Available online 2 April 2014

Keywords:
DONISIO code
High burnup zone
Gadolinium
Fuel performance modelling

ABSTRACT

In this paper we summarize all the models included in the latest version of the DIONISIO code related to the high burnup scenario. Due to the extension of nuclear fuels permanence under irradiation, physical and chemical modifications are developed in the fuel material, especially in the external corona of the pellet. The codes devoted to simulation of the rod behaviour under irradiation need to introduce modifications and new models in order to describe those phenomena and be capable to predict the behaviour in all the range of a general pressurized water reactor. A complex group of subroutines has been included in the code in order to predict the radial distribution of power density, burnup, concentration of diverse nuclides and porosity within the pellet. The behaviour of gadolinium as burnable poison also is modelled into the code. The results of some of the simulations performed with DIONISIO are presented to show the good agreement with the data selected for the FUMEX I/II/III exercises, compiled in the NEA data bank.

1. Introduction

The DIONISIO code has been developed to simulate most of the main phenomena that take place within a fuel rod during the normal operation of a nuclear reactor. The code, which has more than forty interconnected models and a modular structure, predict: temperature distribution, thermal expansion, elastic and plastic strain, creep, irradiation growth, pellet-cladding mechanical interaction, fission gas release, swelling and densification. Axial symmetry is assumed and cylindrical finite elements are used to discretize the domain (Simulación del comportamiento termomecánico de una barra combustible en operación, 2007; Denis and Soba, 2003; Soba and Denis, 2008). The rod is divided into a user defined number of axial segments where a complete axi-symmetric local domain is solved. All the general rod parameters (pressure, fission gas release, free volume of the rod, etc.) are evaluated at the end of every time step averaging the local values obtained. This modification allows taking into account the axial variation of the linear power and, consequently, evaluating the dependence of all the significant rod parameters with that coordinate.

Recently a group of subroutines, designed to extend the application range of the code to high burnup (Kinoshita, 1997; Noirot et al., 2008), has been included. The new calculation tools, which are tuned for UO_2 fuels in LWR conditions, predict the radial distribution of ^{235}U, ^{236}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{242}Pu across the pellet (Newton and Hutton, 2002). Usually codes specialized in reactor physics perform these calculations solving the Boltzmann transport equations in a number of energy intervals (groups) and including adequate considerations in the region of the resonant absorption peaks of ^{238}U. They predict with high precision the radial distribution of neutron flux, burnup and concentration of every species, fissile, fissionable or fertile, gaseous or solid, within the rod, relevant for the overall process, all of them as functions of time. Among the known reactor codes we mention WIMS-E (Hutton et al., 2004), HELIOS (Stammler et al., 1996; HELIOS Methods, 1998), CONDOR (Eduardo Villarino CONDOR CALCULATION PACKAGE PHYSOR, 2002) and HUEMUL (C. Grant, 2014). Without loosing the required completeness, a simplified treatment consisting in reducing the energy spectrum to a single group was included in DIONISIO. Empirical expressions were obtained to represent, with the higher possible approximation degree, the absorption and capture cross sections as functions of the initial enrichment in ^{235}U, the average burnup and the radial coordinate. The curves obtained with a so drastic simplification demand a testing before incorporation in the general fuel behaviour code. This testing is performed via comparison with the reliable reactor codes. With the validated curves already incorporated, the fuel code is expected to give with a reasonable precision the time evolution of the local burnup and hence, the size of the rim zone. The first antecedent in this type of analysis is found in the RADAR model (HELIOS Methods, 1998) which was validated against the WIMS code. The

* Corresponding author. Tel.: +54 011 4839 6796.
E-mail addresses: soba@cnea.gov.ar (A. Soba), lemes@cnea.gov.ar (M. Lemes), megozal@cnea.gov.ar (M.E. González), denis@cnea.gov.ar (A. Denis), lromero@cnea.gov.ar (L. Romero).

http://dx.doi.org/10.1016/j.anucene.2014.03.004
0306-4549/

TUBRNP model, included in the TRANSURANUS code (Schubert et al., 2008) and the RAPID model (Lee et al., 2000) served as a basis for the development of the present work. The original idea of RADAR is conserved but the validity range and scope of the equations are extended.

The general trend to increasing the fuel initial enrichment originates the need of introducing some absorber material in the core. The usual strategy consisting of including Gd_2O_3 as burnable absorber in the UO_2 matrix 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. Among the seven isotopes of gadolinium, those with mass numbers 155 and 157 have particularly high absorption cross section in the thermal energy range. For this reason Gd is burnt in the vicinity of the fuel surface thus shielding the pellet interior from thermal neutrons. The interface between burnt and unburnt Gd shifts towards the pellet centre as irradiation progresses. The isotopes with mass numbers 156 and 158 produced respectively by these reactions have very small absorption cross sections and need not any further consideration from the neutron distribution point of view (Massih et al., 1992). We include the possibility of simulating UO_2 pellets doped with Gd_2O_3 as a burnable poison obtaining the evolution of these isotopes across the pellet radius.

The task described in the preceding paragraph was performed in connection with the reactor cell codes HUEMUL and CONDOR. In Section 2 we describe some of the characteristics of this work and present some results, taking into the account that the main task and detailed description were presented elsewhere (Soba et al., 2013).

Additionally, an expression to describe the burnup induced degradation of the thermal conductivity of UO_2 during the fuel operation time was recently elaborated. The formula also evaluates the conductivity of fuels with some content of Gadolinium in the range from 0 to 8 wt%, which is the usual proportion in the UO_2 fuels with burnable poisons. The new model was firstly compared with conductivity experimental data and was then implemented into the DIONISIO code. Some results of this code aspect were reported in González et al. (2013).

Moreover, empirical expressions representing the amounts of Caesium, Neodymium and Xenon, mainly following Lassmann et al. (1995, 2003) were compared with experimental data and incorporated in DIONISIO as new subroutines.

Finally new models which describe the porosity behaviour and fission gas release in the rim are also developed and included in the code. This work was presented elsewhere (Martín Lemes et al., 2014; Estudio analítico y numérico de los efectos de la irradiación hasta alto quemado en combustibles de reactores de potencia, 2013) but for completeness all the models referred to HBS are presented here. The main aspects are summarized in Section 4 along with some results of comparisons with several experimental data taken from the literature to show the overall performance of the code.

These improvements together with the structural modifications of the program gave origin to the new code version DIONISIO 2.0. Moreover, a considerable number of experiments compiled in IAEA (http://www.iaea.org., 2014; http://www.oecd-nea.org/science/fuel/ifpelst.html., 2014) data bases were simulated with the present code structure. Some of these comparisons are also presented here.

2. One energy group calculation

The balance equations listed below express the variation rate of the concentration of each of the relevant isotopes. They are indicated by N, measured in $atoms/cm^3$, with a subscript formed by the name of the element and the mass number of the isotope. σ and ϕ represent, respectively, the cross section (expressed in barns) and the neutron flux (in $neutrons/(cm^2\,s)$), assuming the energy spectrum reduced to a single group. σ is labeled with a subscript a, c or f to indicate absorption, capture or fission, respectively, and with a superscript to identify the nuclide. The same superscript is used to label the decay constant λ (measured in $1/s$). N and ϕ are considered as functions of the irradiation time (t) and the radial position (r) in the pellet. For the U and Pu isotopes, the cross sections are assumed to depend on the radius, the average burnup (b) and the initial enrichment (q) in ^{235}U measured in $w\%$. For the Gd isotopes, these parameters depend also on the initial content of Gd (g), measured in $w\%$.

$$\frac{\partial C_{U235}}{\partial t} = -C_{U235}(t,r)\sigma_a^{235}(b,r)\phi(t,r) \tag{1}$$

$$\frac{\partial C_{U236}}{\partial t} = -C_{U236}(t,r)\sigma_a^{236}(b,r)\phi(t,r) + C_{U235}(t,r)\sigma_c^{235}(b,r)\phi(t,r) \tag{2}$$

$$\frac{\partial C_{U238}}{\partial t} = -C_{U238}(t,r)\sigma_a^{238}(b,r)\phi(t,r) \tag{3}$$

$$\frac{\partial C_{Pu239}}{\partial t} = -C_{Pu239}(t,r)\left(\sigma_a^{239}(b,r)\phi(t,r) + \lambda^{239}\right) + C_{U238}(t,r)\sigma_c^{238}(b,r)\phi(t,r) \tag{4}$$

$$\frac{\partial C_{Pu240}}{\partial t} = -C_{Pu240}(t,r)\left(\sigma_a^{240}(b,r)\phi(t,r) + \lambda^{240}\right) + C_{Pu239}(t,r)\sigma_c^{239}(b,r)\phi(t,r) \tag{5}$$

$$\frac{\partial C_{Pu241}}{\partial t} = -C_{Pu241}(t,r)\left(\sigma_a^{241}(b,r)\phi(t,r) + \lambda^{241}\right) + C_{Pu240}(t,r)\sigma_c^{240}(b,r)\phi(t,r) \tag{6}$$

$$\frac{\partial C_{Pu242}}{\partial t} = -C_{Pu242}(t,r)\left(\sigma_a^{242}(b,r)\phi(t,r) + \lambda^{242}\right) + C_{Pu241}(t,r)\sigma_c^{241}(b,r)\phi(t,r) \tag{7}$$

$$\frac{\partial C_{Gd155}}{\partial t} = -C_{Gd155}(t,r)\sigma_a^{155}(r,b,q,g)\phi(t,r) \tag{8}$$

$$\frac{\partial C_{Gd157}}{\partial t} = -C_{Gd157}(t,r)\sigma_a^{157}(r,b,q,g)\phi(t,r) \tag{9}$$

Reactor codes generally divide the neutrons energy spectrum in two groups, described as thermal (neutrons with energies below *0.65* eV) and fast (neutrons with higher energies). Both the fast and thermal fluxes are used in the balance Eqs. (1)–(9) to predict the behaviour of each species.

The increased content of Plutonium in the external zone is basically due to the behaviour in the resonance region of the absorption cross section of ^{238}U. The equation used in DIONISIO to express this behaviour was fitted to results of simulations performed with the CONDOR and HUEMUL codes:

$$\sigma_{abs}^{238}(r,b,en) = c_1\left(c_2 + c_3 b_{1000} + c_4 b_{1000}^2 + c_5 b_{1000}^3\right) \times \left(c_6 + c_7 \exp\left(c_8\left(1 - \frac{r}{r_{max}}\right)^{c_9}\right)\right) \tag{10}$$

The function has a shape similar to the expressions used in other codes (Lee et al., 2000). The remaining cross section functions to be introduced in the subroutine are evaluated as follows: the codes CONDOR and HUEMUL are run assuming the conditions of a generic UO_2 pellet; the initial enrichment is varied from 0.7% to 12%; the initial content of Gd (g) is assigned values in the range 4–10%; the final average burnup is given values ranging from fresh fuel to 120 MWd/kgU. With these results, curves are drawn for