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REACTORS DEPARTMENT

ETOBU - SINGLE ENERGY POINT MODEL BURNUP COMPUTER CODE FOR WATER REACTORS

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A B S T R A C T

UABUC is a single energy point reactor burnup computer program in FØRTRAN language. The program calculates the change in the isotopic composition of the uranium fuel as a function of irradiation time with all its associated quantities such as the average point flux, the conversion ratio, macroscopi fuel cross sections, and the point reactivity profile. A step-wise time analytical solution was developed for the nonlinear first order burnup differential equations. The "Westcott" convention of the effective cross sections was used except for plutonium-240 and uranium-238. For plutonium-240, an effective microscopic cross section was derived from the direct physical arguments taking into account the selfshielding effect of plutonium-240 as well as the 1 ev. resonance absorption. For uranium-238, an effective cross section, reflecting the effect of fast fission and resonance absorption was used. The fission products were treated in the three groups with 50, 300, and 800 barns. The yields in the groups were treated as functions of the type of fissionable nuclides, the effective neutron temperature, and the epithermal index. Xenon-135 and samarium-149 were treated seperately as functions of irradiation-time.

INTRODUCTION

This work has been conducted as a part of an integrated reactor physics calculations scheme proposed at the Reactors Department of the ARE Atomic Energy Esablishment. An important part in this scheme is to study the space-time variation in the isotopic fuel composition as burnup proceeds. In order to perform such study usually a numerical matching between a point burnup model and the transport or diffusion equation is required, or conversely a point burnup model is the first step towards the construction of a spatial burnup computer code. This report presents the theory of the point model burnup computer code "UABUC" which has been tested successfully for a reference reactor model of the pressurized heavy water type using natural uranium fuel[1]

HEAVY ISOTOPES REPRESENTATION

Following the irradiation history of a nuclear fuel containing U^{235} and U^{238} mixture, and introducing the physical simplifications[1,2,3] which allow the decoupling of the U^{235} and U^{238} into two separate irradiation chains together with the burnup kinetic equations, it is possible to conclude that a set of first order differential equations may describe the kinetic behaviour of the following isotopes.

U^{235}, U^{236}, N_p^{237}, U^{238}, N_p^{239}, Pu^{239}, Pu^{240}, Pu^{241}, Pu^{242}, Am^{241}, Am^{243}.

With the assumption of steady state flux during a time increment (or flux-time increment), the coefficients of the above mentioned first order differential equations will be constant within the increment limits. The first equation of this set is homogeneous, while the inhomogeneous terms of the following equations involve the

solutions of the preceeding ones only. Therefore, they can be solved in a recuressive manner using the integration factor technique[4] with the result:

$$N_{xy}(\theta) = \sum_{n} H(xy,n).\ E_{xp}\ \left[- T\ (xy,n)(\ \theta - \theta_i)\ \right]$$

where,

N_{xy} (θ) is the volume concentration of nuclides of type xy; having x as the last digit of its atomic number Z and y as the last digit of its mass number A; at fluxtime θ,

(θ_i) is the initial flux time of irradiation step "i" ,

and the functions H(xy,n) and T(xy,n) are defined in reference[1] which can be determined by knowing the average point flux $\bar{\phi}$ and the effective microscopic cross-sections of the different isotopes.

In calculating the quantities N_{xy} (θ), a constant "thermal power density" is assumed and the point average flux is allowed to vary with irradiation. Also, the "Westcott" concept of cross-sections is used except for U^{238} and Pu^{240} where effective cross sections;derived from direct physical arguments of reference[1]; are used.

With expressions for the heavy isotopes concentration $N_{xy}(\theta)$, it is possible to calculate the fuel productive cross-section $\Sigma_f^{\nu}(\theta)$, the conversion ratio (C.R), and the macroscopic absorption cross-section of the heavy isotopes $\Sigma_a^{I}(\theta)$ from the relations:

$$\Sigma_p^{\nu} = \sum_{\overline{xy}} N_{\overline{xy}}\ (\theta)\ \hat{\sigma}_f^{\overline{xy}}\ \nu_{\overline{xy}} \qquad (2),$$

$$C.R. = \frac{\hat{\sigma}_c^{28}\ N_{28}(\theta) + \hat{\sigma}_c^{40}\ N_{40}\ (\theta)}{\hat{\sigma}_a^{25}\ N_{25}\ (\theta) + \hat{\sigma}_a^{49}\ N_{49}(\theta) + \hat{\sigma}_a^{41} N_{41}(\theta)} \qquad (3)\ ,\ \text{and}$$

$$\Sigma_a^T(\theta) = \sum_{xy} N_{xy}(\theta) \cdot \hat{\sigma}_a^{xy}(\theta) \qquad (4)$$

where:

$\hat{\sigma}_c^{xy}$, $\hat{\sigma}_f^{xy}$, and $\hat{\sigma}_a^{xy}$ are the capture, fission, and absorption microscopic cross sections respectively,

ν_{xy} is the number of fast neutron emitted per fission of isotope xy, and $\sum_{xy}$, and $\sum_{xy}$ are summations taken over the fissile materials, and over all the heavy nuclides respectively.

FISSION PRODUCTS REPRESENTATION AND POINT REACTIVITY PROFILE

One of the most important problems related to burnup and long term reactivity calculations is the fission products poisoning. In the very detailed method in which all chains are explicitly represented, one will be interested in something of the order of about two hundreds of fission products described by about two hundreds of simultaneous differential equations. Examples are the "CINDER"[5,6] and "FISSPROD"[7] codes. This type of codes is not quite justified for direct use in burnup calculations due to the large amount of data that have to be handled (or lack of these data) and computer time requirements.

It is for this reason that the fission products will be represented in burnup calculations by the pseudo-scheme type[8,9] as follows:

1. The only fission products treated explicitly; solution of the burnup equations; are those with particularly large capture cross sections and high yields; namely xenon-135 and samarium-149.

2. Other fission products with low capture cross sections will be lumped in groups according to their yields and cross sections through using effective parameters which preserve as many of the intergral properties of the actual situation as are consistent with its complexity.

An expression for the effective macroscopic absorption cross-section of the high cross sections fission products " $\Sigma_a^H(\theta)$" can be obtained by calculating the atomic concentrations of Xe^{135} and Sm^{149} as transient fission products/1/. After some algebraic manipulation it is easy to show that:

$$\Sigma_a^H(\theta) = \sum_{\overline{xy}} N_{\overline{xy}}(\theta)\ \hat{\sigma}_a^h(\overline{xy},\theta),\quad \overline{xy} = 25,49,41,28 \qquad (5)$$

with:

$$\hat{\sigma}_a^h(\overline{xy},\theta) = \hat{\sigma}_f^{\overline{xy}}(\theta)\left\{ \gamma(\overline{xy} \to 19) + \gamma(\overline{xy} \to 09) + \right.$$

$$\left. + \frac{\hat{\sigma}_a^{45}}{\hat{\sigma}_a^{45} + \lambda_{45}^{*}} \left[\gamma(\overline{xy} \to 45) + \gamma(\overline{xy} \to 35) + \gamma(\overline{xy} \to 25) \right] \right\} \qquad (6)$$

where $\gamma(\overline{xy} \to xy)$ is the probability that the nuclides of type "xy" will be formed as a fission product by neutron absorption in nuclide "$\overline{xy}$". Values for $\gamma(\overline{xy} \to xy)$ are given in Table(1), $\hat{\sigma}_a^{45}$ is the Westcott effective microscopic absorption cross section for Xe^{135}, $\hat{\sigma}_f^{\overline{xy}}(\theta)$ is the effective fission cross section for the isotope $\overline{xy}$; and λ_{45}^{*} is the decay constant of Xe^{135} measured in units of $1/\beta$

The present code uses the approach adopted by Walker[10] to calculate the effective, macroscopic absorption cross-section for the low cross sections fission products $\Sigma_a^L(\theta)$. In this approach the low cross sections fission products are treated in three groups with 50, 300 and 800 barns. The yields in the groups are considered as functions of the type of fissionable nuclides, the effective neutron temperature, and

the epithermal index. A detailed description for calculating an effective microscopic absorption cross section fisson products can be found in references[10,14,15,16]. The absorption macroscopic fuel cross section may; therefore; be writhen as :

$$\Sigma_a^F(\theta) = \Sigma_a^H(\theta) + \Sigma_a^L(\theta) + \Sigma_a^I(\theta)$$

To predict the reactivity variation as function of irradiation, the well known expression for the effective multiplication factor $K_{eff}(\theta)\left[= \eta f(\theta).p.\epsilon - \exp(-B_g^2\tau)/(1+B_g^2 L^2(\theta)\right]$ is used together with the appropniate expressions for $L^2(\theta)$ and $\eta f(\theta)$[17,18]. The result appears as:

$$K_{eff} = \frac{\epsilon p.\exp(-B_g^2\tau)}{\Sigma_a^F(0) + \Sigma_o + B_g^2 C}\ \Sigma_F^{\nu}(\theta) \qquad (7)$$

where

$$\Sigma_o = \frac{\Sigma_F^{\nu}(0)}{\eta f(0)} - \Sigma_a^F(0) \qquad (8), \text{and}$$

$$C = \frac{L^2(0)\ \Sigma_F^{\nu}(0)}{\eta f(0)} \qquad (9)$$

In future work,the UABUC code will be extended to include the spatial effect in order to study the in-core fuel performance. Also it has been used to assess the accuracy of the physical simplifications that are introduced in burnup computer codes[19].

Table (1)

Values of the probability functions involved in the calculation of " Σ_a^H "

Nuclide	$\overline{xy}$	$\gamma(\overline{xy} \rightarrow 19) + \gamma(\overline{xy} \rightarrow 09)$		$\gamma(\overline{xy} \rightarrow 45)$		$\gamma(\overline{xy} \rightarrow 35) + \gamma(\overline{xy} \rightarrow 25)$	
		Value	Ref.	Value	Ref.	Value	Ref.
Uranium-235	25	.0113	11	.0030	11	.0810	11
Plutonium-239	49	.0130	5	.0038	5	.0985	5
Plutonium-241	41	.0130	12	.0050	13	.0600	13
Uranium-238	28	.0180	5	.0024	5	.0570	5

$\hat{\sigma}_a^{45}$ = 2.48 x 10^6 barn/11/, and λ_{45} = 2.093 x 10^{-5} sec^{-1}/5/

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