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Calculation of Resonance Region Group Constants of LWR Fuel Cell by using of WIMS69 Groups Library

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Abstract We have established the calculation method to obtain resonance region group constants considering geometric and material properties, Doppler broadening and interaction between resonance isotopes in fuel cell of LWR.

Key words LWR, effective resonance integral, group constant

Introduction

The main problem in preparation of group constants for nuclear reactor physical calculation is to calculate resonance cross sections. In 69 energy group structure of WIMS library the resonance region is defined to lie between 4.0eV and 9.118keV(from 15^{th} group to 27^{th} group).

The WIMS library contains a set of tabulations of the resonance integral for a homogeneous mixture of the resonance isotope and hydrogen[1－4]. By using the equivalence theorem and Carlvik's rational approximation, we obtained the values of effective resonance integral of heterogeneous fuel rod cell of LWR from the tabulation of the resonance integral of WIMS library.

Using interpolation method depending on value of R (ratio of actual resonance integral to infinitely dilute value) and taking account of interaction effects between different resonance isotope, we enhanced correctness of calculation of resonance cross sections.

1. Calculation Method on Group Constants of Resonance Region in Heterogeneous Infinite Lattice

We firstly consider the case of an isolated fuel rod. The first collision probability in fuel rod for neutrons originating in same place, p_{ff}, is the quantity related to the style, size and macroscopic total cross section, Σ_{tF}, of fuel rod and then can not be represented by correct analytic equation. Therefore, in practice, the following rational approximations are applied[4].

$$p_{ff} = \begin{cases} x/(x+1), & \text{Wigner} \\ x/(x+a), & \text{Bell (cylinder } a=1.16) \\ x(2/(x+2)-1/(x+3)), & \text{Carlvik} \end{cases} \qquad (1)$$

where $x = \bar{l}\Sigma_{tF}$ and $\bar{l} = 4V_f / S_f$ is the mean chord length.

In the case of fuel rod with low-enriched UO_2 which is used in LWR, errors of above three approximations for 13 groups in resonance region are from 10 to 18, 5 to 10 and 1 to 2% respectively at the range of x, 0.4 to 5.0.

From calculation experiences, if the error in value of p_{ff} is 10%, the error in calculation of effective resonance integral is about 2% [2].

On the other hand, if the cell in heterogeneous infinite lattice consisting of fuel rods arranged regularly in moderator comes to equivalent cylindrical cell with white boundary condition, there exists the following relation between the first collision probability in fuel rod of this equivalent cell, p_{FF}, and the first collision probability in isolated fuel rod, p_{ff}, of neutron.

$$p_{FF} = p_{ff} + x(1-p_{ff})^2 /(x(1-p_{ff}) + A) \tag{2}$$

where A, the quantity relative to geometric and material properties of cell, is

$$A = \frac{S_b \gamma_b^0}{S_f (t_{fb})^2}, \tag{3}$$

$$\gamma_b^0 = \sum_{i \neq f} P_{bi}^{\infty} + \frac{S_f}{S_b} t_{fb}(1-t_{fb}). \tag{4}$$

where t_{fb} is the probability that neutron escaped isotropically from surface area of fuel rod, S_f, arrives at boundary of cell, S_b, without collision(i.e. transmission probability from S_f to S_b), and P_{bi}^{∞} is the first collision probability in region i of neutron entered isotropically to the boundary of cell, S_b, when the fuel rod is the blackness.

Using the correlation equation, $P_{bi}^{\infty} = (4\Sigma_{ti} V_i / S_b) P_{ib}^{\infty}$, we can provide P_{bi}^{∞} from P_{ib}^{∞}. From the general equation for escape probability, P_{ib}^{∞} is as follows.

$$P_{ib}^{\infty} = \frac{2}{\Sigma_{ti} V_i} \left\{ \int_0^{r_1} [K_{i3}(\tau_{is}^+) - K_{i3}(\tau_{i-1s}^+)] dy + \int_{r_1}^{r_i} [K_{i3}(\tau_{is}^+) - K_{i3}(\tau_{i-1s}^+) + K_{i3}(\tau_{i-1s}^-) - K_{i3}(\tau_{is}^-)] dy \right\} \quad i = \overline{2,\ I}$$

where $K_{i3}(x)$ is the Bickley function of order three.

Therefore,

$$P_{bi}^{\infty} = \frac{8}{S_b} \left\{ \int_0^{r_1} [K_{i3}(\tau_{is}^+) - K_{i3}(\tau_{i-1s}^+)] dy + \int_{r_1}^{r_i} [K_{i3}(\tau_{is}^+) - K_{i3}(\tau_{i-1s}^+) + K_{i3}(\tau_{i-1s}^-) - K_{i3}(\tau_{is}^-)] dy \right\}, \quad i = \overline{2,\ I} \tag{5}$$

where

$$\tau_{is}^+ = \sum_{k=i+1}^{I} \tau_k, \quad \tau_{is}^- = 2\sum_{k=2}^{I} \tau_k + \sum_{k=i+1}^{I} \tau_k, \quad \tau_k = \Sigma_{tk}(x_k - x_{k-1}), \quad x_k = \begin{cases} \sqrt{r_k^2 - y^2}, & r_k \geq y \\ 0, & r_k < y \end{cases}. \tag{6}$$

t_{fb} can be also derived from the general equation for transmission probability.

$$t_{fb} = \frac{4}{S_f} \int_0^{r_1} K_{i3}[\tau(r_{S_f},\ r_{S_b})] dy = \frac{4}{S_f} \int_0^{r_1} K_{i3}\left(\sum_{k=2}^{I} \tau_k \right) dy \tag{7}$$

Applying Carlvik's approximation to p_{ff} in equation (2), substituting it to the equation for

effective resonance integral and rewriting, we can obtain the following effective resonance integral consisting of two terms.

$$I = \sum_{n=1}^{2} \beta_n F(\lambda\sigma_{PF} + \alpha_n\sigma_e) = I_1 + I_2 \tag{8}$$

$$F(\lambda\sigma_{PF} + \alpha_n\sigma_e) = \int \frac{\lambda\sigma_{PF} + \alpha_n\sigma_e}{\sigma_{aF}(E) + \lambda\sigma_{PF} + \alpha_n\sigma_e} \frac{\sigma_{aF}(E)}{E} dE \tag{9}$$

where λ is the intermediate resonance factor, σ_{PF} and σ_{aF} are potential scattering and absorption cross sections of resonance isotope respectively, $\sigma_e = 1/(\bar{l}N_F)$ and N_F are the concentration of resonance isotope.

Quantities, such as $\alpha_1, \alpha_2, \beta_1$ and $\beta_2(=1-\beta_1)$, are represented by the parameter A.

Replacing $\alpha_n\sigma_e$ with $N_M\sigma_{SM}/N_F$, equation (9) reduces to the homogeneous resonance integral; that is, heterogeneous lattice with a given value of $\alpha_n\sigma_e$ has the same resonance integral as homogeneous mixture taking the value of $N_M\sigma_{SM}/N_F$ which equals to $\alpha_n\sigma_e$. This is called the equivalence theorem.

Values of homogeneous effective resonance integral, $F(T_i,\ \sigma_{bj})$, for main resonance isotopes over different temperature, T_i, and background cross section, $\sigma_{bj} = (\lambda\sigma_{PF} + \alpha_n\sigma_e)_j$, are tabulated in multigroup libraries. Therefore, by using the equivalence theorem, we obtained the values of heterogeneous effective resonance integral, $F(T,\ \sigma_b)$, for a given temperature T and a given background cross section σ_b by interpolating from effective resonance integral table.

The fact that effective resonance integral is in proportion to square root of fuel temperature is widely known. However, dependence on σ_b varies with resonance isotope and group and is mainly related to the ratio of actual resonance integral to infinitely dilute value, $R = F(T,\ \sigma_b)/F(T,\ \infty)$ [3].

By using interpolation method depending on value of R, we have written the interpolation equation as

$$\begin{aligned} F(T,\ \sigma_b) = {} & \{F(T_i,\ \sigma_{bj}) + K_i(\sigma_b)[F(T_i,\ \sigma_{bj+1}) - F(T_i,\ \sigma_{bj})]\}(T_{i+1}^{1/2} - T^{1/2})/(T_{i+1}^{1/2} - T_i^{1/2}) + \\ & + \{F(T_{i+1},\ \sigma_{bj}) + K_{i+1}(\sigma_b)[F(T_{i+1},\ \sigma_{bj+1}) - F(T_{i+1},\ \sigma_{bj})]\}(T^{1/2} - T_i^{1/2})/(T_{i+1}^{1/2} - T_i^{1/2}) \end{aligned} \tag{10}$$

where

$$K_i(\sigma_b) = \begin{cases} (\sigma_b^{1/2} - \sigma_{bj}^{1/2})/(\sigma_{bj+1}^{1/2} - \sigma_{bj+1}^{1/2}), & R < 0.50 \\ \ln(\sigma_b/\sigma_{bj})/\ln(\sigma_{bj+1}/\sigma_{bj}), & 0.50 < R < 0.80 \\ (1-(\sigma_{bj}/\sigma_b)^{1/2})/(1-(\sigma_{bj}/\sigma_{bj+1})^{1/2}), & 0.80 < R < 0.95 \\ (1-\sigma_{bj}/\sigma_b)/(1-\sigma_{bj}/\sigma_{bj+1}), & R > 0.95 \end{cases} \tag{11}$$

Absorption cross section of resonance group g is represented by effective resonance integral as follows.

$$\sigma_{ag} = \frac{I_1 + I_2}{\tau_g - (I_1/(\lambda\sigma_{PF} + \alpha_1\sigma_e) + I_2/(\lambda\sigma_{PF} + \alpha_2\sigma_e))}$$

In practice, there are various resonance isotopes in fuel rod and interaction effects arising from overlap of resonances associated with different isotopes must be taken into account.

Then effective resonance integral and resonance absorption cross section of isotope m are written approximately as

$$I'_m = \frac{\beta(\lambda\Sigma_{pF}+\Sigma_{e1})}{\Sigma_{p1,\ m}} F\left(\frac{\Sigma_{p1,\ m}}{N_m}\right) + (1-\beta)\frac{(\lambda\Sigma_{pF}+\Sigma_{e2})}{\Sigma_{p2,\ m}} F\left(\frac{\Sigma_{p2,\ m}}{N_m}\right) = I'_{1m} + I'_{2m} \tag{12}$$

$$\sigma'_{amg} = \frac{I'_{1m} + I'_{2m}}{\left[\beta\frac{\lambda\Sigma_{pF}+\Sigma_{e1}}{\Sigma_{p1,\ m}} + (1-\beta)\frac{\lambda\Sigma_{pF}+\Sigma_{e2}}{\Sigma_{p2,\ m}}\right]\tau_g - \frac{N_m I'_{1m}}{\Sigma_{p1,\ m}} - \frac{N_m I'_{2m}}{\Sigma_{p2,\ m}}} \tag{13}$$

where

$$\Sigma_{pn,\ m} = \overline{\Sigma}_a - N_m\sigma_{am} + \lambda\Sigma_{pF} + \Sigma_{en},\ \ n=1,\ 2 \tag{14}$$

$$\overline{\Sigma}_a = \frac{\sum_m N_m(I^0_{1m} + I^0_{2m})}{\tau_g - \sum_m\left(\frac{N_m I^0_{1m}}{\lambda\Sigma_{pF}+\Sigma_{e1}} + \frac{N_m I^0_{2m}}{\lambda\Sigma_{pF}+\Sigma_{e2}}\right)}. \tag{15}$$

I^0_{1m} and I^0_{2m} are effective resonance integrals of isotope m and they are calculated by equation (9).

2. Calculation Results

The calculations were carried out at a fuel cell in the commercialized PWR with 1 000MW[5]. Main parameters of fuel cell are found in table 1.

Table 1. Main parameters of fuel cell in PWR with 1 000MW

Materials	Constituent	Parameter	Value
Fuel rod material	3% UO_2	Cell step/mm	12.3
		Diameter/mm	9.19
		Density/(g · cm^{-3})	10.41
		Temperature/K	881
Clad material	Zr	Density/(g · cm^{-3})	6.55
		Inside diameter/mm	8.19
		Outside diameter/mm	9.5
		Temperature/K	616
Moderator material	H_2O	Density/(g · cm^{-3})	0.716 8
		Temperature/K	578

The calculation results are found in table 2, where $^{238}\sigma_a$ is the resonance absorption cross section of ^{238}U, k_∞ is the infinite multiplication factor in fuel cell obtained by collision probability method and $\Delta k_\infty / k_\infty$ is the relative deviation with the result by MCNP5(k_∞=1.303 91).

Table 2. $^{238}\sigma_a$ (10^{-24}cm^2) and k_∞ using various approximations for p_{ff}

Group number	Approximations applied to estimation of p_{ff}			Group number	Approximations applied to estimation of p_{ff}		
	Wigner	Bell	Carlvik		Wigner	Bell	Carlvik
15	0.755 81	0.761 72	0.769 20	23	2.171 96	2.293 72	2.295 51
16	0.964 47	0.974 42	0.987 04	24	4.541 66	4.768 90	4.763 42
17	0.557 62	0.570 38	0.583 80	25	5.771 47	6.096 45	6.041 73
18	0.965 38	0.994 53	1.024 06	26	0.206 26	0.206 59	0.207 04
19	1.018 36	1.053 67	1.086 40	27	7.512 97	7.930 97	7.860 67
20	1.258 49	1.306 35	1.339 51	k_∞	1.317 99	1.305 52	1.303 70
21	1.569 71	1.646 48	1.675 65	$\Delta k_\infty \cdot k_\infty^{-1}$/%	1.08	0.12	0.02
22	2.517 40	2.635 31	2.667 21				

As shown in table 2, values of resonance absorption cross section by Wigner's and Bell's approximations are smaller than one by Carlvik's approximation in most of resonance groups. And orders in accuracy of three approximations applied to estimate p_{ff} were represented in calculation results of k_∞, that is, in case using the coarsest approximation of Wigner the relative derivation is more than 1% and, in case of Carlvik's approximation with the highest accuracy the relative derivation is only 0.02%.

Under Carlvik's approximation, calculation results of k_∞ obtained by using various interpolations for background cross section, σ_b, are shown in table 3.

Table 3. Results of k_∞ and relative derivations with the result by MCNP5(k_∞=1.303 91) according to various interpolation methods of σ_b

Interpolation methods	Linear combination	$\sqrt{\sigma_b}$	$\ln\sigma_b$	$\sigma_b^{-1/2}$	$1/\sigma_b$	Method depending on value of R
k_∞	1.307 67	1.304 37	1.300 59	1.296 37	1.291 74	1.303 70
$\Delta k_\infty \cdot k_\infty^{-1}$/%	0.29	0.04	0.25	0.58	0.93	0.02

As shown in table 3, calculation result by interpolation method depending on value of R using equation (10) is more accurate than others and interpolation with type of $\sqrt{\sigma_b}$ is next in the accuracy.

Conclusion

We established numerical method to obtain resonance region group constants which take account of geometric and material properties of LWR heterogeneous fuel lattice by using of WIMS 69 group library. Carlvik's rational approximation is used for the self collision probability in the isolated fuel rod.

We derivated formula for collision and transmission probabilities need to calculate the first collision probability within fuel in infinite array by using the white boundary condition in a cylindrical pin cell. Interaction effects arising from overlap of resonances associated with different isotopes are taken into account in it.

And the correctness of various approximations applied in calculation of resonance region group constants have been compared to each other.

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