Equivalence relations for resonance integral calculation in WIMS-CANDU

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1. Introduction

WIMS-CANDU is a lattice code with a depletion capability for the analysis of reactor physics problems related to a design and safety. Being developed from the WIMS-ANL, WIMS-CANDU uses the equivalence relations to express the resonance integral, which relate the heterogeneous problems to an equivalent homogeneous problem in the case of regular lattices of rods or clusters of rods. In the resonance integration calculation, the effective resonance integrals are obtained by the interpolation from the tables of homogeneous resonance integrals in the data library. Also, WIMS-CANDU uses the Carlvik's method in the calculation of the fuel-to-fuel collision probability, different from WIMS-ANL using Wigner's method. It is well-known that the Carlvik's approximation is more accurate. In order to consider the geometrical irregularity of the array, the modification to the resonance integral due to interaction of the neighboring fuel rods is made using the Dancoff factor.

The purpose of this study is to improve the accuracy of Dancoff factor with the increase of the angle used in the resonance integral calculation and investigated the effect on the multiplication constant and resonance integral for each resonance neutron group. We show that the error in U^{238} capture in the lattice calculation become small with more accurate Dancoff factor.

2. Resonance treatment in WIMS

The resonance treatment in WIMS-CANDU uses the intermediate resonance approximation to calculate the group-averaged resonance integrals as a function of the background scattering cross-section. Equivalence relations are used to relate the heterogeneous geometry to an equivalent homogeneous one in reactor lattices. The effective resonance cross-sections are calculated by the interpolation from the resonance integrals in the data library. To arrive at an equivalence relation to the fuel-to-fuel collision probability p_{FF} in the lattice, p_{FF} is expressed as a sum of rationals

 $p_{FF} = \sum_n \beta_n x/(x+\alpha_n)$ with $\sum_n \beta_n = 1$, (1) where $x=4V_f \sum_f /S_f$ and in which case the equivalence relation for the resonance cross integral of the heterogeneous system becomes a sum of the homogeneous integrals

$$\boldsymbol{R}\boldsymbol{I} = \boldsymbol{\Sigma}_n \boldsymbol{\beta}_n \boldsymbol{R}\boldsymbol{I}(\boldsymbol{\sigma}_p + \boldsymbol{\alpha}_n \boldsymbol{\sigma}_e) , \qquad (2)$$

where σ_p is the potential scattering cross-section of the fuel, per absorber atom, and $\sigma_e = S_f / 4V_f N$ the escape cross-section, N being the absorber number density.

Tracking the neutrons born in the fuel, one obtains

 $p_{FF} = p_{ff} + x(1 - p_{ff})^2 / \{x(1 - p_{ff}) + A + B\}$, (3) in terms of the single rod self-collision probability p_{ff} and a constant *A* and *B* of probability of a fuel and a cell boundary.

As an approximation method of p_{ff} , WIMS-CANDU uses the Wigner's method to calculate the collision probability in an annular model of fuel, cladding, coolant and moderator. It approximates the single rod self-collision probability, p_{ff} , by a single rational term $p_{ff} = x/(x+a)$, where *a* is a Bell factor. But it is well known that an approximation of p_{ff} by a single rational is never accurate, as can be seen in Figure 1. In fact, a Bell factor is interpreted as a correction parameter in the equivalence relation, which yields the proper value for the resonance integral. Consequently, instead of an introduction of a Bell factor, one could use an improved approximation for $p_{ff} = 2x/(x+2)-x/(x+3)$, expressed by a sum of two rationals and proposed by Carlvik(1962). Its accuracy is shown in Figure 1.



Figure 1. Percentage error in $1-p_{ff}$ for different approximations

Now a substitution of $p_{ff} = 2x/(x+2)-x/(x+3)$ into the equation (3) gives

 $\boldsymbol{p}_{FF} = \boldsymbol{x}(\beta/(\boldsymbol{x}+\alpha_l) + (l-\beta)/(\boldsymbol{x}+\alpha_2)), \quad (4)$

with

$$\chi_{2,1} = \{(5A+6) \pm \sqrt{A^2 + 36A + 36}\}/2(A+1),$$
(5)

 $\beta = \{(4A+6)/(A+1) - \alpha_l\}/(\alpha_2 - \alpha_l).$ (6)

Also, it leads to the equation of a resonance integral with the parameters $\alpha_{l_1} \alpha_{2}$ and β , that is,

$$\boldsymbol{R}\boldsymbol{I} = \boldsymbol{\beta} \cdot \boldsymbol{R}\boldsymbol{I}(\sigma_p + \alpha_1 \cdot \sigma_e) + (1 - \boldsymbol{\beta}) \cdot \boldsymbol{R}\boldsymbol{I}(\sigma_p + \alpha_2 \cdot \sigma_e) \quad (7)$$

Instead of the Wigner's approximation, one applies and implements an improved method proposed by Carlvik with WIMS-CANDU, in order to calculate the collision probability in an annular model of fuel, cladding and coolant, and, if relevant, moderator.

3. Calculation of Dancoff factor

The Dancoff factor is defined as the reduction factor of the fuel escape probability compared to that of an isolated fuel pin, when all fuel pins are black. In other words, it is the first-flight blackness of all materials, except fuel, for a neutron leaving a fuel pin, when all fuel pins are black. For a black fuel pin, $\gamma_f = 4V_f \Sigma_f / S_f (1 - 1)^2 + 1$ p_{ff})=1. Here, γ_f means the first-flight blackness, that is, the probability of neutrons entering the fuel with a cosine distribution through S_f to collide inside the fuel. From the definition of Dancoff factor,

 $\begin{array}{l} D=&lim_{\{\gamma f\rightarrow 1\}}(1\text{-}P_{FF})/(1\text{-}p_{ff})=1\text{-}1/(1\text{-}A\text{+}B),\\ \text{where } A=&S_b\gamma_b^{0/}S_ft_{fb}^{-2}, \ B=&S_b/S_ft_{fb}^{-2} \ (f(1\text{-}g)/(1\text{-}f(1\text{-}g))). \ \text{For }B=&0, \ D \ \text{agrees with the result } D_{\infty} \ \text{for the infinite lattice.} \end{array}$

The corrections of Dancoff factor for non-infinite lattice effects are made the using geometrical considerations. For each pin the surrounding n pin cell positions are investigated and

- 1- $D_i = (1-D_\infty) \Sigma_i W_i T_i$
- 2- $T_i = 2E_3(\tau_i)$
- 3- $E_3(\tau) = \int_{-\infty}^{\infty} e^{-\tau x} / x^3 dx$ 4- $\Sigma_j w_j = 1$ for j=1, n.

Here, τ_i is the optical distance from the edge of pin cell i to the edge of the nearest pin cell in the direction j. T_{i} is the corresponding transmission probability. The weight w_i is the normalized to $\Sigma_i w_i = 1$. The following table is shown for n=8 and for the CANDU-6 model of WIMS-CANDU.

Resonance group	Energy range (lower energy limit)	Dancoff factor
15	5.5300E+03	0.2247
16	3.5191E+03	0.2244
17	2.2394E+03	0.2271
18	1.4251E+03	0.2183
19	9.0690E+02	0.2146
20	3.6726E+02	0.2165
21	1.4873E+02	0.2207
22	7.5501E+01	0.2156
23	4.8052E+01	0.2160
24	2.7700E+01	0.2161
25	1.5968E+01	0.2162
26	9.8770E+00	0.2163
27	4.0000E+00	0.2164

4. Conclusion

In order to improve the accuracy of the Dancoff factor calculation, we made an increase the number of the angles for each neutron group and isotope and investigated the variation of the Dancoff factor and keffective.

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