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Criticality Calculation for Cluster Fuel Bundles Using Monte Carlo Generated Grey Dancoff Factor

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Abstract

The grey Dancoff factor calculated by Monte Carlo method is applied to the criticality calculation for cluster fuel bundles. Dancoff factors for five symmetrically different pin positions of CANDU37 and CANFLEX fuel bundles in full three-dimensional geometry are calculated by Monte Carlo method. The concept of equivalent Dancoff factor is introduced to use the grey Dancoff factor in the resonance calculation based on equivalence theorem. The equivalent Dancoff factor which is based on the realistic model produces an exact fuel collision probability and can be used in the resonance calculation just as the black Dancoff factor. The infinite multiplication factors based on the black Dancoff factors calculated by collision probability or Monte Carlo method are overestimated by about 2mk for normal condition and 4mk for void condition of CANDU37 and CANFLEX fuel bundles in comparison with those based on the equivalent Dancoff factors.

I. Introduction

The equivalence relation between a homogeneous and a heterogeneous geometry has been used in the calculation of the resonance cross section in most core physics codes. The equivalence relation can be established if the fuel collision probability in the heterogeneous geometry can be expressed as a summation of rational terms. The accuracy of the resonance integral calculation depends on how accurately the fuel collision probability is expressed by rational terms and the fuel collision probability is related with the Dancoff factor in closely packed lattices.

The calculation of the Dancoff factor for an actual reactor is very difficult because of the non-uniformities found around the control or absorber rod or in irregularly located fuel pins like CANDU fuel bundles. Though several approximate methods and algorithms have been developed, the errors due to the Dancoff factors have not been evaluated sufficiently in the reactor physics calculation.[1]

In this study, black and grey Dancoff factors, i.e., for perfectly and partially absorbing fuel rods, respectively, are calculated by the Monte Carlo method for the cluster type fuel bundles. The calculated Dancoff factors are then applied to the criticality calculation using the WIMSD code.[2] The concept of equivalent Dancoff factor is introduced in this paper to use the grey Dancoff factor in the equivalence theorem.

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Ⅱ. Resonance Absorption in Heterogeneous Systems

The resonance absorption in a heterogeneous system can be calculated by solving the neutron slowing-down equation applied for a system of two regions, fuel and moderator. Only the fuel region contains resonance absorbing material, while both regions may contain moderating nuclei.[5]

The neutron flux distribution in the fuel region can be calculated numerically from the slowing-down equation with given fuel collision probability, P_{FF}. Resonance integrals and effective cross sections can then be calculated from the neutron flux distribution with fine group cross sections as follows:

$$RI = \int \Sigma_a(E)\phi_F(E)dE, \tag{1}$$

$$\overline{\Sigma} = \frac{\int \Sigma(E)\phi_F(E)dE}{\int \phi_F(E)dE}, \tag{2}$$

where the integration is over the cross section library group in question.

Due to the difficulties and calculation time in directly solving the slowing-down equation for heterogeneous media, the equivalence relation between a homogeneous and a heterogeneous medium has been used as a practical method of good accuracy for the resonance treatment in most reactor physics codes.[4] The resonance integral of a heterogeneous medium may be interpolated from tabulated homogeneous resonance integrals through parameters denoting the heterogeneity of the medium in the equivalence theorem. The homogeneous resonance integrals may be calculated by solving the slowing-down equation directly for various conditions of the reactor.

The equivalence relation between a homogeneous and a heterogeneous medium can be established if $P_{FF}(E)$ can be approximated as a summation of rational terms as follows:

$$P_{FF}(E) = \sum_n \left\{ \frac{\Sigma_t^A(E)}{\Sigma_t^A(E)+\Sigma_{esc}} \right\}, \tag{3}$$

where Σ_t^A is total cross section of the absorber and Σ_{esc} is escape cross section determined by the geometrical configuration of the medium, respectively.[5]

The accuracy of the resonance integral for the heterogeneous medium based on the equivalence theorem depends on how accurately the fuel collision probability is expressed by the rational terms. The fuel collision probability is related to the Dancoff factor which is the probability that a neutron emitted from the surface of a fuel element under consideration with a cosine shape angular distribution enters another fuel element without having a collision with nuclei in the moderator or in the cladding, and depends on the material properties and geometrical configuration.

The fuel collision probability P_{FF} for the infinite regular lattice becomes[6]

$$P_{FF} = \frac{(\beta - C_b)p_{ff} + xC_b(1 - p_{ff})\{p_{ff} + \beta(1 - p_{ff})\}}{(\beta - C_b) + xC_b(1 - p_{ff})}, \tag{4}$$

where $A_n = \prod_{i=1}^{n} (1 - G_{0i})$,

$C_n = \prod_{i=1}^{n} (1 - G_{i-1,i})^2$,

G_{ij} : the probability that a neutron born uniformly in region i will have its first collision in region j,

p_{ff} : fuel collision probability for an isolated fuel rod,

V_f, Σ_f : volume and total cross section of fuel rod,

C_b : black Dancoff factor,

$\beta = \frac{A_n^2}{C_n}$ and $x = \Sigma_f \frac{4V_f}{S_f}$.

Eq. (4) can be converted to the summation of rational terms if p_{ff} is given as a rational form.

If the rods in the lattice are located irregularly such as in CANDU37 or CANFLEX, the approximations used in deriving the above equations are no longer valid and even the calculation of the black Dancoff factor is very complicated and needs additional approximations.

Monte Carlo method was used in this paper to calculate Dancoff factors. With the introduction of "grey Dancoff factor," C_g, where fuel rods are considered to be partially absorbing as in the actual nuclear reactors, the approximations can be avoided and the fuel collision probability for the lattice of fuel rods can be expressed in simple form as

$$P_{FF}^{g} = p_{ff} + (1 - p_{ff}) C_g. \tag{5}$$

The equivalent Dancoff factor (C_e) is then introduced here to apply the grey Dancoff factor in the resonance calculation based on the equivalence theorem. The equivalent Dancoff factor is "grey-equivalent black Dancoff factor" which produces accurate fuel collision probability that is exactly the same with the one calculated using Eq. (5) and the fuel collision probability has a suitable form for the equivalence relation. The equivalent Dancoff factor is defined as follows using Eqs. (4) and (5):

$$P_{FF}^{e} = \frac{(\beta - C_e) p_{ff} + x C_e (1 - p_{ff}) \{ p_{ff} + \beta (1 - p_{ff}) \}}{(\beta - C_e) + x C_e (1 - p_{ff})}. \tag{6}$$

Ⅲ. Monte Carlo Dancoff Factor Calculation

Assuming constant source strength of the emerging neutrons on the whole surface of the fuel region, one can calculate the Dancoff factor as[7]

$$C = \frac{\int d\boldsymbol{s} \int_{\boldsymbol{n} \cdot \Omega > 0} d\Omega \, \boldsymbol{n} \cdot \boldsymbol{\Omega} \, \exp[- \Sigma_t^M l_M(\boldsymbol{s}, \boldsymbol{\Omega}) - \Sigma_t^C l_C(\boldsymbol{s}, \boldsymbol{\Omega})]}{\int d\boldsymbol{s} \int d\Omega \, \boldsymbol{n} \cdot \boldsymbol{\Omega}}, \tag{7}$$

where $\boldsymbol{n}$ = normal vector of the surfaces in the point $\boldsymbol{s}$,

l_M, l_C = neutron path lengths through moderator and cladding in the direction $\boldsymbol{\Omega}$, respectively,

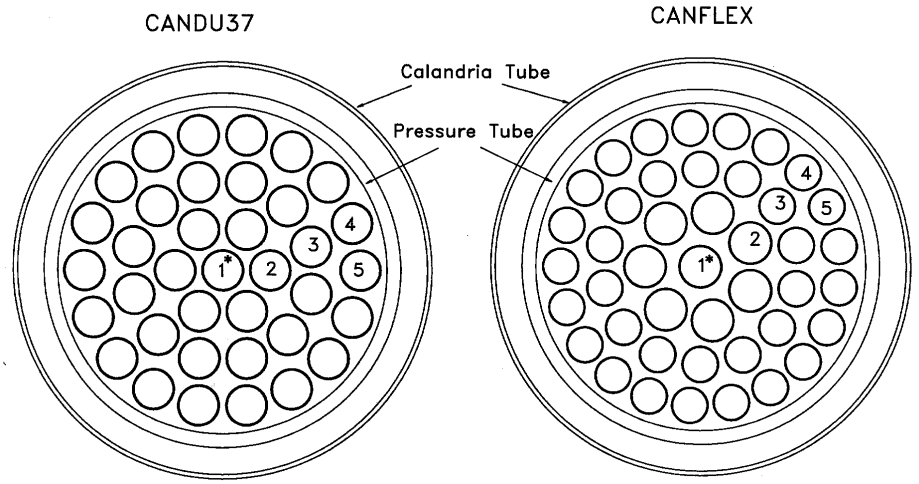
Σ_t^M, Σ_t^C = total macroscopic cross section of moderator and cladding, respectively.

After the random variables for the location and direction of the emitted neutron are sampled and the lengths traveled in different material regions are determined, the score is calculated. Each neutron started is traced until it collides with fuel (black Dancoff factor) or escapes through the outer boundaries, including axial surfaces. The Dancoff factor is calculated as the average of the scores over all histories.

The algorithm is modified to allow the neutrons to pass repeatedly through fuel region as well as moderator and cladding for the grey Dancoff factor calculation. The probability

of getting absorbed in the fuel is obtained by summation of the probabilities for each of the fuel regions crossed by the path.

A Monte Carlo program G-DANCOFF that calculates grey Dancoff factor as well as black Dancoff factor was written in FORTRAN-77 and compiled in the HP-9000/735 workstation and verified through comparisons with Carlvik method[8] and DANCOFF-MC[1]. The Dancoff factors were calculated for the five symmetrically different fuel pin locations of CANDU37 and CANFLEX fuel bundles (Fig. 1).



*pins for which Dancoff factors are calculated.

Fig. 1 Cross Sectional Diagram of CANDU37 and CANFLEX Fuel Bundles

Ⅳ. Criticality Calculation for CANDU37 and CANFLEX Fuel Bundles Using WIMSD code

The resonance treatment in the WIMSD code is based on the equivalence theorem and the collision probability method. The cluster is divided into two regions for the resonance integral calculation in the WIMSD code, inner and outer region. Pins in the outermost ring belong to outer region. Other pins in the cluster belong to inner region and are assumed to consist of infinite array of pins.

The resonance integrals for the inner pins and cluster-average pin are calculated from Dancoff factors given in the input file using the equivalence relation. The resonance integral for the outer pins is calculated to preserve the cluster-average resonance integral in WIMSD.[9]

In the Monte Carlo method, the resonance integral for the outer pins is calculated using the inner and outer Dancoff factors as follows:[10]

$$RI^{outer} = \frac{\sqrt{\sigma_p + (1 - C^{outer})\sigma_e}}{\sqrt{\sigma_p + (1 - C^{inner})\sigma_e}} \; RI^{inner} , \tag{8}$$

where σ_p and σ_e are potential and escape cross sections, respectively.

The inner and cluster Dancoff factors were calculated as averages of the pins' Dancoff factors included in each region in the Monte Carlo method.

A DSN (discrete ordinates) option was used in the transport calculation. 69 group cross section library where 13 groups belong to resonance energy region was used in the criticality calculation. WIMSD criticality calculations for normal (coolant density 0.8079 g/cc) and void (coolant density 0.01 g/cc) conditions were performed to see the effect of

Table 1. Dancoff Factors for CANDU37 and CANFLEX Used in WIMSD Calculation

	E[1]	Normal[2]						Void[2]					
		Inner			Cluster			Inner			Cluster		
			Monte Carlo			Monte Carlo			Monte Carlo			Monte Carlo	
		WIMSD	Black	Equiv.	WIMSD	Black	Equiv.	WIMSD	Black	Equiv.	WIMSD	Black	Equiv.
	15	.7669	.7589	.6178	.6118	.6165	.5644	.9498	.9241	.7348	.7468	.7449	.6743
	16	.7656	.7576	.6173	.6107	.6155	.5637	.9490	.9233	.7348	.7462	.7443	.6740
	17	.7655	.7575	.6173	.6107	.6154	.5637	.9490	.9234	.7348	.7462	.7443	.6741
C	18	.7651	.7572	.6173	.6104	.6152	.5636	.9493	.9236	.7354	.7464	.7445	.6744
A	19	.7669	.7588	.6180	.6118	.6165	.5645	.9508	.9250	.7357	.7475	.7456	.6750
N	20	.7654	.7575	.6174	.6107	.6155	.5637	.9497	.9240	.7354	.7467	.7448	.6746
D	21	.7676	.7595	.6182	.6123	.6170	.5648	.9513	.9255	.7357	.7479	.7460	.6752
U	22	.7727	.7643	.6212	.6163	.6209	.5680	.9577	.9315	.7391	.7528	.7509	.6790
3	23	.7765	.7678	.6240	.6193	.6238	.5706	.9639	.9373	.7432	.7576	.7555	.6830
7	24	.7876	.7781	.6313	.6280	.6322	.5780	.9803	.9527	.7534	.7700	.7679	.6933
	25	.7867	.7773	.6314	.6273	.6316	.5777	.9806	.9530	.7543	.7703	.7682	.6939
	26	.7502	.7444	.6210	.5994	.6055	.5609	.9641	.9375	.7613	.7577	.7557	.6920
	27	.8023	.7914	.6365	.6392	.6428	.5852	.9911	.9628	.7546	.7783	.7760	.6973
	15	.7743	.7769	.6384	.6271	.6324	.5877	.9596	.9365	.7320	.7664	.7566	.6865
	16	.7730	.7758	.6380	.6261	.6315	.5871	.9589	.9359	.7321	.7660	.7561	.6863
	17	.7729	.7757	.6379	.6260	.6314	.5870	.9590	.9359	.7322	.7660	.7561	.6863
C	18	.7725	.7754	.6380	.6257	.6311	.5869	.9592	.9362	.7327	.7662	.7563	.6867
A	19	.7741	.7768	.6386	.6269	.6323	.5877	.9603	.9372	.7328	.7671	.7572	.6871
N	20	.7728	.7756	.6381	.6259	.6314	.5870	.9595	.9364	.7327	.7664	.7565	.6868
F	21	.7747	.7774	.6387	.6275	.6327	.5880	.9608	.9377	.7327	.7674	.7575	.6872
L	22	.7788	.7813	.6411	.6307	.6359	.5906	.9659	.9425	.7354	.7714	.7613	.6902
E	23	.7816	.7840	.6434	.6330	.6381	.5927	.9708	.9471	.7387	.7752	.7650	.6934
X	24	.7901	.7922	.6495	.6397	.6446	.5986	.9838	.9594	.7468	.7853	.7748	.7015
	25	.7891	.7913	.6495	.6390	.6440	.5983	.9841	.9596	.7477	.7855	.7750	.7021
	26	.7549	.7608	.6408	.6125	.6201	.5826	.9709	.9472	.7568	.7753	.7651	.7019
	27	.8031	.8039	.6536	.6498	.6539	.6048	.9924	.9675	.7467	.7919	.7812	.7043

[1] Resonance Energy Group in the 69 Groups of WIMSD Cross Section Library
[2] Normal : Coolant Density 0.8079 g/cc
Void : 0.01 g/cc

Table 2. k_{∞} Comparison

		WIMSD	Monte Carlo	
			Black	Equiv.
CANDU37	Normal[1]	1.1221 (0.2039)[2]	1.1224 (0.2293)	1.1201
	Void[1]	1.1370 (0.3590)	1.1368 (0.3493)	1.1333
CANFLEX	Normal	1.1230 (0.1568)	1.1238 (0.2420)	1.1214
	Void	1.1390 (0.4103)	1.1392 (0.4266)	1.1349

[1] Normal : Coolant Density 0.8079 g/cc
Void : 0.01 g/cc
[2] $\Delta k = 100*(k_{\infty} - k_{\infty}^{equiv})$

the Dancoff factor on k_∞ in actual conditions. Table 1 provides the Dancoff factors calculated by WIMSD and the Monte Carlo method. Table 2 provides the calculated infinite multiplication factors.

The equivalent Dancoff factors for CANDU37 and CANFLEX fuel bundles are smaller than the black Dancoff factors by about 10% for cluster average pin and about 20% for the inner pins in the normal condition. The differences in k_∞ due to the differences in the equivalent and black Dancoff factor are about 2mk for the normal condition and 4mk for the void condition.

V. Conclusions

The black and grey Dancoff factors for CANDU37 and CANFLEX fuel bundles (that consist of complicated fuel clusters) were calculated using the Monte Carlo method. The calculated Dancoff factors were applied to the criticality calculation using the WIMSD code.

The concept of equivalent Dancoff factor was introduced in this paper to use the grey Dancoff factor in the equivalence theorem. The infinite multiplication factors based on the black Dancoff factors calculated by collision probability method as in WIMSD or Monte Carlo method were overestimated by about 2mk for the normal condition and 4mk for the void condition of CANDU37 and CANFLEX compared with those based on the equivalent Dancoff factors.

The equivalent Dancoff factor is based on the realistic model at which actual geometrical configuration and fuel cross section are considered and produces exact fuel collision probability. The equivalent Dancoff also has a suitable form to be used in the equivalence relation and can be used just as the black Dancoff factor in the current reactor physics codes.

The equivalent Dancoff factor can remove and evaluate errors that occur in the resonance calculation using the black Dancoff factor and can be used in the accurate resonance calculation for any type of fuels without difficulties.

References

1. S. Fehér, J. E. Hoogenboom, P. F. A. de Leege, and J. Valkó, "Monte Carlo Calculation of Dancoff Factors in Irregular Geometries," *Nucl. Sci. Eng.*, **117**, 227 (1994).
2. *WIMSD - A Neutronics Code for Standard Lattice Physics Analysis*, NEA Data Bank (1997).
3. G. I. Bell and S. Glasstone, *Nuclear Reactor Theory*, Van Nostrand Reinhold Company, New York (1970).
4. W. Rothenstein, "Resonance Absorption Calculation in Thermal Reactors," *Prog. Nucl. Energy*, **5**, 95 (1980).
5. R. J. J. Stamm'ler and M. J. Abbate, *Methods of Steady-State Reactor Physics in Nuclear Design*, Academic Press (1983).
6. K. Kowalska, *S-WIMS Manual*, NEA Data Bank (1972).
7. H. Okuno and Y. Komura, *DANKE: A Monte Carlo Computer Program for Calculating the Dancoff Correction Factor for Spheres, Rods and Slabs*, JAERI-M94-049, Japan Atomic Energy Research Institute (1994).
8. I. Carlvik, "The Dancoff Correction in Square and Hexagonal Lattices," *Nucl. Sci. Eng.*, **29**, 325 (1967).
9. Y. Ronen, *CRC Handbook of Nuclear Reactors Calculations*, Vol. 1, CRC Press, Inc (1986).
10. M. Edenius, H. Häggblom, and B. H. Forssén, *CASMO-3 - A Fuel Assembly Burnup Program Methodology Version 4.4*, Studsvik Nuclear (1989).