

AN APPROACH FOR EFFECTIVE DANCOFF FACTOR CALCULATION

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ABSTRACT

In this paper, an approach for effective Dancoff factor calculation based on equivalence principle and its application in the SCALE-4.4a code system is described. This procedure is founded on principle of conservation of neutron absorption for resolved resonance range in a heterogeneous medium and an equivalent medium consisting of an infinite array of two-region pin cells, where the presence of other fuel rods is taken into account through a Dancoff factor. The neutron absorption in both media is obtained using fine-group elastic slowing-down calculations. This procedure is implemented in a design oriented lattice physics code, which is applicable for any geometry where the method of collision probability is possible to apply to get a flux solution. Proposed procedure was benchmarked for the recent exercise that represents a system with a fuel double heterogeneity, i.e., fuel in solid form (pellets) surrounded by fissile material in solution, and for an example where the radial dependence of resonance absorption within the fuel was studied by carrying out a calculation for a pin divided into several resonant regions.

Key Words: Equivalence principle, effective Dancoff factor

1. INTRODUCTION

The usual step in reactor criticality calculations is to start with an elementary cell of the lattice, in which the neutron slowing down and thermalization problems can be treated with optical reflecting or isotropic reflecting (white boundary condition). However, even this is too complicated in the resonance energy range.

As a first approximation in the resonance self-shielding calculations, a single fuel lump (usually a fuel rod) in an infinite moderator is considered, and the presence of other fuel rods is taken into account by applying a certain correction, generally called the Dancoff correction [1]. The theory has been known for a long time, and several analytical [2] and numerical [3-6] methods and algorithms are widely used. Recently it has been suggested [7] that the accuracy of computing the Dancoff factor has not improved sufficiently, particularly in the case of complicated and irregular geometries, while the accuracy of modern reactor physics code systems has become much better than it was some two decades ago. An additional complication is that present-day reactor physics codes generally provide for the automatic calculation of the Dancoff correction, and the user is not always aware of the degree of approximation involved.

One method commonly used for solving the neutron slowing-down equation is based on two-region (fuel and moderator) collision probability representation of a heterogeneous lattice cell. Several analytical methods have been proposed to account for a detailed variation of the neutron flux across the energy range of each resonance in this two-region model, the most rigorous of which

is the Nordheim Integral Technique [8]. This technique is implemented in the NITAWL-II code [9], which is applied in all SCALE-4.4a code system analytical sequences [10] that include problem-dependent cross-section processing.

In the Nordheim method, the Breit-Wigner single-level model is used for the cross section processing, and the slowing-down source in the fuel region, due to neutron scatter with resonance nuclide as well as with two admixed moderator (non-absorbing) nuclides, is calculated explicitly over a fine mesh in the lethargy variable. The moderator region is assumed to contain a non-absorbing moderator with an associated $1/E$ variation of the slowing-down flux. Finally, the first-flight collision probabilities, used for spatial transport, are modified for lattice-cell geometry by Dancoff factor that accounts for transmission from the fuel region through the moderator to neighboring absorbers. The Dancoff factor, in this context, is the probability that a neutron emerging from the surface of one fuel lump will enter another absorber lump without any collision in the moderator. This definition is also used in other numerical and Monte Carlo methods for calculation of Dancoff factor [3-7]. For the most widely used arrangements, such as regular square or hexagonal lattices, the NITAWL-II code provides Dancoff factors, however, in the more complex geometries, the Dancoff factors are to be supplied as input by the user. In most other calculation schemes [11,12], the Dancoff correction plays a similar role.

In order to provide a solution for any geometry for which a flux solution by collision probability method is possible, and to include resonance interference and overlap effects in the SCALE-4.4a code system, a procedure based on the equivalence principle is proposed for effective Dancoff factor calculation. This procedure equalizes the absorption self-shielded cross section in the chosen energy range of a heterogeneous medium to an equivalent medium containing the single fuel lump with considering resonant nuclide where the presence of other fuel regions are taken into account by applying the effective Dancoff factor. The neutron absorption in both media is calculated using fine-group elastic slowing-down calculations. This procedure is implemented in the VEGA2DAN sequence of the VEGA2 design oriented lattice physics code [13]. The physical principles and mathematical methods used in the proposed procedure and the verification results are described in subsequent sections.

2. EFFECTIVE DANCOFF FACTOR CALCULATION

The proposed procedure is based on an idea that it is possible to include the collision probability definition and resonance interference effects in the Dancoff correction theory by preserving the absorption self-shielded cross section for chosen energy range in a heterogeneous medium and an equivalent one characterized with effective Dancoff factor. There are two reasons for selecting the energy range with lower boundary $E_l = 1$ eV and upper boundary $E_u = 300$ eV for thermal reactor applications. The first reason is connected with characteristics of the ENDF/B-V evaluation, which includes all resolved resonances of ^{235}U and ^{239}Pu in this range. This evaluation was chosen for generating the 238- and 44-group Criticality Safety Reference Libraries [14] used in the SCALE-4.4a code system. The second reason is that more than 90% of resonant absorption by ^{238}U in thermal reactors takes place in selected energy range.

To obtain a very detailed solution versus neutron energy, the slowing-down module CESD [13] from the VEGA2 code is used. This module solves the multigroup slowing-down equation for a heterogeneous geometry with the collision probability method. The energy mesh was chosen to obtain a very good representation of cross sections for heavy nuclides.

2.1. The Fine-Group Elastic Slowing-Down Calculation

In general case with any number of resonant nuclides and zones (a zone is a volume small enough for flat-flux approximation), the collision-probability approach leads to the neutron slowing-down equation,

$$\Sigma_{ti}(E)\phi_i(E)V_i = \sum_{j=1}^I P_{ji}(E) \left[\sum_{k=1}^{K_j} R_j^k(E) + Q_j(E) \right] V_j, \quad (1)$$

where it is assumed that the medium is perfectly reflected and the scattering is isotropic. Here Σ_{ti} is the total cross section, Φ_i is the energy-dependent flux in zone i , P_{ij} is the first-flight collision probability from zone i to zone j , R_j^k is the elastic slowing-down operator for nuclide k in zone j , and Q_j is the neutron source in zone j .

Since the resonance interference effects were studied only for resolved resonances, that cause the largest effect for thermal reactors (i.e., for $E < 300$ eV), the neutron source in Eq. (1) is approximated as a lethargy-independent source between $E_{ls} = 2.25$ keV and $E_{us} = 3.35$ keV. Also, it is assumed that the neutrons are uniformly and isotropically emitted in the whole moderator ($i \in M$),

$$Q_i(E) = \begin{cases} 1/E, & E_{ls} < E < E_{us}, i \in M \\ 0, & E < E_{ls}, E > E_{us}, i \notin M \end{cases}. \quad (2)$$

The elastic slowing-down operator R_j^k for nuclide k in zone j is defined as

$$R_j^k(E) = \int_E^{\bar{E}_k} \frac{N_j^k \sigma_s^k(E') \phi_j(E') dE'}{(1 - \alpha_k) E'}, \quad (3)$$

where $\bar{E}_k = \min(E/\alpha_k, E_{su})$, $\alpha_k = ((A_k - 1)/(A_k + 1))^2$ and A_k is the atomic mass of nuclide k .

The quantity to be preserved $\bar{\Sigma}_{ai}$, is

$$\bar{\Sigma}_{ai} = \sum_{k=1}^{K_i} N_i^k \bar{\sigma}_{ai}^k, \quad (4)$$

where

$$\bar{\sigma}_{ai}^k = \frac{E_l}{E_u} \frac{\int_{E_l}^{E_u} \sigma_a^k(E) \phi_i(E) dE}{\int_{E_l}^{E_u} \phi_i(E) dE}. \quad (5)$$

The value of absorption cross section $\bar{\sigma}_{ai}^k$ for nuclide k in zone i , and reference values of absorption cross section σ_a^k for nuclide k as a function of dilution cross section σ_0 , are used in the VEGA2DAN sequence to determine the effective dilution cross section σ_{0i}^k for each nuclide k in each zone i . For this purpose the Segev interpolation scheme [15] is applied. Application of these dilution cross sections in the NITAWL-II code enables to include the resonance interference effects between different nuclides and spatial variation of the shielded cross sections. On the other hand, the macroscopic value of absorption cross section $\bar{\Sigma}_{ai}$ is used for effective Dancoff factor (c_i) calculation in zone i . This factor is convenient for utilization in all SCALE-4.4a system sequences, which include problem dependent cross section processing. Finally, the macroscopic value of absorption cross section $N_i^k \bar{\sigma}_{ai}^k$ is applied in VEGA2DAN sequence for calculation of effective Dancoff factor (c_i^k) in zone i containing the mixture of resonant nuclide k and one or two admixed moderator nuclides (defined in accordance with the Nordheim treatment). In this case, Dancoff factor c_i^k is favorable for the stand-alone utilization of the NITAWL-II code.

2.2. The equivalence principle

Using the Nordheim model for the elastic slowing-down, the equivalent neutron flux $\varphi_i(E)$ in fuel zone i is approximated with

$$\varphi_i(E) = \frac{1 - P_i(E)}{\Sigma_{ti}(E)} R_i(E) + \frac{P_i(E)}{E}, \quad (6)$$

where $P_i(E)$ is probability that a neutron originating in the fuel zone i will make its next collision in the moderator zones and $R_i(E)$ is elastic slowing-down operator in zone i . For general case, the elastic slowing-down operator $R_i(E)$ is defined as

$$R_i(E) = \sum_{k=1}^{K_j} \frac{\bar{E}_k}{E} \int_E \frac{N_i^k \sigma_s^k(E') \varphi_i(E') dE'}{(1 - \alpha_k) E'}. \quad (7)$$

In Eq. (6), the flux in the moderator zones is normalized to 1 above resonances, and a reciprocity relation is used to eliminate the escape probability from moderator zones. For simple case of one fuel rod in an infinite moderator, $P_i(E)$ is equivalent to the escape probability from the fuel $P_{0i}(E)$. If the fuel zone is more complicated, as in most practical cases of fuel lattices, and if the fuel zone is not totally black, i.e., some neutrons will pass through fuel zone without collision, the escape probability has to be modified by a Dancoff correction [8]

$$P_i(E) = \frac{P_{0i}(E)(1 - c_i)}{1 - [1 - \Sigma_{ti}(E)\bar{\ell}_i P_{0i}(E)]c_i}, \quad (8)$$

where $\bar{\ell}_i$ is the average chord length in the fuel zone i . The escape probability $P_{0i}(E)$ is function of geometry type and size as represented by a characteristic dimension $\bar{\ell}_i$. Also, it is explicit function of macroscopic total cross section in the fuel zone $\Sigma_{ti}(E)$. The analytic expressions for escape probability $P_{0i}(E)$ were developed by Case, deHoffman and Placzek [16] in slab, cylindrical and spherical geometry, and by Smith and Murray [17] for spherical shell (with central black zone). For cylindrical shell from r_{i-1} to r_i (also with central black zone) this probability is calculated by using Gauss-Jacobi integration of expression

$$P_{0i} = \frac{2}{\pi(r_i^2 - r_{i-1}^2)\Sigma_{ti}} \left\{ 2 \int_0^{r_{i-1}} [Ki_3(0) - Ki_3(\tau_1)]dy + \int_{r_{i-1}}^{r_i} [Ki_3(0) - Ki_3(\tau_2)]dy \right\}, \quad (9)$$

where Ki_3 is the third order Bickley function [18],

$$Ki_3(x) = \int_0^{\pi/2} \sin^2 \theta \exp\left(-\frac{x}{\sin \theta}\right) d\theta,$$

and where τ_1 and τ_2 denote optical path length

$$\tau_1 = \Sigma_{ti} \left(\sqrt{r_i^2 - y^2} - \sqrt{r_{i-1}^2 - y^2} \right),$$

and

$$\tau_2 = 2\Sigma_{ti} \sqrt{r_i^2 - y^2}.$$

An iterative strategy, in which the equivalent neutron flux $\phi_i(E)$, obtained for Dancoff factor c_i from previously iteration, is used to determine the new value of Dancoff factor by preserving the "exact" value of the shielded absorption cross section $\bar{\Sigma}_{ai}$, is based on the following equation,

$$\begin{aligned} \varphi_i(E) = & \varphi_i(E) \left[1 - \Sigma_{ti}(E) \bar{\ell}_i P_{0i}(E) \right] c_i + \left[1 - P_{0i}(E) \right] \frac{R_i(E)}{\Sigma_{ti}(E)} + \\ & \left[\Sigma_{ti}(E) \bar{\ell}_i P_{0i}(E) + P_{0i}(E) - 1 \right] \frac{R_i(E)}{\Sigma_{ti}(E)} c_i. \end{aligned} \quad (10)$$

In this iterative procedure, the new value of effective Dancoff factor c_i is calculated from the expression (that forces the shielded absorption cross section $\bar{\Sigma}_{ai}$ to be preserved)

$$c_i = \frac{a_{2i} + a_{4i} - \bar{\Sigma}_{ai}(b_{2i} + b_{4i})}{-a_{1i} - a_{3i} + a_{4i} + \bar{\Sigma}_{ai}(b_{1i} + b_{3i} - b_{4i})}, \quad (11)$$

where

$$\begin{bmatrix} a_{1i} \\ a_{2i} \\ a_{3i} \\ a_{4i} \\ b_{1i} \\ b_{2i} \\ b_{3i} \\ b_{4i} \end{bmatrix} = \begin{bmatrix} \int_{E_l}^{Eu} \Sigma_{ai}(E) \varphi_i(E) \left[1 - \Sigma_{ti}(E) \bar{\ell}_i P_{0i}(E) \right] dE \\ \int_{E_l}^{Eu} \frac{\Sigma_{ai}(E)}{\Sigma_{ti}(E)} \left[1 - P_{0i}(E) \right] R_i(E) dE \\ \int_{E_l}^{Eu} \frac{\Sigma_{ai}(E)}{\Sigma_{ti}(E)} \left[\Sigma_{ti}(E) \bar{\ell}_i P_{0i}(E) + P_{0i}(E) - 1 \right] R_i(E) dE \\ \int_{E_l}^{Eu} \Sigma_{ai}(E) \frac{P_{0i}(E)}{E} dE \\ \int_{E_l}^{Eu} \varphi_i(E) \left[1 - \Sigma_{ti}(E) \bar{\ell}_i P_{0i}(E) \right] dE \\ \int_{E_l}^{Eu} \frac{1}{\Sigma_{ti}(E)} \left[1 - P_{0i}(E) \right] R_i(E) dE \\ \int_{E_l}^{Eu} \frac{1}{\Sigma_{ti}(E)} \left[\Sigma_{ti}(E) \bar{\ell}_i P_{0i}(E) + P_{0i}(E) - 1 \right] R_i(E) dE \\ \int_{E_l}^{Eu} \frac{P_{0i}(E)}{E} dE \end{bmatrix}. \quad (12)$$

As pointed out previously, the CESD algorithm is applied in the VEGA2DAN sequence of the VEGA2 code for the solution of a fixed-source slowing-down equation (1) in an arbitrary geometry, using 20000 microgroups in the resolved energy domain. The recent work [19] has shown that this solution leads to acceptable agreement with Monte Carlo results. To calculate

integrals in Eq. (12), the so-called formalism of Riemann integration is used. This integration is performed using the same 20000-group cross sections stored in an auxiliary data library that could be accessed by VEGA2DAN during their calculations. This data library was generated from the ENDF/B-VI.4 evaluation with the pre-processing codes RECENT and SIGMA1 [20].

The convergence of Dancoff factor iteration to fine criteria (0.0001) may take as many as 10 iterations. In order to simplify the first-flight collision probability calculations, particularly in complicated two-dimensional geometries, an approximate option based on the N-term rational representation of collision probabilities is implemented in the VEGA2DAN sequence. In this option, the assumption that the fuel compositions are identical in all fuel zones is used. Here, as in the case of non-overlapping resonances, the collision probabilities are function of a single variable only, namely, of the total cross section of the fuel.

3. RESULTS

The proposed procedure was benchmarked for the recent example that represents the system with a fuel double heterogeneity, i.e., the fuel in solid form (pellets) surrounded by fissile material in the water solution [21]. The need for this type of analysis arises in several situations such as the dissolution of fuel elements in acid and TMI-2 type reactor accidents. Complementary reference calculations, obtained by various international contributors [21], confirm that the major source of dispersion in the standard design-oriented method is the incorrect determination of effective resonance absorption by ^{238}U . The largest discrepancies are showed for the benchmark problem 20. This problem represents spherical pellets (with diameter of 1 cm) of UO_2 (2.5% enriched uranium) dissolved continuously in a borated water solution (1500 ppm) at several pellet packing densities ($\text{PF} = V_{\text{fuel}}/V_{\text{cell}}$). The analysis of obtained results [21] has shown that standard design-oriented codes, as for instance the NITAWL code, coupled with the XSDRNPM code [22] via the CSAS control sequence [23], and APOLLO code [24], that permit the evaluation of more realistic self-shielded resonance cross sections within various spatial regions, but ignore the pellet-fission liquor shadowing effect, underestimate the reactivity loss, at 50% dissolution, by about 4000 pcm.

The new results obtained with the proposed procedure, implemented in the calculation based on the utilization of VEGA2DAN, NITAWL-II and XSDRNPM-S codes (via the CSAS control sequence), are presented in Fig. 1. The VEGA2DAN code was used to calculate effective Dancoff factors in the pellet and fission liquor zones (characterized with spherical and spherical shell geometry). This stage enables to account for ^{238}U resonance mutual self-shielding effect in the pellet-fissile liquor interaction. The NITAWL-II code was used for preparation of shielded cross sections in the resolved resonance domain (using Dancoff factors obtained with VEGA2DAN code). Finally, the effective multiplication factor (k_{∞}) for the pellet-fissile liquor cell with the white boundary condition was obtained by XSDRNPM-S code (performing one-dimensional discrete ordinates $S_{16}(P_3)$ calculation). These results were compared with reference results obtained by the MCNP-4B code [25] and continuous-energy library VMCCS [26], generated from ENDF/B-VI.4 evaluation. As can be seen in Fig. 1, the precision of the proposed procedure, as well as the VEGA2 code based on the subgroup procedure and multigroup library

(also, generated from ENDF/B-VI.4), is similar to the more demanding calculations based on the MCNP-4B code and ENDF/B-VI.4 library.

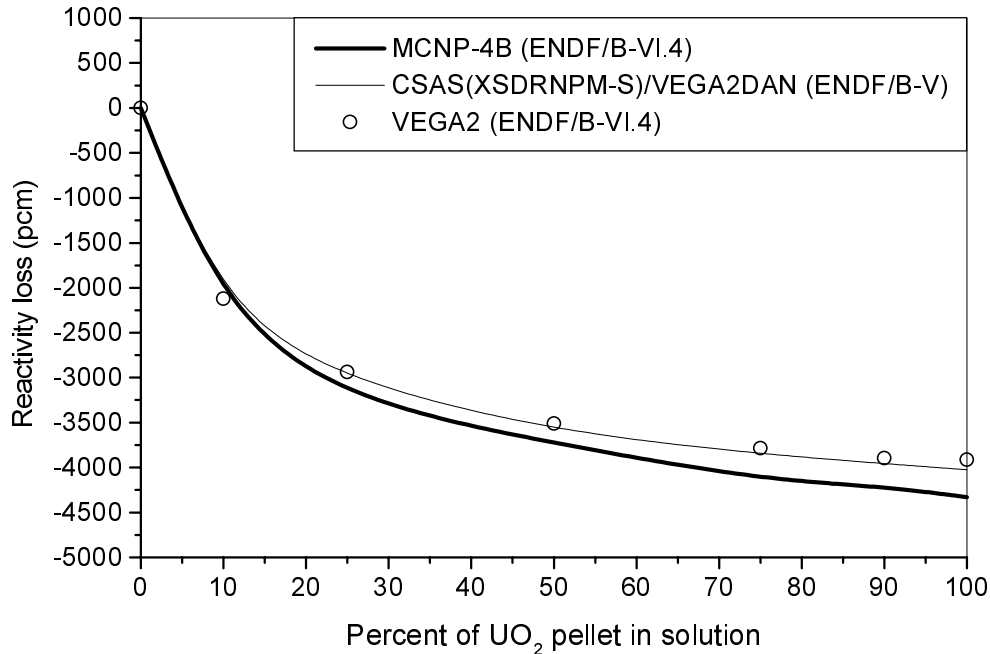


Figure 1. Comparison of calculated reactivity loss as function of fuel pellet solution, for a packing fraction ($PF=V_{\text{fuel}}/V_{\text{cell}}$) equal to 0.4 (the benchmark problem 20, Ref. [21])

The second benchmark represents a reflected pressurized water reactor (PWR) cell with square lattice pitch of 1.33 cm, containing the UO₂ (3.3 w/o ²³⁵U) fuel rod and clad (Zircaloy-4) of radii 0.41 cm and 0.475 cm, respectively. The mixture composition of this pin cell is given in Table I.

Table I. Mixture composition of PWR pin cell

Mixture	Nuclide	Atomic number density (10^{24} atoms cm^{-3})
Fuel (900K)	²³⁵ U	$7.500 \cdot 10^{-4}$
	²³⁸ U	$2.200 \cdot 10^{-2}$
	O	$4.550 \cdot 10^{-2}$
Clad (615K)	Cr	$7.598 \cdot 10^{-5}$
	Fe	$1.286 \cdot 10^{-4}$
	Zr	$4.254 \cdot 10^{-2}$
	Hf	$4.482 \cdot 10^{-6}$
Moderator (585K)	H	$4.633 \cdot 10^{-2}$
	O	$2.317 \cdot 10^{-2}$

For this benchmark the radial dependence of the resonance absorption within the fuel was studied by performing a multigroup calculation for a fuel pin divided into ten resonant regions of equal volumes. The current (version 4.4a) and previous versions of SCALE code systems do not

treat cells with the same nuclide in more than one fuel zone. The basic problem is that the NITAWL-II code treats each resonance of each nuclide totally independently, with no interaction with other zones except through the Dancoff factor. The SCALE generates the Dancoff factor assuming that nuclide occurs only in the current zone. So, it is not possible to treat the two or more zones case properly using the NITAWL-II code via CSAS control sequence. In the present paper, the Dancoff factors were calculated with the VEGA2DAN code. The 44-group shielded cross sections (derived from the ENDF/B-V evaluation) were prepared with the NITAWL-II code for each fuel layer, and the absorption rate of ^{238}U in the energy range from 10^{-5} eV to 20 MeV were obtained with the KENO-V.a Monte Carlo code [27]. The Dancoff factors obtained with VEGA2DAN code for the ten-layer model of PWR pin cell benchmark are given in Table II.

Table II. Dancoff factors for the ten-layer model of PWR pin cell

Layer (Fuel region)	Radius [cm]	Dancoff factor
1	0.129653	0.915
2	0.183358	0.961
3	0.224566	0.967
4	0.259307	0.970
5	0.289914	0.970
6	0.317585	0.969
7	0.343031	0.966
8	0.366715	0.959
9	0.388960	0.939
10	0.410000	0.741

The results obtained for the ten-layer model, where the self-shielded cross sections were prepared separately for each layer with effective Dancoff factor previously calculated, are compared with those obtained for the one-layer model, where the self-shielded cross sections calculated for the whole fuel pin were used for each layer. The Dancoff factor for the whole fuel pin is equal to 0.317. Results obtained with the KENO-V.a code by using these two models, and results obtained with the MCNP-4B Monte Carlo code and an auxiliary MCNP-4B library prepared for the working temperatures of this benchmark on the basis of ENDF/B-V evaluation, are presented in Table III. For each run of the KENO-V.a and MCNP-4B Monte Carlo codes, 10^7 neutron histories were taken into account. In this way, a standard deviation of the ^{238}U absorption rate less than 0.1% was ensured. As expected, a strong resonance self-shielding effect was observed for the spatial dependence of ^{238}U absorption rate. On the basis of these results, it can be seen that proposed procedure consistently improves the agreement of multigroup SCALE-4.4a code system (based on the Dancoff correction theory) with the MCNP-4B continuous-energy Monte Carlo code.

Table III. Monte Carlo calculation of the ^{238}U absorption ($\text{cm}^{-3} \text{s}^{-1}$) in the PWR fuel rod with linear heat rate of 95 W cm^{-1}

Layer (Fuel region)	MCNP-4B	KENO-V.a	
		One-layer model (Percent difference to MCNP-4B)	Ten-layer model (Percent difference to MCNP-4B)
1	2.2640+12 ^(a)	2.7602+12 (21.9)	2.3419+12 (3.4)
2	2.2961+12	2.7736+12 (20.8)	2.3809+12 (3.7)
3	2.3378+12	2.7884+12 (19.3)	2.4239+12 (3.7)
4	2.3812+12	2.8036+12 (17.7)	2.4612+12 (3.4)
5	2.4390+12	2.8207+12 (15.7)	2.5221+12 (3.4)
6	2.5120+12	2.8381+12 (13.0)	2.5916+12 (3.2)
7	2.6178+12	2.8569+12 (9.1)	2.6886+12 (2.7)
8	2.7911+12	2.8776+12 (3.1)	2.8465+12 (2.0)
9	3.1848+12	2.9032+12 (-8.8)	3.1846+12 (0.0)
10	5.2629+12	2.9330+12 (-44.3)	5.1963+12 (-1.3)

^(a) 2.2640+12 means $2.2640 \cdot 10^{12}$.

4. CONCLUSION

This paper shows that procedure for Dancoff factor calculation based on equivalence principle between a heterogeneous medium and an equivalent medium consisting of an infinite array of simple pin cells can provide to account for resonance interference and overlap effects. The advantage of this procedure is apparent in complicated, irregular geometries where other methods are not applicable satisfactory. The increase in the computational time is not significant with today's computers, and more important, the time spent on computation of Dancoff factors is still only a fraction of time needed to run criticality problems.

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