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RESONANCE COMPUTATIONS FOR CELLS WITH FUEL ANNULI*

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ABSTRACT

Two methods have been developed for the computation of resonance integrals in cells containing annular fuel regions. Both are based on rational approximations. One is a generalization of a one-term rational approximation method developed by Segev for a cell with a single fuel annulus. The second modifies the earlier Chen-Gelbard two-term method originally used for double-heterogeneity calculations. Both methods were tested, in cells with two fuel annuli, for various U^{235} and U^{238} resonances. Both gives resonance integrals accurate enough for practical purposes. The two-term fits are substantially more accurate in some NR cases, but are somewhat more difficult to correct for finite resonance widths.

I. INTRODUCTION

Fuel assemblies with fuel and moderator contained in concentric annular tubes are of some practical interest. One typical example of such an assembly is that of the Savannah River reactors in which two fuel annuli, along with structure and coolant regions, are present as shown schematically in Ref. 1. In general, the rigorous treatment of resonance absorption in a cell consisting of multiple fuel annuli would require the use of an integral transport theory code, such as the RABANL option of MC^2-2, that treats the neutron transport between regions and the slowing down equation in great detail. Such an approach is time-consuming and is usually not considered unless rigor is absolutely required. For routine design calculations, simplified methods based on rational approximations and the NR/IR approximation are usually preferred when used in conjunction with the widely accepted Bondarenko scheme based codes. Furthermore, the latter approach is much more convenient in treating the unresolved resonances.

This paper describes two types of rational approximations, based on one and two terms respectively, that can provide adequate treatment of resonance absorption in a cell consisting of multiple annuli. The fact that the fuel cells can be considered as 1D infinite cylinders simplifies the problem significantly. The NR fluxes can be computed readily using the highly efficient collision probability routine taken from the existing MC^2-2/SDX code, whereby various parameters required by the rational approximations can be determined for a wide range of situations of practical interest. Both methods are believed to be useful for design calculations.

II. ONE TERM FIT

We consider, preliminarily, the case of a single cell containing only a fuel region (region 0) and a moderator region (region 1). Suppose for simplicity that region 0 contains only one resonant absorber, mixed with a scattering diluent of constant macroscopic cross section Σ_m. Assume the diluent as well as the moderator in region 1 are, essentially, infinitely heavy. Then

$$V_0 \Sigma_{t0}\phi_0(u) = (1 - P_0) \frac{V_0}{(1 - \alpha)} \int_{u-\varepsilon}^{u} du' e^{-(u-u')} \Sigma_{s0}(u') \phi_0(u') du'$$

$$+ V_0(1-P_0)\Sigma_m + P_1 V_1 \Sigma_{t1},$$

and, using reciprocity,

$$\Sigma_{t0}\phi_0(u) = (1 - P_0) \frac{1}{(1 - \alpha)} \int_{u-\varepsilon}^{u} du' e^{-(u-u')} \Sigma_{s0}(u') \phi_0(u') du' \qquad (1)$$

$$+ (1 - P_0) \Sigma_m + P_0 \Sigma_{t0}.$$

Now let

$$P_0 = \Sigma_e/(\Sigma_e + \Sigma_{t0}) \qquad (2)$$

without, for the moment, defining Σ_e. Putting Eq. (2) into Eq. (1) we get

$$(\Sigma_e + \Sigma_{t0}) \phi_0(n) = \frac{1}{(1 - \alpha)} \int_{u-\varepsilon}^{u} e^{-(u-u')} \Sigma_{s0}(u')\phi_0(u')du' \qquad (3)$$

$$+ (\Sigma_e + \Sigma_m) .$$

Equation (3) is formally the same as the slowing-down equation in an ("equivalent") infinite medium, a medium containing heavy scatterers with cross sections Σ_e and Σ_m. Equation (4), in the NR limit, takes the form

$$\phi_0(u) = (\Sigma_{p0} + \Sigma_m + \Sigma_e)/[\Sigma_{t0}(u) + \Sigma_e] . \qquad (4)$$

In Wigner's rational approximation for an isolated rod, $\Sigma_e = \Sigma_e^{iso} = 1/\bar{\ell}_0$ where $\bar{\ell}_0$ is the rod's mean-chord-length, $\bar{\ell}_0 = 4V_0/S_0$. We then have $P_0 = 1/(1 + \Sigma_t \bar{\ell}_0)$, an expression which is asymptotically correct in the black limit. In the more general case P_0 is generally written as in Eq. (3), but with[2,3]

$$\Sigma_e = \Sigma_e^{iso} \frac{a(1 - C)}{[1 + (a - 1)C]} , \quad \Sigma_e^{iso} = 1/\bar{\ell}_0, \quad \bar{\ell}_0 \equiv 4V_0/S_0. \qquad (5)$$

Here C is the Dancoff factor, i.e., the probability, in the black-fuel limit, that a neutron, drawn from an isotropic flux at a rod surface, will be reabsorbed in the rod after reflection; a is the Bell factor, which improves the accuracy of Eq. (5) as the rod gets gray. Prescriptions for setting a will be found in Refs. (2) and (3). Since these prescriptions are not applicable, directly, to our geometry we will not discuss them here. Our procedure for computing a will be discussed below, after modification of the above analysis to cover cells with several annular fuel regions. The case of a cell with a single fuel annulus has already been treated by Segev.[4] Here we generalize Segev's method to cells with several fuel annuli.

Consider any fuel annulus k with the outer radius R_k sandwiched between two moderator regions in a cell consisting of multiple annuli. The escape probability of fuel region k must be equal to the sum of the probabilities of neutrons escaping through two surfaces and eventually make their collisions somewhere in the lattice. Hence, one has

$$\begin{aligned} 1 - P_{kk} = & \left[P_{k,k-1}\,\gamma_{k-1} + P_{k,k-1}\,(1-\gamma_{k-1})\,(1-G_{k-1,k})\,\gamma_{k+1}\right. \\ & \left. + - - - - - -\right] + \left[P_{k,k+1}\,\gamma_{k+1} + P_{k,k+1}\,(1-\gamma_{k+1})\right. \\ & \left.(1-G_{k+1,k+2})\,\gamma_{k+2} + - - - - -\right] \end{aligned} \tag{6}$$

where $G_{j\pm1,i}$ is the probability that neutrons entering region i from region $i\pm1$ and make their collision in region i, and γ's are the 'sticking' probabilities for moderator regions. Here, $G_{i\pm1,i}$ is related to $P_{i,i\pm1}$ by

$$G_{i\pm1,i} = \Sigma_{ti}\,\frac{4\,V_i}{S_i^{\pm}}\,P_{i,i\pm1} \tag{7}$$

where V_i and $S_i^{\pm}$ are volume and outer/inner surfaces in question.

Equation (6) can be reduced to much simpler form if one follows the procedures proposed by Segev.[4] His assumptions, when applied to the present case, are just Sauer's rational approximation[5] for $P_{i,i\pm1}$ of interest, i.e.

$$P_{i,i\pm1} = \frac{v_i}{1 + \frac{v_i}{s_i^{\pm}}\,\bar{\ell}\Sigma_{ti}} \tag{8}$$

where v_j and $s_j^{\pm}$ are volume and surface fractions respectively,

$$s_i^{+} = \frac{R_i}{R_i + R_{i-1}}\,; \qquad s_i^{-} = \frac{R_{i-1}}{R_i + R_{i-1}}\,. \tag{9}$$

The substitution of Eqs. (8) and (9) into Eq. (6) under the black limit yields the escape probabilities for various annuli as a function of $\bar{\ell}\,\Sigma_t$ and sticking probabilities of the adjacent moderator regions from which the escape cross sections in the conventional form can be obtained. To cast the results into the conventional form defined by Eq. (5), it can be shown readily that, for any fuel annulus k with the outer radius R_k, the quantities Σ_{ek}^{iso} (actually with intra-cell Dancoff corrections) and C_k under the 'black' limit becomes

$$\Sigma_{ek}^{iso} = \frac{1}{\bar{\ell}} \cdot \frac{\gamma_{k+1} R_k + \gamma_{k-1} R_{k-1}}{R_k + R_{k-1}} ; \qquad \text{for } k < N-1 \tag{10}$$

$$= \frac{1}{\bar{\ell}} \cdot \frac{R_k + \gamma_{k-1} R_{k-1}}{R_k + R_{k-1}} ; \qquad \text{for } k = N-1$$

$$C_k = 0; \qquad \text{for } k < N-1 \tag{11}$$

$$= 1 - \frac{\gamma_{k+1} R_k + \gamma_{k-1} R_{k-1}}{R_k + \gamma_{k-1} R_{k-1}} ; \qquad \text{for } k = N-1$$

where N is assumed to be the outermost non-fuel region and the 'sticking' probabilities γ's are

$$\gamma_{k-1} = 1 - T_{k-1}^{00} - T_{k-1}^{IO} \tag{12}$$

$$\gamma_{k+1} = 1 - T_{k+1}^{IO}; \qquad \text{for } k < N-1 \tag{13}$$

$$= \left(1 - T_{k+1}^{OI}\right) + T_{k+1}^{OI}\left(1 - T_{k+1}^{00} - T_{k+1}^{IO}\right) ; \qquad \text{for } k = N-1$$

Here, T_k^{00}, T_k^{IO} and T_k^{OI} denote the transmission probabilities from outer surface to outer surface, outer-to-inner and inner-to-outer, respectively. For any given non-fuel cross section for an energy group, these quantities can be evaluated rigorously and efficiently using the method proposed in Ref. (6). Thus, the intra and inter cell Dancoff corrections are specified without the need of changing the traditional expression.

The expressions described above obviously reduces to that of Segev when the cell with only one annular fuel region is considered. It is also worth noting that the cell with annuli can be considered as the most fundamental configuration in the lattice physics. In the limit, when R_{k-1}/R_k approaches zero (or pin cell), $T^{OI} = T^{IO} = 0$ and $(1 - T^{00}/\Sigma_t\bar{\ell})$ reduces asymptotically to the well known escape probability of Inglis[7] for fuel pin as shown in Ref. 7. In another limit when R_{k-1}/R_k approaches unity (or plate cells), T^{00} vanishes and T^{OI} reduces analytically to $2E_3(\tau)$, the well-known transmission probability for the plate. Thus, the pin and plate configurations may be considered as the limiting cases of the annular cell.

To introduce Bell factors, we again assume that Σ_e is given by Eq. (5), but now Σ_e^{iso} is defined by Eq. (10). In the geometries considered here no analytic expression for an optimum a is available. We note, however, that the NR flux is the flux in a purely absorbing cell in which (a) $\Sigma_{ak}^{NR} = \Sigma_{tk}$: (b) $S_k = \Sigma_{Mk}$ in moderator regions, and (c) $S_k = (\Sigma_p + \Sigma_m)_k$ in fuel regions. Here S_k is the source density in region k. If the fuel regions are all of the same enrichment, this NR flux becomes a function of a single total fuel cross section, a function which can easily be computed by collision probability methods. The Bell factor in Eq. (5) can then be adjusted to a value such that Eq. (5) agrees with the computed NR fluxes reasonably well over the range of resonance cross sections encountered in a given multigroup. Here we only consider cells with a single fuel enrichment, and determine a by the above procedure.

II. TWO-TERM FIT

A procedure for fitting parameters in two-term rational approximations was proposed in Ref. 8. There, because the cell geometry was very complicated, the transport computations used in the parameter-fitting process were carried out by Monte Carlo. As a result the fitting process was fairly expensive, so that it had to be regarded as a benchmarking tool rather than a design method. Here: (a) we show that the proposed fitting process, in special situations, can be used for design and (b) we describe some changes in the fitting process, introduced to improve its performance.

Computational Method, Two-term Fit

We again assume, in all work reported here, that the fuel compositions are identical in all annuli, though we place no restrictions on the number of, or dimensions of, the annular fuel regions. The fitting process proceeds as follows:

1. In each multi-group select three fuel cross sections, $\Sigma_{tf} = \Sigma_1$, Σ_2, Σ_3. Later more will be said about the choice of these Σ_{tf}'s, but now we assume only that Σ_3 is large enough so that, when $\Sigma_{tf} = \Sigma_3$, the fuel regions will be fairly black.

2. Calculate the NR flux, ϕ^ν, for each of the three Σ_ν. In these calculations all materials are treated as pure absorbers. Total cross sections in non-fuel regions are set equal to the true total cross sections within the multi-group while Σ_{tf} is set, in turn, to each of the three Σ_ν's. The source in each non-fuel region is equal to its total cross section, while the source in the fuel is taken to be equal to Σ_p. Compute ϕ_o^ν from the relation[5]

$$\phi^\nu = \Sigma_p/\Sigma_\nu + (1 - \Sigma_p/\Sigma_\nu)\phi_o^\nu,$$

where ϕ_o^ν is the flux due only to the sources outside the fuel. We will fit ϕ_o, in each fuel region, to the form

$$\phi_o \approx G \equiv (a + C_1C_2C_3\,x)/[(1 + C_1C_3\,x)(1 + C_2C_3\,x)], \qquad (14)$$

where $x \equiv \Sigma_{tf}\bar{\ell}$.

Here $\bar{\ell}$ is the mean-chord-length of the fuel region in question, while a, C_1, C_2 and C_3 are fitting parameters. It should be understood that these parameters are different in each fuel region but, for simplicity, region indices will be omitted. It is the purpose of our fitting process to construct a rational approximation of form Eq. (14) such that

$$G^{\nu} \equiv G(\Sigma_{tf} = \Sigma_{\nu}) = \phi_o^{\nu} \ , \ \nu = 1, 2, 3 \tag{15}$$

with a, C_1, C_2 and C_3 all real and positive. The restriction on admissible values of a and C_1 makes it necessary to use four parameters to fit three fluxes. Note that it is ϕ_o which is being fit here to a two-term rational approximation, and that there are really three terms in ϕ.

3. Initially, set $C_3 = 1/(\Sigma_3 \phi_o^3 \bar{\ell})$.

4. Define:

$$\tau_{\nu} \equiv C_3 \Sigma_{\nu} \bar{\ell},$$
$$\Delta\tau \equiv \tau_2 - \tau_1, \ \Delta G = \phi_o^2 - \phi_o^1,$$
$$\Delta(G\tau) \equiv \phi_o^2 \tau_2 - \phi_o^1 \tau_1,$$
$$\Delta(G\tau^2) \equiv \phi_o^2 \tau_2^2 - \phi_o^1 \tau^2{}_1,$$
$$C_{20} \equiv -\Delta G/\Delta(G\tau)$$
$$C_{2\infty} \equiv \Delta(G\tau)/[\Delta\tau - \Delta(G\tau^2)].$$

It can be shown[5] that

$$C_1 = (C_{20} - C_2)/(1 - C_2/C_{2\infty}). \tag{16}$$

5. (a) If $C_{2\infty} < 0$ set $C_2 = 2C_1$ and solve (3) for the larger C_1.

Then determine a from (1).

(b) If $C_{2\infty} > C_{20}$, (and we assume that C_{20} is positive), then set $C_2 = C_{20}/2$ and get C_1 from (3). Again get a from (1).

(c) If $0 < C_{2\infty} < C_{20}$ set $C_2 = 2C_{20}$ and again get C_1 from (3).

6. Given a, C_1 and C_2, recompute C_3 from

$$\phi_o^3 = (a + C_1 C_2 C_3 \Sigma_3 \bar{\ell})/[(1 + C_1 C_3 \Sigma_3 \bar{\ell})(1 + C_2 C_3 \Sigma_3 \bar{\ell})] \ , \tag{17}$$

taking the largest root of the quadratic. Return to 4 and loop to convergence. Convergence to fine criteria may take as many as 20 iterations, but has never been troublesome.

Rationale for the above procedure is basically the same as in Ref. 6, but some significant changes have been made, here, in the original algorithm. First, because Σ_3 is sometimes not very much larger than the other Σ's the initial value, set in step 3, is not always adequate. It is therefore corrected iteratively. Secondly, the case (a) option in Ref. 6 has been changed to our 5a because we find that, in the original algorithm we often get $C_1 \approx C_2$, a numerically undesirable situation. Finally, and for the same reason, the a = 1 option of Ref. 6 was eliminated.

The fitted fluxes are not insensitive to the values of the Σ_ν which must, therefore, be adjusted preliminarily. This is done by first computing $\phi(\Sigma)$ for perhaps 20 Σ's in the range from Σ_p to Σ_{max}, where Σ_{max} is the maximum fuel cross section which will be encountered in the group. Then the accuracy of the fitted $G(\Sigma)$ is examined for each Σ. The Σ_ν are then readjusted to improve the fit in regions where it seems inadequate. Generally, we have started from $\Sigma_1 \approx 4\Sigma_p$, $\Sigma_3 \approx \Sigma_{max}$, $\Sigma_2 \sim \frac{1}{2}(\Sigma_1 + \Sigma_3)$. Finally, the accuracy of selected resonance integrals may be tested by quadrature over the true and fitted fluxes and the Σ_ν's may be fine-tuned to improve the accuracy of the multi-term integrals.

III. COMPUTATIONAL RESULTS AND DISCUSSIONS

NR resonance integrals have been computed, using the methods described in Sections I and II above, for five U^{235} resonances and eight U^{238} resonances, in the geometry described in Ref. 1. All resonances parameters are listed in Table I. For comparison, high precision resonance integrals, also in NR, were computed by quadrature over NR fluxes evaluated (by collision probability methods) as detailed functions of total fuel cross section. Relative errors are shown in Table II for one-term computations, in Table III for two-term fits. All inner-ring results were obtained with a = 2.19, outer ring results for 1 = 1.65. For two-term fits in the highly enriched configurations $\Sigma_1 = 0.4$, $\Sigma_2 = 2.$, $\Sigma_3 = 10$, all in cm^{-1}. In all the low-enrichment cases $\Sigma_1 = 0.6$, $\Sigma_2 = 10.$, $\Sigma_3 = 20$. The highly-enriched fuel regions contained substantial quantities of aluminum diluent. Therefore, self-shielding effects were small and both methods were extremely accurate. For low enrichments (and medium enrichments cases not shown here), the two-term resonance integrals were substantially better than the one-term integrals. In all cases considered, again including a wide range of configurations not shown here, errors in two-term resonance integrals were under 1%, errors in the one-term integrals under 4%. Thus, in resonance integral computations, both methods seem adequate for practical purposes.

To what extent they are adequate for Doppler calculations is, at this time, much less clear. For the smallest resonances treated here, errors in the Doppler effect may be very large, especially when the change in resonance integral due to temperature becomes comparable to the errors in the resonance integrals themselves. For large resonances one sees errors of up to ≈10% for two-term fits, up to ≈ 15% for one-term fits. Of course, the same difficulty in computing Doppler coefficients is encountered in the simplest pin-cell lattices, so that no new difficulties have been caused by the added geometric complexity.

Generally one finds, as is to be expected, that the two-term resonance integrals are substantially more accurate than one-term integrals, but the use of two-term expansions does seem to have at least one disadvantage. For two-region cells the one-term approximation converts the integral equation for the flux into an equation formally the same as the slowing-down equations in an ("equivalent") infinite medium. Therefore, it is possible to estimate the NR-approximation error by comparing an infinite medium NR computation with an accurate solution (pretabulated, in practice) of the infinite medium slowing-down equations. The equivalence relation is no longer rigorous in a general multiregion cell: it can still be used, however, as an approximation from which resonance-width corrections may be estimated.

On the other hand, there is no longer a simple equivalence relation if the one-term rational approximation is replaced by a multi-term approximation. For the same reason, the traditional IR-approximation becomes less obvious when the equivalence relation is in doubt. Estimation of errors induced by the NR approximation is, therefore, more difficult than in the one-term case, though by no means impossible.

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Table I. Representative Resonances Used for Test Calculations

a. U^{235}

E_o eV	Γ_n	Γ_f	Γ_γ	σ_o
19.297	0.31936E-02	0.60179E-01	0.30348E-01	0.22991E+04
16.088	0.36099E-03	0.19617E-01	0.31383E-01	0.56881E+03
13.996	0.53723E-03	0.47000E+00	0.26000E-01	0.10065E+03
8.180	0.11234E-02	0.91000E-01	0.31170E-01	0.14501E+04
1.140	0.15161E-04	0.11620E+00	0.34600E-01	0.11481E+03

b. U^{238}

E_o eV	Γ_n	Γ_γ	σ_o
189.60	0.16700E+00	0.23050E-01	0.12068E+05
165.30	0.34000E-02	0.23360E-01	0.20015E+04
145.60	0.91190E-03	0.23000E-01	0.68204E+03
102.50	0.71640E-01	0.24410E-01	0.18948E+05
66.01	0.24610E-01	0.23680E-01	0.20104E+05
36.67	0.33910E-01	0.22920E-01	0.42372E+05
6.67	0.15100E-02	0.22530E-01	0.24522E+05

Table II. Relative Errors in Resonance Integrals As Results of One-Term Rational Approximations

a. U^{235}

	High Enrichment (85%)		Low Enrichment (8%)	
	Inner	Outer	Inner	Outer
E_o eV	ε,%	ε,%	ε,%	ε,%
19.297	0.762	-0.333	-3.043	-1.246
16.088	0.787	1.046	-1.120	-0.076
13.996	0.419	0.562	-0.425	-0.003
8.181	0.752	0.012	-2.699	-0.968
1.140	0.457	0.615	-0.481	-0.0009

Table II. Relative Errors in Resonance Integrals As Results of One-Term Rational Approximations (Cont.)

b. U^{238}

E_o eV	High Enrichment (85%) Inner ε,%	High Enrichment (85%) Outer ε,%	Low Enrichment (8%) Inner ε,%	Low Enrichment (8%) Outer ε,%
189.6	0.783	0.239	-0.012	2.116
165.3	0.217	0.284	-3.809	-2.105
145.6	0.076	0.097	-2.598	-0.614
102.5	0.780	-0.103	0.319	2.671
66.01	0.859	0.459	0.798	3.094
36.67	1.281	-1.434	0.085	2.430
6.67	0.802	-0.583	0.259	2.664

Table III. Relative Errors in Resonance Integrals as Results of Two-Term Rational Approximation

a. U^{235}

E_o eV	High Enrichment (85%) Inner ε,%	High Enrichment (85%) Outer ε,%	Low Enrichment (8%) Inner ε,%	Low Enrichment (8%) Outer ε,%
19.297	0.003	-0.0004	0.343	0.119
16.088	-0.031	-0.032	0.918	0.353
13.996	-0.341	-0.433	0.478	0.151
8.181	0.088	0.113	0.505	0.239
1.140	-0.321	-0.407	0.523	0.169

Table III. Relative Errors in Resonance Integrals as Results of Two-Term Rational Approximation (Cont.)

b. U^{238}

E_o / eV	High Enrichment (85%) Inner ε,%	High Enrichment (85%) Outer ε,%	Low Enrichment (8%) Inner ε,%	Low Enrichment (8%) Outer ε,%
189.6	0.239	0.331	-0.0006	-0.384
165.3	-0.379	-0.478	-0.235	-0.410
145.6	-0.187	-0.235	0.962	0.505
102.5	0.159	0.215	0.042	-0.402
66.01	0.355	0.469	-0.068	-0.406
36.67	-0.460	-0.706	-0.005	-0.438
6.67	-0.027	-0.052	-0.008	-0.238

Table IV. Fitted Parameters for Two-Term Rational Approximation

Parameters	High Enrichment (85%) Inner	High Enrichment (85%) Outer	Low Enrichment (8%) Inner	Low Enrichment (8%) Outer
C_1	0.53936	0.65761	0.31073	0.31906
C_2	0.39901	0.41879	0.76151	0.58332
C_3	1.1221	0.93639	1.1340	1.0321
a	0.96956	0.96370	1.1188	0.98509