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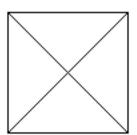
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# COMPUTING CONTROL ROD WORTHS IN THERMAL RESEARCH REACTORS

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# COMPUTING CONTROL ROD WORTHS IN THERMAL RESEARCH REACTORS

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# ABSTRACT

Simple diffusion theory cannot be used to evaluate control rod worths in thermal reactors because of steep flux gradients that occur within the absorber material. However, reliable control rod worths can be calculated within the framework of diffusion theory if the control material is characterized by a set of mesh-dependent effective diffusion parameters or if group-dependent current-to-flux ratios are specified on the absorber surface.

For thin slab absorbers the effective diffusion parameters are functions of a pair of blackness coefficients. Methods for calculating these blackness coefficients in the  $P_1$ ,  $P_3$  and  $P_5$  approximations, with and without scattering, are discussed, and equations for the corresponding mesh-dependent effective diffusion parameters are derived.

For control elements whose geometry does not permit a thin slab treatment, other methods are needed for determining the effective diffusion parameters. One such method, based on reaction rate ratios, is presented.

An alternate method for calculating control rod worths isolates the absorber from the diffusion-theory calculation by specifying group-dependent current-to-flux ratios on the absorber surface. Neutron transport calculations are used to determine these current-to-flux ratio internal boundary conditions subject to limits set by radius-dependent black absorber rods.

These methods are illustrated for a number of absorber materials and geometries. Computed control rod worths are compared with detailed Monte Carlo calculations and, where possible, with experimental measurements. In general, control rod worths based on these diffusion-theory methods are found to be consistent with those from Monte Carlo calculations and with measured values.

#### **1. INTRODUCTION**

Research reactor control rods are composed of materials which strongly absorb thermal neutrons. In such materials the low-energy neutron flux varies rapidly as a function of position, which causes steep flux gradients near the absorber surface. Under these conditions Fick's law of diffusion is invalid, and so, without special methods, diffusion theory cannot be used to calculate control rod worths in thermal research reactors. Higher order methods, such as Monte Carlo techniques, are commonly used for this purpose. However, reasonably accurate control rod worths can be computed within the framework of diffusion theory by characterizing the absorber material by means of a group-dependent set of effective diffusion parameters (D<sub>eff</sub> and  $\Sigma_{a-eff}$ ) or by specifying group-dependent neutron current-to-flux ratios (i.e. internal boundary conditions) on the absorber surface.

The purpose of this paper is to show how effective diffusion parameters and internal boundary conditions can be calculated. Using these techniques, control rod worths are computed and compared with results of detailed Monte Carlo calculations and with measured values.

## 2. EFFECTIVE DIFFUSION PARAMETERS

Methods used to determine effective diffusion parameters depend on the geometry of the absorber. If the control rod can be described by one or more thin slab absorbers (i.e. thickness << transverse dimensions), effective diffusion parameters can be written in terms of a pair of "blackness coefficients" which are defined below. For non-slab-like absorbers effective diffusion parameters can be determined from a reaction rate ratio matching requirement. In either case, the effective diffusion parameters depend on the neutronic properties of the absorber and on the mesh structure within it, but not on the outside media. For those high energy groups for which  $\Sigma_s >> \Sigma_a$  for the control material, normal diffusion theory is valid so the determination of effective diffusion parameters is unnecessary for these groups.

#### 2.1 Thin Slab Geometry

For control materials in the shape of thin slabs, mesh-dependent effective diffusion parameters can be expressed in terms of a pair of energy-dependent blackness coefficients,  $\alpha$  and  $\beta$ . For an absorber slab of thickness  $\tau$  the blackness coefficients are defined by the equations

$$\alpha \equiv (J_1 + J_r) / (\phi_1 + \phi_r), \text{ and } \beta \equiv (J_1 - J_r) / (\phi_1 - \phi_r)$$

where  $\phi$  and J are the asymptotic neutron fluxes and currents <u>into</u> the slab on the left-hand and right-hand surfaces of the slab. Because of these definitions, the blackness coefficients depend only on the properties of the absorber slab.

## 2.1.1 Blackness Coefficients

Blackness theory<sup>1-3</sup> provides a mechanism for evaluating the blackness coefficients. The theory assumes:

- 1. The coolant slab is uniform and of infinite lateral extent.
- 2. There are no neutron sources within the control slab due to fission, n2n, or scattering from other energies.
- 3. Neutron scattering within the slab is isotropic.
- 4. Diffusion theory is applicable to all regions within the reactor except for the control slab.
- 5. Blackness coefficients evaluated for infinite slabs are applicable to finite slabs whose transverse dimensions are very large relative to the thickness.

Because of the first two assumptions, the one-dimensional monoenergetic Boltzmann transport equation can be solved by expanding the angular flux within the slab into spherical harmonics in order to determine surface fluxes and currents. The fourth assumption is normally violated at locations just outside a strongly absorbing slab. Therefore, the flux shape determined by using blackness-modified diffusion parameters is likely to be erroneous at such locations. The last assumption is necessary because quantities analogous to  $\alpha$  and  $\beta$  for finite slabs do not exist. However, it is reasonable to expect this assumption to provide a good approximation.

To illustrate how the blackness coefficients are calculated,  $\alpha$  and  $\beta$  are evaluated in the P<sub>1</sub> approximation, with and without scattering, in the Appendix. Although the algebra is lengthy, the Appendix outlines how the same methods are extended to calculate the blackness coefficients in the P<sub>3</sub> and P<sub>5</sub> approximations. More details on these higher order approximations are given in Ref. 3. For very strong absorbers ( $\Sigma_a / \Sigma_s >> 1$ ) a modified form of the zero-scatter P<sub>1</sub> approximation, namely

$$\alpha_{0m}(P_1) = 0.4692 \left[1 - 2E_3(\Sigma_a \tau)\right] / \left[1 + 3E_4(\Sigma_a \tau)\right]$$

$$\beta_{0m}(P_1) = 0.4692 \left[1 + 2E_3(\Sigma_a \tau)\right] / \left[1 - 3E_4(\Sigma_a \tau)\right],$$

gives good results. In these equations  $E_3$  and  $E_4$  are the exponential integrals of the absorber thickness expressed in absorption mean free paths. The blackness coefficients, especially  $\beta$ , are very sensitive to neutron scattering and so these approximations fail when scattering becomes significant. In such cases the coefficients should be evaluated in the  $P_5$  approximation.

Broad-group blackness coefficients are most accurate if they are obtained by fluxweighting the fine-group values. Thus,

$$< \alpha > = \sum_{i} \alpha_{i} (\phi_{l} + \phi_{r})_{i} / \sum_{i} (\phi_{l} + \phi_{r})_{i}$$

$$<\beta>=\sum_{i}\beta_{i}(\phi_{l}-\phi_{r})_{i}/\sum_{i}(\phi_{l}-\phi_{r})_{i}$$

where the summations are over the number of fine groups which make up the broad group. The fine group surface fluxes ( $\phi_1$  and  $\phi_r$ ) may be obtained from a one-dimensional P<sub>1</sub>, S<sub>8</sub> transport calculation.

It is usually sufficient to calculate  $\langle \alpha \rangle$  and  $\langle \beta \rangle$  only for the thermal and epithermal groups. Normally, blackness coefficients for the fast groups are not needed because for these energies  $\Sigma_s \rangle > \Sigma_a$  for the absorber and so normal diffusion theory applies without any need for effective diffusion parameters.

# 2.1.2 Effective Diffusion Parameters

The  $\alpha$  and  $\beta$  blackness coefficients form a pair of internal boundary conditions applicable on the surfaces of the absorber slab. However, most diffusion codes are not programmed to handle internal boundary conditions of this type. Therefore, it is convenient to determine a set of effective diffusion parameters ( $D_{eff}$  and  $\Sigma_{a-eff}$ ) in terms of the blackness coefficients which preserve the current-to-flux ratios on each side of the absorber slab. These effective diffusion parameters depend on the mesh interval size h and therefore allow the use of a very course mesh in the absorber for the diffusion-theory calculations.

Expressions for the effective diffusion parameters are derived in the Appendix, so only the results are given here. For the case where the diffusion code, such as  $DIF3D^4$ , determines fluxes at the center of the mesh intervals,

$$\begin{split} k &= (1/\tau) \; [ \; \beta^{1/2} + \alpha^{1/2} \; ] \; / \; [ \; \beta^{1/2} - \alpha^{1/2} \; ] \; , \\ D_{eff} &= (h/2) \; (\alpha + \beta) \; [(1 + \cosh \, kh)/2] \; (\tanh \, k\tau) \; / \; (\sinh \, kh) \; , \; and \\ \Sigma_{a\text{-eff}} &= D_{eff} \; [\cosh \, kh - 1] \; / \; h^2 \; . \end{split}$$

The equations for k and  $\Sigma_{a-eff}$  are also valid for use in diffusion codes which calculate fluxes on the mesh boundaries. For this case, however, the expression for  $D_{eff}$  becomes (see Ref. 3)

$$D_{eff} = (h/2) (\alpha + \beta) (\tanh k\tau) / (\sinh kh)$$

For an effectively black absorber  $\alpha \rightarrow \beta \rightarrow 0.4692$  and k tends to infinity. Effective diffusion parameters can be obtained for this limiting case by setting  $k\tau$  equal to an arbitrarily large, but finite, value such as  $k\tau = 10$ . In this limit the effective diffusion parameters corresponding to mesh-centered fluxes reduce to

$$D_{eff} = \alpha \tau / (2n)$$
 and  $\Sigma_{a-eff} = [\alpha n / (4\tau)] e^{k\tau/n}$ 

where n=1,2,... determines the mesh interval size  $h = \tau/n$ .

#### 2.1.3 Examples

Blackness coefficients and effective diffusion parameters have been evaluated for several control materials commonly used in research reactors in slab geometry. Tables 1-3 summarize the results for slabs of natural cadmium, a Ag-In-Cd alloy, and natural hafnium. The thickness of the cadmium sheet ( $\tau = 0.1016$  cm) corresponds to that used in the 30-MW Oak Ridge Research Reactor (now shut down) and the Swedish R2 Reactor. Flat blades of the Ag-In-Cd alloy were assumed to be 0.310 cm thick with a density of 9.32 g/cm<sup>3</sup> and a composition of 4.9 wt % Cd, 80.5 wt % Ag, and 14.6 wt % In. The natural hafnium slab is 0.50 cm thick, which equals the thickness of the square hafnium annulus used in the control elements of Japan's JRR-3 reactor.

For each of these materials broad-group blackness coefficients were evaluated in the P<sub>1</sub>, P<sub>3</sub> and P<sub>5</sub> approximations. Fine-group flux weighting was used to determine the P<sub>5</sub> average values  $\langle \alpha(P_5) \rangle$  and  $\langle \beta(P_5) \rangle$  and the modified zero-scattering P<sub>1</sub> average values  $\langle \alpha_{0m}(P_1) \rangle$  and  $\langle \beta_{0m}(P_1) \rangle$ . For comparison purposes, Table 1 also includes the unmodified zero-scattering P<sub>5</sub> average values  $\langle \alpha_0(P_5) \rangle$  and  $\langle \beta_0(P_5) \rangle$ . Note that the effective diffusion parameters (D<sub>eff</sub> and  $\Sigma_{a-eff}$ ) given in these tables depend on the mesh interval size h and are

TABLE 1 BROAD GROUP BLACKNESS COEFFICIENTS AND EFFECTIVE DIFFUSION PARAMETERS FOR A CADMIUM SLAB OF THICKNESS $\tau$ = 0.1016 cm								
Quantity	Group 1	Group 2	Group 3	Group 4	Group 5			
$\begin{array}{c} E_{u}(eV) \\ \Sigma_{a}/\Sigma_{s} \\ D(cm) \\ \Sigma_{a}(cm^{-1}) \\ L(cm) \\ \tau/L \\ \Sigma_{a}\tau \end{array}$	1.0E+07 5.7044E-03 2.2107E+00 1.3852E-03 39.95 0.0025 1.4074E-04	8.208E+5 3.5980E-02 1.2857E+00 1.1291E-02 10.67 0.0095 1.1472E-03	5.531E+03 4.6885E-01 6.6445E-01 1.6113E-01 2.031 0.0500 1.6371E-02	1.855 3.3797E+00 4.5743E-01 8.1813E-01 0.7477 0.1359 8.3122E-02	0.6249 2.7866E+02 2.6851E-02 6.7436E+01 0.01995 5.093 6.8515E+00			
No. of Fine Groups	1	1	32	14	21			
$\begin{array}{c} \alpha(P_{1}) \\ \alpha(P_{3}) \\ \alpha(P_{5}) \\ < \alpha(P_{5}) > \\ < \alpha_{o}(P_{5}) > \\ < \alpha_{om}(P_{1}) > \\ \end{array}$ $\begin{array}{c} \beta(P_{1}) \\ \beta(P_{3}) \\ \beta(P_{5}) \\ < \beta(P_{5}) > \\ < \beta_{o}(P_{5}) > \\ < \beta_{om}(P_{1}) > \end{array}$	7.2308E-05 7.2304E-05 7.2304E-05 7.2304E-05 7.0502E-05 6.5998E-05 2.6866E+01 2.6868E+01 2.6868E+01 2.6868E+01 4.7447E+03 4.4454E+03	5.7402E-04 5.7374E-04 5.7371E-04 5.7371E-04 5.7111E-04 5.3636E-04 2.0183E+01 2.0183E+01 2.0183E+01 2.0183E+01 5.8022E+02 5.4537E+02	8.0056E-03 7.9567E-03 7.9516E-03 7.2171E-03 7.1182E-03 6.8076E-03 1.3004E+01 1.3002E+01 1.3002E+01 1.3795E+01 1.8903E+02 1.7754E+02	3.8077E-02 3.7162E-02 3.7089E-02 3.6251E-02 3.5965E-02 3.4988E-02 6.2145E+00 6.2051E+00 6.2034E+00 8.6248E+00 1.5660E+01 1.4706E+01	4.9904E-01 4.7188E-01 4.6980E-01 4.4449E-01 4.4473E-01 4.4368E-01 4.9955E-01 4.7241E-01 4.7035E-01 4.7099E-01 4.7134E-01 4.6984E-01			
EDP's* $h = \tau$ : $D_{eff}$ $\Sigma_{a-eff}$ $h = \tau/2$ : $D_{eff}$	1.3649E+00 1.4233E-03 1.3649E+00	1.0253E+00 1.1294E-02 1.0253E+00	7.0079E-01 1.4214E-01 7.0070E-01	4.3814E-01 7.1662E-01 4.3768E-01	2.3926E-02 1.5556E+02 1.4800E-02			
$egin{array}{c} D_{eff} \ \Sigma_{a-eff} \end{array}$	1.3649E+00 1.4233E-03	1.0253E+00 1.1294E-02	7.0070E-01 1.4210E-01	4.3768E-01 7.1511E-01	1.4800E-02 3.6893E+01			

\*Effective Diffusion Parameters ( EDP's) based on < $\alpha(P_5)$ > and < $\beta(P_5)$ > values.

TABLE 2 BROAD GROUP BLACKNESS COEFFICIENTS AND EFFECTIVE DIFFUSION PARAMETERS FOR A Ag-In-Cd SLAB OF THICKNESS $\tau$ = 0.310 cm								
Quantity	Group 1	Group 2	Group 3	Group 4	Group 5			
$\begin{array}{c} E_{u}(eV) \\ \Sigma_{a}/\Sigma_{s} \\ D(cm) \\ \Sigma_{a}(cm^{-1}) \\ L(cm) \\ \tau/L \\ \Sigma_{a}\tau \end{array}$	1.0E+07	8.208E+5	5.531E+03	1.855	0.6249			
	O.01388	0.06620	0.9549	9.2358	14.916			
	1.8067E+00	9.6634E-01	3.0846E-01	1.2755E-01	1.0813E-01			
	3.8027E-03	2.6855E-02	5.9217E-01	3.9909E+00	6.5510E+00			
	21.80	5.999	0.7217	0.1788	0.1285			
	0.0142	0.0517	0.4295	1.7338	2.4125			
	1.1788E-03	8.3250E-03	1.8357E-01	1.2372E+00	2.0308E+00			
No. of Fine Groups	1	1	32	14	21			
$\alpha(P_1)$ $\alpha(P_3)$ $\alpha(P_5)$ $<\alpha(P_5)>$ $<\alpha_{om}(P_1)>$	5.8971E-04	4.1294E-03	8.0743E-02	3.5099E-01	4.3407E-01			
	5.8948E-04	4.1191E-03	7.8255E-02	3.2980E-01	4.0888E-01			
	5.8946E-04	4.1184E-03	7.8052E-02	3.2762E-01	4.0657E-01			
	5.8946E-04	4.1184E-03	5.3232E-02	3.0963E-01	3.8747E-01			
	5.5110E-04	3.8370E-03	5.2921E-02	3.0990E-01	3.9047E-01			
$\beta(P_1)$	7.7410E+00	4.9746E+00	1.8153E+00	6.6227E-01	5.4799E-01			
$\beta(P_3)$	7.7410E+00	4.9738E+00	1.8052E+00	6.3920E-01	5.2324E-01			
$\beta(P_5)$	7.7410E+00	4.9736E+00	1.8037E+00	6.3730E-01	5.2151E-01			
$<\beta(P_5)>$	7.7410E+00	4.9736E+00	2.4627E+00	7.1679E-01	5.4003E-01			
$<\beta_{om}(P_1)>$	5.3069E+02	7.5151E+01	8.2595E+00	7.8897E-01	5.6342E-01			
$h = \tau:$ $D_{eff}$ $\Sigma_{a-eff}$	1.1998+00	7.7091E-01	3.8713E-01	1.1110E-01	8.3704E-02			
	3.8032E-03	2.6592E-02	3.5102E-01	3.5168E+00	8.8489E+00			
$h = \tau/2:$ $D_{eff}$ $\Sigma_{a-eff}$	1.1998E+00	7.7075E-01	3.7964E-01	9.7419E-02	6.4097E-02			
	3.8031E-03	2.6581E-02	3.4721E-01	2.6505E+00	4.7032E+00			

TABLE 3 BROAD GROUP BLACKNESS COEFFICIENTS AND EFFECTIVE DIFFUSION PARAMETERS FOR A HAFNIUM SLAB OF THICKNESS $\tau$ = 0.500 cm								
Quantity	Group 1	Group 2	Group 3	Group 4	Group 5			
$\begin{array}{c} E_{u}(eV) \\ \Sigma_{a}/\Sigma_{s} \\ D(cm) \\ \Sigma_{a}(cm^{-1}) \\ L(cm) \\ \tau/L \\ \Sigma_{a}\tau \end{array}$	1.0E+07	8.208E+5	5.531E+03	1.855	0.6249			
	O.01075	0.05192	0.6362	11.1581	6.5293			
	1.1018E+00	7.5354E-01	3.9258E-01	2.1924E-01	3.1425E-01			
	3.2572E-03	2.2812E-02	4.7998E-01	5.2020E+00	2.9832E+00			
	18.39	5.747	0.9044	0.2052	0.3246			
	0.0272	0.0870	0.5529	2.436	1.540			
	1.16286-03	1.1406E-02	2.3999E-01	2.6010E+00	1.4916E+00			
No. of Fine Groups	1	1	32	14	21			
$\alpha(P_1)$ $\alpha(P_3)$ $\alpha(P_5)$ $<\alpha(P_5)>$ $<\alpha_{om}(P_1)>$	8.1451E-04	5.6485E-03	1.0356E-01	4.5802E-01	3.8305E-01			
	8.1413E-04	5.6328E-03	1.0046E-01	4.3288E-01	3.6102E-01			
	8.1410E-04	5.6316E-03	1.0016E-01	4.3074E-01	3.5886E-01			
	8.1410E-04	5.6316E-03	1.0208E-01	4.1096E-01	3.5165E-01			
	7.6051E-04	5.2312E-03	1.0070E-01	4.1707E-01	3.5647E-01			
$\beta(P_1)$	4.3542E+00	2.8878E+00	1.1282E+00	5.1022E-01	5.8520E-01			
$\beta(P_3)$	4.3541E+00	2.8869E+00	1.1191E+00	4.8566E-01	5.6261E-01			
$\beta(P_5)$	4.3541E+00	2.8868E+00	1.1179E+00	4.8394E-01	5.6093E-01			
$<\beta(P_5)>$	4.3541E+00	2.8868E+00	1.2135E+00	5.1162E-01	5.7023E-01			
$<\beta_{om}(P_1)>$	3.8416E+02	5.4857E+01	4.8787E+00	5.3505E-01	6.2356E-01			
$h = \tau:$ $D_{eff}$ $\Sigma_{a-eff}$	1.0885E+00	7.2169E-01	3.0337E-01	1.2790E-01	1.4256E-01			
	3.2570E-03	2.2570E-02	4.4583E-01	8.3555E+00	3.6695E+00			
$h = \tau/2:$ $D_{eff}$ $\Sigma_{a-eff}$	1.0885E+00	7.2134E-01	2.9685E-01	9.2318E-02	1.1541E-01			
	3.2567E-03	2.2548E-02	4.2667E-01	3.7061E+00	2.2719E+00			

based on the  $\langle \alpha(P_5) \rangle$  and  $\langle \beta(P_5) \rangle$  values. Recall that the effective diffusion parameters, and the blackness coefficients upon which they depend, are functions only of the properties of the slab and are independent of the surrounding media.

Unmodified diffusion parameters (D and  $\Sigma_a$ ) may be used for those groups for which  $\Sigma_a / \Sigma_s \ll 1$  and/or  $\tau / L \ll 1$ , where L is the diffusion length of neutrons in the absorber. On this basis effective diffusion parameters are needed for groups 3-5 for slabs of natural hafnium and the Ag-In-Cd alloy. For cadmium, however, effective diffusion parameters are really needed only for group 5. For this group the thickness of the cadmium sheet in absorption mean free paths ( $\Sigma_a \tau$ ) is about 5.1, which means that the cadmium sheet absorbs over 99% of all the incident group 5 neutrons (i.e. group 5 is approximately black). Table 1 shows that in the P<sub>5</sub> approximation  $\alpha(P_5) = 0.4698$ , which nearly equals the black limit of 0.4692. This unique property of cadmium results from the very large absorption resonance at about 0.18 eV.

These tables also show that for  $\Sigma_a \tau > 1$  the modified-zero-scattering approximation gives remarkably good values for the blackness coefficients. Even for  $\Sigma_a \tau$  as low as about 0.2,  $\langle \alpha_{0m}(P_1) \rangle$  is quite satisfactory. However, in this range of  $\Sigma_a \tau$  values  $\langle \beta_{0m}(P_1) \rangle$  is badly over-calculated because of its sensitivity to neutron scattering effects. Where applicable, however, the modified-zero-scattering approximation is very useful because these blackness coefficients can be easily calculated.

## 2.2 Other Geometries

For control rod geometries which cannot be approximated by a one-dimensional slab treatment, quantities analogous to the  $\alpha$  and  $\beta$  blackness coefficients do not exist so other methods are needed to determine effective diffusion parameters. Since analytical expressions for the effective diffusion parameters cannot be obtained for multi-dimensional control rods, an iterative technique is used to determine  $D_{eff}$  and  $\Sigma_{a-eff}$ . It is assumed that a set of effective diffusion parameters can be found which depend on the nuclear cross sections of the absorber, its dimensions, and the mesh spacing used in diffusion-theory calculations to describe the control rod, but which are independent of the environment outside the lumped absorber.

To determine the effective diffusion parameters a control cell characteristic of the rod and its surroundings is defined. This cell, with reflective boundary conditions, explicitly models the lumped absorber, its immediate environment, and a surrounding fuel region. For this cell Monte Carlo calculations are performed to determine for each energy group the capture rate in the absorber lump relative to the fission rate in the fuel region. This same cell is used for diffusion-theory calculations choosing the same mesh structure in the absorber which will be used later for global diffusion calculations. Beginning with the highest energy group, D and  $\Sigma_a$  values are adjusted in a series of diffusion-theory calculations until the absorption rate in the absorber lump relative to the fission rate in the surrounding fuel region equals that obtained from the Monte Carlo calculation. This process is repeated on a group-by-group basis. Effective diffusion parameters are those adjusted values of D and  $\Sigma_a$  which result in a match to the Monte Carlo reaction rate ratios. An arbitrary relationship between D<sub>eff</sub> and  $\Sigma_{a-eff}$  may be defined such as

$$\mathbf{D}_{\rm eff} = [3 \ \Sigma_{\rm a-eff}]^{-1} \, .$$

As for the slab case, effective diffusion parameters are not needed for those high-energy groups for which  $\Sigma_s \gg \Sigma_a$ .

This method is commonly used by the University of Michigan in two-group calculations of the worths of the shim-safety rods in the Ford Nuclear Reactor (FNR)<sup>5</sup>. However, it is a rather laborious procedure when more energy groups are used in the diffusion-theory calculations. Therefore, other procedures, described below, are normally used in the ANL-RERTR program to calculate control rod worths within the framework of diffusion theory.

# 3. INTERNAL BOUNDARY CONDITIONS

Since diffusion theory fails near the surface of a strong neutron absorber, a pair of group- and mesh-dependent effective diffusion parameters can be used to calculate reactivity effects of the absorber. An alternate approach is to isolate the absorber from the diffusion-theory calculation by applying group-dependent internal boundary conditions at the absorber surface.

The internal boundary condition, A, is of the form

$$D \phi' + A \phi = 0$$

where  $\phi'$  is the normal derivative of the flux at the absorber surface. Thus,

$$A=\text{-}D~\varphi^{\prime}\,/\,\varphi=J\,/\,\varphi=D\,/\,d=\lambda_{tr}\,/\,3~d$$

where  $d \equiv extrapolation$  distance into the absorber,

 $\lambda_{tr} \equiv$  the neutron transport mean free path in the diffusing medium, and

 $A \equiv$  the internal boundary condition defined as the current-to-flux ratio at the absorber surface.

Transport calculations are used to determine the group-dependent current-to-flux ratios. It is assumed that the material-dependent internal boundary condition is the same at every

point on the surface of the absorber. However, current-to-flux ratios used in diffusiontheory calculations should never exceed the black absorber limit.

# 3.1 Current-to-Flux Ratios for Black Absorbers

For a plane black boundary (i.e. no return neutrons) the extrapolation distance has the value  $d = 0.7104\lambda_{tr}$  which corresponds to a current-to-flux ratio  $A = \lambda_{tr} / 3d = 0.4692$ . The extrapolation distance for a black cylindrical rod is a function of the radius, R, and the transport mean free path,  $\lambda_{tr}$ , of neutrons in the surrounding medium. Figure 1 is a plot of the current-to-flux ratio evaluated at the surface of a black cylindrical absorber of infinite length as a function of  $R/\lambda_{tr}$ . These black-rod internal boundary conditions were calculated from extrapolation distances given in Ref. 6. Note that in the limit as  $R/\lambda_{tr}$  approaches infinity, the current-to-flux ratio becomes that of a planar black boundary. Using the least squares process, data from Fig. 1 were fit to a polynomial of the form

$$(J/\phi)_{black} = \sum_{i} a_{i} (R/\lambda_{tr})^{i}$$

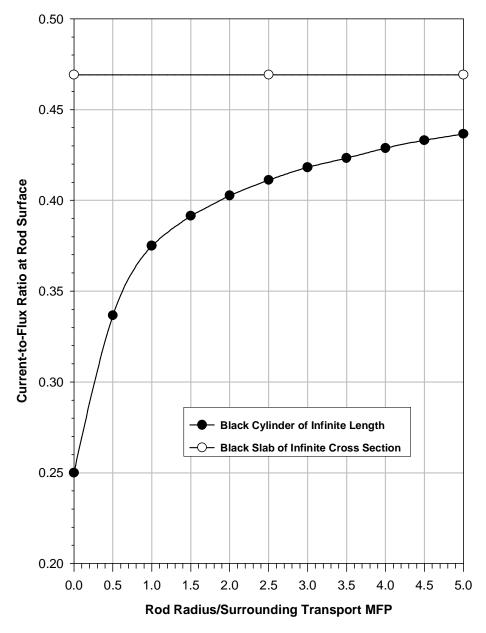
where the coefficients are:

<u>i</u>	$\underline{a}_{\underline{i}}$
0	2.49993E-01
1	2.50031E-01
2	-1.87744E-01
3	7.70505E-02
4	-1.56659E-02
5	1.00392E-03
6	1.17961E-04
7	-1.52381E-05

# 3.2 Current-to-Flux Ratios for Non-Black Absorbers

For non-black absorber materials the surface current-to-flux ratios are energy-dependent. For this case the internal boundary conditions can be calculated from a discrete-ordinate transport calculation using finely spaced mesh intervals in order to determine group-dependent fluxes and currents at the surface of the absorber. If any of the values exceed the values given in Fig. 1, they should be replaced with the black absorber limits. Internal boundary conditions are not needed for those upper energy groups for which  $\Sigma_a / \Sigma_s \ll 1$  and/or  $\tau / L \ll 1$  where L is the diffusion length and  $\tau$  is the minimum transverse dimension of the absorber material.

For the very special case of an absorber slab placed within a symmetric neutron field,  $\phi_l = \phi_r$  and  $J_l = J_r$ . The surface current-to-flux ratio then equals the  $\alpha$  blackness coefficient discussed earlier.



INTERNAL BOUNDARY CONDITIONS FOR BLACK CONTROL RODS

Figure 1

# 3.3 Example

Until recently, the shim-safety rods used in the University of Michigan Ford Nuclear Reactor consisted of a borated stainless steel material. Table 4 (from Ref. 5) gives the transverse dimensions and composition of these shim-safety rods. To obtain a set of internal boundary conditions, the rod, the surrounding moderator, and fuel were represented in cylindrical geometry. Since most thermal neutrons are absorbed near the surface of the shim-safety rod, the radius of the "equivalent" cylindrical rod was chosen so as to preserve the surface area of the actual rod. This cylindrical rod was divided into three concentric zones with the outer and middle zones having thicknesses of 1 mm and 3 mm, respectively. Full-density borated stainless steel was used in the outer and middle zones, but the density in the inner zone was reduced so as to preserve the total amount of material in the equivalent rod. Multigroup cross sections were generated for each control zone and for all the other regions outside the shim rod using the WIMS-D4M code<sup>7</sup>. Onedimensional  $P_1$  S<sub>8</sub> transport calculations were performed with the TWODANT code<sup>8</sup> in order to determine group-dependent current-to-flux ratios on the surface of the equivalent cylindrical rod. Table 5 summarizes the current-to-flux ratios obtained in this manner. This table also shows the internal boundary conditions calculated for the  $TiB_2(95\%^{-10}B)$ -Al6351 shim rods now used in the Ford Nuclear Reactor. Based on  $\Sigma_a / \Sigma_s$ ,  $\tau / L$ , and  $\Sigma_a \tau$ values, where  $\tau$  is the minimum thickness of the actual shim rod, Table 5 shows that internal boundary conditions are not needed for the fast groups 1 and 2 and that the rod is black to group-4 neutrons. Therefore, the polynomial fit to Fig. 1 was used to determine the group-4 current-to-flux ratios.

# 4. CONTROL ROD WORTH EVALUATIONS

Because of their strong neutron-absorbing character, special methods are needed to determine control rod worths in diffusion theory calculations. As discussed in the above paragraphs, one such method is to determine a pair of group- and mesh-dependent effective diffusion parameters for the absorber rod. An alternate method is to isolate the absorber material from the diffusion calculation by applying a group-dependent set of internal boundary conditions (current-to-flux ratios) at the absorber surface. Using these methods, control rod worths have been calculated for several control rod materials.

TABLE 4 COMPOSITION AND GEOMETRY OF THE FNR SHIM-SAFETY RODS								
	Composition (atoms/b-cm)							
Nuclide	Borated Stainless Steel	TiB <sub>2</sub> (95%	<sup>10</sup> B)-Al6351					
<sup>10</sup> B <sup>11</sup> B Mg Al Si Ti V Cr Mn Fe Ni Cu Zn	1.108E-3 5.184-3 1.640E-2 5.644E-2 1.130E-2	1.5749E-3 7.5390E-5 4.0978E-4 5.7161E-2 5.9104E-4 1.0158E-3 1.6293E-5 1.5962E-5 1.8129E-4 1.4862E-4 1.4131E-5 2.6122E-5 5.0734E-5						
	Geome	try						
Dimens	ions (cm)	Borated SS	TiB <sub>2</sub> -Al6351					
Effective Length Rectangular-Like Cros	s Soction:	60.960	60.960					
Major Axis Minor Axis Radius of Rounded		5.668 2.198 1.099	5.715 2.222					
Radius of Rounded			0.635					

TABLE 5 INTERNAL BOUNDARY CONDITIONS FOR THE FNR SHIM-SAFETY RODS									
	Borated Stainless Steel Rods								
Quantity	Group 1	Group 2	Group 3	Group 4					
$E_{u}(eV)$ $\Sigma_{a}/\Sigma_{s}$ D(cm) $\Sigma_{a}(cm^{-1})$ L(cm) $\tau/L$ $\Sigma_{a}\tau$	1.0000E+07 6.8727E-03 1.6583E+00 1.8958E-03 2.9576E+01 7.4318E-02 4.1669E-03	8.2100E+05 6.4574E-03 8.8032E-01 3.3825E-03 1.6132E+01 1.3625E-01 7.4347E-03	5.5300E+03 1.5990E-01 3.1743E-01 1.4756E-01 1.4667E+00 1.4986E+00 3.2434E-01	6.2500E-01 2.6788E+00 9.5010E-02 2.5676E+00 1.9236E-01 1.1426E+01 5.6436E+00					
IBC = J/φ	2.5331E-02 TiB	1.1123E-02 ₂(95% <sup>10</sup> B)-Al6351 R	8.1122E-02	4.0956E-01					
$\begin{array}{c} \Sigma_{a}/\Sigma_{s} \\ D(cm) \\ \Sigma_{a}(cm^{-1}) \\ L(cm) \\ \tau/L \\ \Sigma_{a}\tau \\ IBC = J/\phi \end{array}$	3.6927E-03 3.1275E+00 6.6305E-04 6.8680E+01 3.2360E-02 1.4736E-03 1.3262E-02	1.4154E-02 1.6415E+00 3.6092E-03 2.1326E+01 1.0422E-01 8.0214E-03 -6.9260E-03	1.7049E+00 1.1959E+00 1.7942E-01 2.5818E+00 8.6082E-01 3.9876E-01 1.1656E-01	3.7923E+01 9.3876E-02 3.4624E+00 1.6466E-01 1.3498E+01 7.6952E+00 4.1097E-01					

**NOTE:** These tables show that:

- 1. IBC's are not needed for groups 1 and 2 since  $\Sigma_a/\Sigma_s \ll 1$ .
- 2. IBC's are needed for groups 3 and 4.
- 3. IBC for group 4 is that of a black rod since  $\Sigma_a \tau >> 1$ .

# 4.1 Cadmium Control Elements

Control elements used in the Oak Ridge Research Reactor (ORR) and the Swedish R2 Reactor have the same design. The poison section consists of a water-filled square cadmium annulus 2.345 in. (5.956 cm) on a side, 30.5 in. (77.47 cm) long, and 0.040 in. (0.1016 cm) thick. Since the width-to-thickness ratio is very large, effective diffusion parameters obtained earlier for a cadmium slab of this thickness (see Table 1) are applicable. For the reasons given earlier, effective diffusion parameters are needed only for the group 5 thermal neutrons ( $E_n < 0.625$  eV). Table 1 shows that for this group the cadmium thickness in absorption mean free paths is greater than 5. Therefore, the cadmium sheet is effectively black to group 5 neutrons with a corresponding current-toflux ratio equal to 0.4692. It was shown in Ref. 3 that the worth of a cadmium slab of this thickness calculated with effective diffusion parameters obtained from the spectrumweighted P<sub>5</sub> blackness coefficients ( $<\alpha(P_5)>$  and  $<\beta(P_5)>$  and calculated using the group-5 black internal boundary condition gave nearly identical results both of which agreed with the result of a Monte Carlo calculation within  $1\sigma$  statistics. Therefore, control rod worths for the ORR and R2 reactors were calculated using the black internal boundary condition for group 5 neutrons incident on the cadmium absorber and normal diffusion theory for all the other groups.

Table 6 summarizes 3D calculations for control rod worths in the R2 reactor. Note that all the diffusion-theory worth calculations agree within  $1\sigma$  of the corresponding VIM<sup>9</sup>-Monte Carlo results. These values are taken from Ref. 3, which includes a description of the R2 reactor core configuration.

The ORR 179-AX5 core<sup>10</sup> was water-reflected with all-fresh  $U_3Si_2$  (4.8 gU/cm<sup>3</sup>) LEU fuel. It contained 14 standard (19-plate) fuel elements and 4 shim rods each with an upper cadmium poison section and a lower 15-plate fuel follower section. Differential rod worths were measured by the positive period method. The integral rod worth was obtained by integrating the differential measurements from the lower to the upper limit of the shim rod displacement.

Measured and calculated integral worths for the D6 shim rod in ORR Core 179-AX5 are compared in Table 7. As with the Swedish R2 reactor, the black internal boundary condition  $(J/\phi = 0.4692)$  was applied at the surface of the cadmium absorber for the thermal group ( $E_n < 0.625 \text{ eV}$ ) in the diffusion-theory calculations. Table 7 also shows that the DIF3D-diffusion and the VIM-Monte Carlo total worth calculations are in good agreement, but are about 5.6% larger than the measured value. This difference is typical of ORR worth measurements discussed in Ref. 10 and is partly the result of approximate corrections to the experimental data for delayed photoneutrons and temperature feedback effects. Note that the integrated worth and the total worth, based on rod-in and rod-out eigenvalue calculations, agree to within less that 1%. However, these integral and total

TABLE 6EIGENVALUES AND CADMIUM CONTROL ROD WORTHS FOR THE SWEDISH R2REACTOR								
Fuel <sup>a</sup>	FuelaRod Config. $K_{eff}$ -DIF3Db $\Delta \rho^{c}$ -% $\delta k/k$ $k_{eff}$ -VIM $\Delta \rho^{c}$ -% $\delta k/k$							
HEU 25019 " "	All Out All In At 50% Only G3 Out	1.1602 0.9654 1.0826 1.0233	17.39 6.18 11.53	1.1662±0.0025 0.9700±0.0022 1.0862±0.0024 1.0266±0.0024	17.34±0.30 6.32±0.27 11.66±0.29			
LEU 32616         All Out         1.1562         1.1537±0.0020           "         All In         0.9655         17.09         0.9656±0.0025         16.89±0.31           "         At 50%         1.0816         5.97         1.0790±0.0026         6.00±0.27           "         Only G3 Out         1.0184         11.70         1.0191±0.0025         11.45±0.28								
<sup>a</sup> The HEU 25019 notation stands for HEU fuel with 250 g <sup>235</sup> U per 19-plate element. <sup>b</sup> The DIF3D calculations were done for group 5 of cadmium made black.								

 $^{c}\Delta\rho = (k_{out} - k_{in})/k_{out}k_{in}.$ 

TABLE 7 D6 INTEGRAL ROD WORTH FOR ORR CORE 179AX5							
	Integratio	n Limits, In.	а	Integ	ral worth, % δk/k		
LL =	= 0.0	UL =	26.56	Calc.	Exp.	C/E	
				7.239	6.855	1.056	
			Total Worth				
Code	R-out, In.	R-in, In.	R-bank, In.	k-out	k-in	% δk/k	
VIM DIF3D	26.56 26.56	0.0 0.0	17.72 17.72	1.0400±0.0018 1.0371	0.9666±0.0020 0.9641	7.299±0.273 7.309	
<sup>a</sup> Integratic	<sup>a</sup> Integration of the differential rod worth from the lower to the upper limit gives the total rod worth.						

		FE	FE	FE		
	FE	FF D4	FE	FF D6	FE	
	FE	FE	FE	FE	FE	
	FE	FF F4	FE	FF F6	FE	

# WATER-REFLECTED LEU CRITICAL 179AX5

FE = 19-plate standard fuel element

FF = 15-plate fuel follower element

worths are not expected to be exactly the same because of differences in the rod bank elevations.

#### 4.2 Ag-In-Cd Control Elements

Some research reactors use control elements consisting of flat forked blades composed of the Ag-In-Cd alloy described earlier. For this alloy and for a thickness  $\tau = 0.310$  cm, Table 2 gives the effective diffusion parameters based on the flux-weighted P<sub>5</sub> blackness coefficients,  $\langle \alpha(P_5) \rangle$  and  $\langle \beta(P_5) \rangle$ , for mesh intervals of  $h = \tau$  and  $h = \tau/2$ . These blackness-modified diffusion parameters were used in 3D diffusion-theory calculations to determine control rod worths in the 10-MW IAEA Generic Reactor<sup>11</sup>. For this reactor the 23-plate fuel elements use fresh LEU U<sub>3</sub>Si<sub>2</sub> - Al dispersion fuel with a <sup>235</sup>U loading of 390 g per fuel element.

DIF3D-diffusion and VIM-Monte Carlo results for eigenvalues and reactivities are compared in Table 8. They all agree within the 1 $\sigma$  Monte Carlo statistics. Based on effective diffusion parameters calculated from the Ag-In-Cd blackness coefficients, the worth of Rod 3 was determined for mesh intervals of h =  $\tau$ ,  $\tau/2$ ,  $\tau/3$ , and  $\tau/4$ . Table 8 shows that the calculated rod worth is nearly independent of the mesh interval size. However, the results suggest a maximum value of h= $\tau/2$  be used for determining the effective diffusion parameters from the blackness coefficients.

# 4.3 Hafnium Control Elements

Control elements for the Japanese 20-MW JRR-3 reactor<sup>12</sup> consist of square waterfilled natural hafnium boxes 6.36 cm on a side and 0.50 cm thick. Using the methods described earlier, Table 3 shows the evaluated blackness coefficients for a hafnium slab of this thickness and a density of 13.3 g/cm<sup>3</sup>. The effective diffusion parameters were evaluated using the spectrum-averaged P<sub>5</sub> blackness coefficients.

Three-dimensional DIF3D diffusion and VIM Monte Carlo calculations were used to calculate control rod worths in the JRR-3 reactor. The standard fuel element has 20 plates whereas the control rod follower element has 16 plates of fresh LEU fuel. Using effective diffusion parameters corresponding to a mesh interval  $h = \tau/2$ , Table 9 compares DIF3D and VIM eigenvalues and control rod worths for the JRR-3 reactor.

TABLE 8 XYZ CALCULATIONS FOR THE 10-MW IAEA GENERIC REACTOR FOR FRESH LEU U₃Si₂ FUEL WITH Ag-In-Cd CONTROL BLADES							
Rod Configuration	Code	h-cm	k <sub>eff</sub>	Δρ <sup>a</sup> -% δk/k			
All Out All Out	VIM DIF3D		1.1922±0.0031 1.1903				
All In All In	VIM DIF3D⁵	h = τ/2	1.0296±0.0031 1.0309	13.25±0.36 12.99			
Rod 3 Out Rod 3 Out Rod 3 Out Rod 3 Out Rod 3 Out	VIM DIF3D <sup>b</sup> DIF3D <sup>b</sup> DIF3D <sup>b</sup> DIF3D <sup>b</sup>	$h = \tau$ $h = \tau/2$ $h = \tau/3$ $h = \tau/4$	1.0838±0.0033 1.0790 1.0813 1.0818 1.0816	8.39±0.36 8.66 8.47 8.43 8.44			
<sup>a</sup> Based on the Ag-In-Cd blackness-modified diffusion parameters. <sup>b</sup> $\Delta \rho = (k_{out} - k_{in})/k_{out}k_{in}.$							

# LOCATIONS of the Ag-In-Cd CONTROL BLADES in the 10-MW IAEA GENERIC REACTOR

С	С	С	С	С	С
		ROD 1			
				ROD 2	
	ROD 3		Irr. Pos.		
				ROD 4	
Irr Pos.		ROD 5			
С	С	С	С	С	С

TABLE 9         EIGENVALUES AND HAFNIUM CONTROL ROD WORTHS FOR THE JRR-3 REACTOR						
Rod Config.	K <sub>eff</sub> -DIF3D	$\Delta  ho^{a}$ -% δk/k	k <sub>eff</sub> -VIM	Δρ <sup>a</sup> -% δk/k		
All Out At 50% All In	1.2291 1.1224 0.8689	7.74 33.74	1.2227±0.0023 1.1143±0.0024 0.8763±0.0028	7.96±0.25 32.33±0.39		
${}^{a}\Delta\rho = (k_{out} - k)k_{out} k.$						

D <sub>2</sub> O TANK						
			А		С	
			В		RR	
						Ē



Figure 2. FNR 27-Element Water-Reflected LEU Core

#### 4.4 Borated Stainless Steel Control Elements

Shortly after the conversion of the Ford Nuclear Reactor (FNR) from HEU to LEU fuel, full-length rod worth measurements were made in the 27-element fresh LEU core (Fig. 2) in December 1981. Total rod worths were obtained by integrating incremental worths, measured by the positive period technique, from the lower to the upper limit of rod movement. The results of these measurements are reported in Ref. 13.

The shape and composition of the borated stainless steel shim-safety rods used in this UAl<sub>x</sub>-Al core are described in Table 4. This table shows that the FNR shim-safety rods cannot be approximated by a thin slab treatment and so blackness theory cannot be used to evaluate their worth. However, rod worths were evaluated for this 27-element core configuration using the MCNP Monte Carlo code<sup>14</sup>, the DIF3D code with internal boundary conditions (IBC's) for groups 3 and 4 (see Table 5), and the DIF3D code with effective diffusion parameters (EDP's) obtained by matching reaction rate ratios<sup>15</sup>. Table 10 compares measured and calculated rod worths and includes the University of Michigan results based on their two-group reaction rate matching process described in Ref. 5. For all these calculations the rod worth was determined by computing the reactivity difference between rod-in and rod-out cases with the regulating rod (RR) fully withdrawn. The Monte Carlo and diffusion calculations with IBC's are three-dimensional whereas the diffusion calculations with EDP's are two-dimensional XY calculations. None of the calculations account for the beam tubes associated with the  $D_2O$  tank on the north side of the core, nor do the calculations account for the rod bank and regulating rod elevations corresponding to the differential worth measurements, since this data is Nevertheless, Table 10 shows very acceptable agreement among the unavailable. measured and calculated rod worth values. Note that the rod worths are increased by about 7% when they are evaluated for the case where the regulating rod is withdrawn 50% and the rod bank is withdrawn 67%.

## 4.5 Titanium Diboride Aluminum Control Elements

In October 1995 the FNR borated stainless steel shim-safety rods were replaced with borated aluminum rods composed of an alloy of titanium diboride in 6351 aluminum. The boron in the TiB<sub>2</sub> has a <sup>10</sup>B enrichment > 95%. Table 4 compares the geometry and compositions of the TiB<sub>2</sub>(95%<sup>10</sup>B)-Al6351 shim-safety rods with the former borated stainless steel ones while Table 5 compares the internal boundary conditions. These IBC's were used in 3-dimensional DIF3D calculations to determine the worths of the borated aluminum rods in the 27-element FNR core (Fig. 2). These rod-out and rod-in calculations were done with the rod bank and the regulating rod fully withdrawn. Table 11 summarizes the results and compares the rod worths with those obtained earlier

TABLE 10 FNR EIGENVALUES AND SHIM-SAFETY ROD WORTHS FOR THE 27-ELEMENT FRESH UAI <sub>x</sub> LEU CORE							
% Rod Withdrawal		Code	Geom	Eigenvalue	Rod Worth, % δk/k		
Reg. Rod	Bank	Rod				Meas.	Calculated
100.0	100.0	A: 100.0	MCNP DIF3D: IBC's DIF3D: EDP's	XYZ XYZ XY	1.03234±0.00070 1.03632 1.02208		
100.0	100.0	A: 0.0	MCNP DIF3D: IBC's DIF3D: EDP's UM-2DB: EDP's	XYZ XYZ XY XY	1.00999±0.00074 1.0145 0.99910	2.220	2.144±0.098 2.109 2.250 2.279
50.0	66.7	A: 100.0 A: 0.0	DIF3D: IBC's DIF3D: IBC's	XYZ XYZ	1.02035 0.99751		2.244
100.0	100.0	B: 0.0	MCNP DIF3D: IBC's DIF3D: EDP's UM-2DB: EDP's	XYZ XYZ XY XY	1.00938±0.00070 1.01176 0.99782	2.320	2.203±0.095 2.342 2.379 2.648
50.0	66.7	B: 100.0 B: 0.0	DIF3D: IBC's DIF3D: IBC's	XYZ XYZ	1.02106 0.99529		2.535
100.0	100.0	C: 0.0	MCNP DIF3D: IBC's DIF3D: EDP's UM2DB: EDP's	XYZ XYZ XY XY	1.01084±0.00073 1.01450 0.99944	2.283	2.060±0.097 2.075 2.216 2.247
50.0	66.7	C: 100.0 C: 0.0	DIF3D: IBC's DIF3D: IBC's	XYZ XYZ	1.02040 0.99778		2.222

TABLE 11 COMPARISON OF THE BORATED STAINLESS STEEL AND THE TiB2-AI SHIM-SAFETY ROD WORTHS IN THE FNR 27-ELEMENT CORE							
Rod	Withdrawal <sup>a</sup>	Code	Eigenvalue	Rod Worth Ratio % δk/k		atio	
	%		(TiB <sub>2</sub> -Al)	TiB <sub>2</sub> -Al	B-SS	Calc'd	Meas. <sup>b</sup>
A	100.0	DIF3D: IBC's	1.03568				
А	0.0	DIF3D: IBC's	1.01074	2.383	2.109	1.130	1.148
В	0.0	DIF3D: IBC's	1.00801	2.650	2.342	1.131	1.095
С	0.0	DIF3D: IBC's	1.01113	2.345	2.075	1.130	1.096

<sup>a</sup>For these calculations the regulating rod (RR) and the other shim-safety rods were fully withdrawn.

<sup>b</sup>The TiB<sub>2</sub>-Al/B-SS rod worth ratio was calculated for the 27-element core (Fig. 2). However, the measured ratio is based on rod calibrations made in the October 1995 core when the borated stainless steel shim-safety rods were replaced with  $TiB_2(95\%^{10}B)$ -Al6351.

(Table 10) for the borated stainless steel material. The worth of the newer rods is about 13% larger than that of the original rods. This increase in rod worth is the result of the larger circumference (6.8%) and the larger <sup>10</sup>B concentration (42%) of the TiB<sub>2</sub>-Al6351 shim-safety rods relative to the borated stainless steel ones (see Table 4). Although both shim rod materials are black to thermal neutrons ( $E_n$ <0.625 eV), the higher <sup>10</sup>B concentration results in greater epithermal absorption in the TiB<sub>2</sub>-Al6351 (compare the group-3 IBC's in Table 5). Shim-safety rod worths for both materials were measured in the FNR October 1995 core<sup>16</sup>. Table 11 compares the measured TiB<sub>2</sub>-Al/B-SS worth ratios in this core with the values calculated for the 27-element core configuration. The average calculated and measured ratios are 1.13 and 1.11, respectively. Different core configurations and core burnup may be responsible for the somewhat different worth ratios.

#### 5.0 SUMMARY AND CONCLUSIONS

The most reliable method for calculating control rod worths makes use of a Monte Carlo code, such as MCNP<sup>14</sup>, which can model the reactor, the fuel assemblies, and the shim-safety rods in considerable detail. For diffusion-theory calculations, however, special methods are needed because of steep flux gradients near the surface of strong neutron absorbers. These special methods fall into two categories. In the first category, pairs of group- and mesh-dependent effective diffusion parameters are found for the absorber. In the second category the absorber is isolated from the diffusion calculation by specifying group-dependent internal boundary conditions (current-to-flux ratios) on the surface of the absorber material. High-order transport calculations are required to determine the effective diffusion parameters or the internal boundary conditions. In general, these special methods are needed in multigroup diffusion calculations only for the low-energy groups. For those intermediate and fast groups for which  $\sum_{a} \sum_{s} << 1$  for the absorber the unmodified diffusion parameters may be used. Potentially, the effective diffusion parameter method is somewhat more accurate than the method using internal boundary conditions. This is because the first method uses two adjusted parameters ( $D_{eff}$  and  $\Sigma_{a-eff}$ ) for each group whereas the second uses only one  $(J/\phi)$ . For symmetric situations where fluxes and currents are the same on each side of the absorber, the two methods give essentially identical results.

This paper describes methods for calculating effective diffusion parameters and internal boundary conditions. For slab-like absorbers (thickness much less than transverse dimensions), the effective diffusion parameters are expressed in terms of the  $\alpha$  and  $\beta$  blackness coefficients and the mesh spacing in the absorber. For best results, spectrum-weighted blackness coefficients evaluated in the P<sub>5</sub> approximation are used. For those low-energy groups for which  $\Sigma_a / \Sigma_s >> 1$ , the modified zero-scatter approximation may be used for the blackness coefficients, namely  $\alpha_{0m}$  and  $\beta_{0m}$ . For non-slab-like absorbers effective diffusion parameters are found by adjusting the absorber cross sections until the reaction rate ratio for absorption in the rod to fission in a neighboring fuel region matches

that of a corresponding Monte Carlo or discrete ordinates transport calculation. Fine-mesh transport calculations are used to determine internal boundary conditions from fluxes and currents at the surface of the absorber. However, values must not be used which exceed radius-dependent current-to-flux ratios for perfectly black absorbers. Methods for calculating these "black" limits are discussed.

All these methods are illustrated by calculating control rod worths for a number of absorber materials (Cd, Ag-In-Cd, Hf, borated stainless steel, and  $TiB_2$ -Al6351) in several research reactors. In general, diffusion-theory worth calculations using these methods are found to be in reasonable agreement with detailed Monte Carlo results and with experimental measurements.

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## APPENDIX

#### **Blackness Coefficients and Effective Diffusion Parameters in Slab Geometry**

Mesh-dependent effective diffusion parameters are often used to calculate control rod worths within the limitations of diffusion theory. For slab absorbers these effective diffusion parameters are functions of a pair of blackness coefficients. This appendix illustrates a method for calculating the blackness coefficients in the  $P_1$  approximation with and without scattering in the absorber slab and discusses how the method may be extended to the  $P_3$  and  $P_5$  approximations. Equations are derived for the effective diffusion parameters as functions of the blackness coefficients and the mesh interval size within the absorber.

## A.1 Matching Conditions on the Absorber Surfaces

Consider the three-region slab configuration shown below.

$$I \qquad \begin{vmatrix} I \\ x=0 \end{vmatrix} \qquad II \qquad III \qquad III$$

The absorber region (Region II) extends from x=0 to  $x=\tau$  and is assumed to be a sourcefree region which scatters neutrons isotropically. Since the angular fluxes  $\psi(x,\mu)$  incident on Region II from Regions I and III must be continuous at the boundaries,

$$\psi_{II}(0,\mu) = \psi_{I}(0,\mu), \quad \mu > 0$$
  
 $\psi_{II}(\tau,\mu) = \psi_{III}(\tau,\mu), \quad \mu < 0$ 

where  $\mu$  is the cosine of the angle between the flux direction and the normal to the slab. The boundary fluxes in Regions I and III may be expanded into a power series over the range of  $\mu$  (-1 to 1). Thus,

$$\psi_I(0,\mu) = \sum_{n=0}^L A_n \mu^n$$
$$\psi_{III}(\tau,\mu) = \sum_{n=0}^L B_n \mu^n$$

Maynard (Ref. 1) has shown that the angular flux continuity requirement leads to the matching conditions

$$\sum_{n=0}^{L} \left[ \left( \frac{(-1)^{n}}{m+n+1} - R_{mn} \right) A_{n} - (-1)^{n} T_{mn} B_{n} \right] = 0$$

$$\sum_{n=0}^{L} \left[ \left( \frac{1}{m+n+1} - R_{mn} \right) B_{n} - (-1)^{n} T_{mn} B_{n} \right] = 0$$

and

$$\sum_{n=0}^{L} \left[ \left( \frac{1}{m+n+1} - (-1)^{n} R_{mn} \right) B_{n} - T_{mn} A_{n} \right] = 0$$

if the absorber (Region II) is source-free and scatters neutrons isotropically. It turns out that either the even or odd moments can be matched. The odd moments are usually chosen. Thus, only odd values of m are used in these matching equations with  $m_{max} = L$ .  $R_{mn}$  and  $T_{mn}$  are reflection and transmission coefficients defined by the equations

$$R_{mn}(\Sigma_{t}\tau,\Sigma_{s}/\Sigma_{t}) = (-1)^{m} \int_{-1}^{0} \mu^{m} \psi_{n}(0,\mu) d\mu$$
$$T_{mn}(\Sigma_{t}\tau,\Sigma_{s}/\Sigma_{t}) = \int_{0}^{1} \mu^{m} \psi_{n}(\tau,\mu) d\mu$$

 $R_{mn}$  and  $T_{mn}$  are the reflected and transmitted contributions to the outgoing  $m_{th}$  moments due to the incoming flux. They are defined to be positive and are functions only of the absorber thickness ( $\tau$ ) and its macroscopic scattering and absorption cross sections ( $\Sigma_s$  and  $\Sigma_a$ ).

## A.2 Evaluation of the Reflection and Transmission Coefficients

For the purpose of evaluating  $R_{mn}$  and  $T_{mn}$  it is convenient to assume that Regions I and III are voids and that a  $\mu^n$  (n=0,1,2,...) source distribution is incident on the absorber slab from the left. For this source distribution the monoenergetic one-dimensional Boltzmann transport equation is solved for the surface angular fluxes  $\psi_n(0,\mu)$  and  $\psi_n(\tau,\mu)$ . Using the one-dimensional option of the TWODANT code<sup>8</sup> (i.e. ONEDANT), an angular quadrature of 24 (S<sub>24</sub>), and double  $P_N$  quadrature constants,  $R_{mn}$  and  $T_{mn}$  can be readily integrated by the Gauss-Legendre quadrature method. Thus,

$$R_{mn} = (-1)^m \sum_{i=1}^{N/2} \mu_i^m \Psi_n(0,\mu_i) W_i, \qquad \mu < 0$$

$$T_{mn} = \sum_{i=1}^{N/2} \mu_i^m \Psi_n(\tau, \mu_i) W_i, \qquad \mu > 0$$

where N is the angular quadrature order  $(S_N)$  and  $W_i$  are the required Gauss-Legendre weights which are normalized so that in the range from i=1 to i=N/2 they sum to unity. The abscissas ( $\mu_i$ ) and weights ( $W_i$ ) are given below for N=24.

<u>Abscissas</u>	<u>Weights</u>
±0.99078	0.023588
$\pm 0.95206$	0.053470
$\pm 0.88495$	0.080039
±0.79366	0.101580
±0.68392	0.116750
$\pm 0.56262$	0.124570
±0.43738	0.124570
±0.31608	0.116750
±0.20634	0.101580
±0.11505	0.080039
±0.04794	0.053470
±0.00922	0.023588

For the special case of a pure absorber slab ( $\Sigma_s = 0$ )  $R_{mn}$  is zero and  $T_{mn}$  can be easily evaluated. For this case the transmitted angular flux is the product of the incident flux  $\mu^n$  and the probability of a neutron passing through the slab without absorption ( $e^{-\Sigma_a \tau/\mu}$ ). Thus,

$$T_{mn}(\Sigma_{a}\tau) = \int_{0}^{1} \mu^{m} \psi_{n}(\tau,\mu) d\mu = \int_{0}^{1} \mu^{m+n} e^{-\Sigma_{a}\tau/\mu} d\mu = E_{m+n+2}(\Sigma_{a}\tau)$$

where  $E_{m+n+2}(\Sigma_a \tau)$  is the exponential integral of order m+n+2.

# A.3 Evaluation of the Blackness Coefficients

In the regions outside the control blade the angular fluxes satisfy the monoenergetic, one-dimensional, time-independent Boltzmann transport. To obtain analytical expressions for the blackness coefficients the angular fluxes on the surfaces of the absorber are expanded into a series which in the P<sub>L</sub> approximation becomes

$$\Psi(x,\mu) \cong \frac{1}{2} \sum_{n=0}^{L} (2n+1) \Psi_n(x) P_n(\mu)$$

where  $\psi_n(x)$  is the nth spherical harmonic moment and where  $P_n(\mu)$  is the nth Legendre polynomial. The spherical harmonic moments are given by the equation

$$\Psi_n(x) = \int_{-1}^{1} \Psi(x,\mu) P_n(\mu) d\mu$$

Although the higher order moments are more complicated,  $\psi_0(x)$  and  $\psi_1(x)$  are just the neutron flux and neutron current, respectively.

In the  $P_1$  approximation (L=1=m) the angular fluxes on the left-hand and right-hand surfaces of the absorber plate become

$$\Psi_{I} \equiv \Psi_{I}(0,\mu) = \sum_{n=0}^{L=1} A_{n}\mu^{n} = A_{0} + A_{1}\mu$$

$$= \frac{1}{2} \sum_{n=0}^{L=1} (2n+1) \psi_n(0) P_n(\mu) = \frac{1}{2} \psi_0(0) P_0(\mu) + \frac{3}{2} \psi_1(0) P_1(\mu) = \frac{1}{2} \psi_0 + \frac{3}{2} \psi_1 \mu = \frac{1}{2} \phi_1 + \frac{3}{2} J_1 \mu$$

Similarly,

$$\Psi_{\rm r} \equiv \Psi_{\rm III}(\tau,\mu) = B_0 + B_1\mu = \frac{1}{2}\phi_{\rm r} - \frac{3}{2}J_{\rm r}\mu$$

Hence,

$$\mathbf{A}_0 = \frac{1}{2} \phi_1, \qquad A_1 = \frac{3}{2} J_1, \qquad \mathbf{B}_0 = \frac{1}{2} \phi_r, \qquad B_1 = -\frac{3}{2} J_r$$

Note that  $B_1$  is negative because the blackness coefficients are defined in terms of currents into the absorber slab. Adding the Maynard matching equations for the L = 1 case gives

$$(\frac{1}{2} - R_{10} - T_{10})(A_0 + B_0) - (\frac{1}{3} + R_{11} + T_{11})(A_1 - B_1) = 0$$

Using the above values for  $(A_0 + B_0)$  and  $(A_1 - B_1)$  this equation becomes

$$(\frac{1}{2} - R_{10} - T_{10})(\phi_1 + \phi_r)(\frac{1}{2}) - (\frac{1}{3} + R_{11} + T_{11})(J_1 + J_r)(\frac{3}{2}) = 0$$

The  $\alpha$  blackness coefficient in the P approximation is therefore

$$\alpha \equiv \frac{(J_1 + J_r)}{(\phi_1 + \phi_r)} = \frac{(1/2)(1 - 2R_{10} - 2T_{10})}{(1 + 3R_{11} + 3T_{11})} .$$

Using the same procedure but subtracting the Maynard matching equations gives the  $\beta$  blackness coefficient.

$$\beta \equiv \frac{(J_1 - J_r)}{(\phi_1 - \phi_r)} = \frac{(1/2)(1 - R_{10} + 2T_{10})}{(1 + 3R_{11} - 3T_{11})}$$

Note that the  $\beta$ -equation can be obtained from the  $\alpha$ -equation by simply changing the sign of the transmission coefficients. This is a general result which is also valid in the P<sub>3</sub> and P<sub>5</sub> approximations.

As discussed above, for the case of zero scattering the reflection coefficients vanish and the transmission coefficients reduce to exponential integrals. Thus, the no-scattering  $P_1$  approximation for the blackness coefficients becomes

$$\begin{split} \alpha_{_0} &= \frac{(1/2)[1\!-\!2E_{_3}(\Sigma_{a}\tau)]}{1\!+\!3E_{_4}(\Sigma_{a}\tau)} \\ \beta_{_0} &= \frac{(1/2)[1\!+\!2E_{_3}(\Sigma_{a}\tau)]}{1\!-\!3E_{_4}(\Sigma_{a}\tau)} \ . \end{split}$$

Recall that improved values are obtained for these blackness coefficients by using the modified forms ( $\alpha_{0m}$  and  $\beta_{0m}$ ) in which the (1/2) coefficient is replaced with the value 0.4692.

These P<sub>1</sub> approximations for the blackness coefficients show that they are functions only of the properties of the absorber slab ( $\Sigma_a$ ,  $\Sigma_s$ , and  $\tau$ ). This is also true for the higher order approximations. Although the algebra is tedious, these same methods can be used to find the blackness coefficients in the P<sub>3</sub> and P<sub>5</sub> approximations. However, for these cases the spherical harmonic moments  $\psi_n(x)$  need to be evaluated on the surfaces of the control slab for n=2,3,4 and 5.

To calculate these higher-order spherical harmonics it is assumed that the control blade is surrounded by an homogenized fuel zone. For this medium the monoenergetic, onedimensional, time-independent Boltzmann equation is multiplied by  $(2n + 1)P_n(\mu)$  and integrated over all  $\mu$ . Using the recurrence relation

$$(n + 1)P_{n+1}(\mu) + nP_{n-1}(\mu) = (2n + 1)\mu P_n(\mu)$$
,

this integration leads to a set of first-order coupled differential equations for the spherical harmonics which, in the  $P_L$  approximation, are subject to the requirement that  $\psi_n(x) = 0$  for n>L. Solutions to these differential equations are of the form

$$\psi_n(x) = g_n(v) e^{vx/v}$$

where  $\lambda$  is the total mean free path of neutrons in the homogenized fuel regions outside the absorber slab. Substituting this solution into the differential equations for the spherical harmonics leads to a recurrence relation for the  $g_n(v)$ 's with  $g_0(v)$  defined to be unity. In the  $P_L$  approximation  $\psi_{L+1}(x) = 0$  which requires  $g_{L+1}(v) = 0$ . This condition leads to the allowed values of v which are positive and which are (L-1)/2 in number. Recall that in the  $P_L$  approximation only odd values of L are used. Since the blackness coefficients are functions only of the properties of the absorber slab, it is necessary to assume that the surrounding fuel regions are infinite in extent (no leakage) with either isotropic or linear anisotropic scattering.

Following these procedures Ref. 3 shows that

 $g_{0}(v) = 1$   $g_{1}(v) = 0$   $g_{2}(v) = -1/2$   $g_{3}(v) = 5/(6v)$   $g_{4}(v) = 3/8 - 35/(24v^{2})$   $g_{5}(v) = -[9g_{4}(v) + 4v g_{3}(v)]/(5v)$  $g_{6}(v) = -[11g_{5}(v) + 5v g_{4}(v)]/(6v)$ 

In the P<sub>3</sub> approximation there is one allowed v-value since (L-1)/2 = 1 and this value is obtained from the requirement that  $g_4 = 0$ . Thus,  $v_2(P_3) = (35)^{1/2}/3$ . Similarly, in the P<sub>5</sub> approximation  $v_2(P_5) = 1.2252109$  and  $v_3(P_5) = 3.2029453$ . These values of v and  $g_n(v)$  determine the higher order spherical harmonics evaluated on the absorber slab surfaces. Thus,

Spherical Harmonics in the P<sub>3</sub> Approximation

$\psi_{0l} = \phi_l + a_2$	$\psi_{0r} = \phi_r + b_2$
$\psi_{11}=J_1$	$\psi_{1r}$ = - $J_r$
$\psi_{21} = g_2(\nu_2) a_2$	$\psi_{2r} = g_2(\nu_2) b_2$
$\psi_{31} = g_3(v_2) a_2$	$\psi_{3r} = -g_3(v_2) b_2$

Spherical Harmonics in the P<sub>5</sub> Approximation

$\psi_{0l} = \phi_l + a_2 + a_3$	$\psi_{0r}=\phi_{0r}+b_2+b_3$
$\psi_{11}=J_1$	$\psi_{1r} = - J_r$
$\psi_{21} = g_2(\nu_2) a_2 + g_2(\nu_3) a_3$	$\psi_{2r} = g_2(\nu_2) \ b_2 + g_2(\nu_3) \ b_3$
$\psi_{31} = g_3(\nu_2) a_2 + g_3(\nu_3) a_3$	$\psi_{3r} = -g_3(v_2) b_2 - g_3(v_3) b_3$
$\psi_{41} = g_4(\nu_2) a_2 + g_4(\nu_3) a_3$	$\psi_{4r} = g_4(\nu_2) \ b_2 + g_4(\nu_3) \ b_3$
$\psi_{51} = g_5(\nu_2) \ a_2 + g_5(\nu_3) \ a_3$	$\psi_{5r} = -g_5(v_2) b_2 - g_5(v_3) b_3$

where  $a_2$ ,  $a_3$ ,  $b_2$ , and  $b_3$  are arbitrary constants which are eliminated in the evaluation of the blackness coefficients.

With these values for the spherical harmonics the blackness coefficients can be calculated in the  $P_3$  and  $P_5$  approximations following the same approach as was used above for the  $P_1$  approximation. As before, the continuity requirement of the angular fluxes at the surfaces of the absorber slab determines the expansion coefficients  $A_n$  and  $B_n$  in terms of the spherical harmonics  $\psi_{nl}$  and  $\psi_{nr}$ . To determine the blackness coefficient  $\alpha$  in the  $P_3$  approximation, for example, Maynard's matching equations are added together for m=1 and for m=3. From these two equations the constant  $(a_2 + b_2)$  is eliminated and from the resulting equation  $\alpha(P_3)$  is determined. By subtracting the equations and eliminating the constant  $(a_2 - b_2)$ ,  $\beta(P_3)$  is obtained.  $\beta(P_3)$  can also be found by simply changing the sign of all the transmission coefficients  $(T_{nn})$  in the final expression for  $\alpha(P_3)$ .

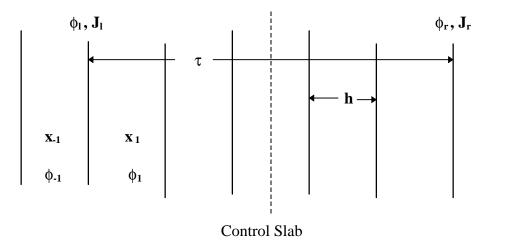
Although the algebra is very tedious, the same procedure is used to find  $\alpha(P_5)$  and  $\beta(P_5)$ . For this case Maynard's two matching equations are added together for m=1, m=3, and m=5. From these three equations the constants  $(a_2 + b_2)$  and  $(a_3 + b_3)$  are eliminated and the resulting equation solved for  $\alpha(P_5)$ . Changing the signs of the reflection coefficients in this equation determines  $\beta(P_5)$ .

For more details regarding these procedures see Ref. 3. As for the P<sub>1</sub> case, the P<sub>3</sub> and P<sub>5</sub> blackness coefficients are functions only of the properties of the absorber slab ( $\tau$ ,  $\Sigma_a$ , and  $\Sigma_s$ ).

#### A.4 Evaluation of the Effective Diffusion Parameters

The effective diffusion parameters are chosen so as to preserve the current-to-flux ratios on the surfaces of the control slab as given by the blackness coefficients. Since these effective diffusion parameters are to be used in a finite difference solution of the diffusion equation, they contain an explicit dependence on the mesh interval size, h. This allows the use of a very coarse mesh in the absorber for diffusion calculations. Equations will be derived for the effective values of D and  $\Sigma_a$  for use in those diffusion codes, such as DIF3D<sup>4</sup>, which evaluate fluxes at the center of mesh intervals. The same methods may be used to determine the effective diffusion parameters for codes which evaluate fluxes on mesh interval boundaries. These techniques for determining mesh-dependent effective diffusion parameters as functions of  $\alpha$  and  $\beta$  were first proposed by E. M. Gelbard.<sup>17</sup>

Consider the following diagram.



It is convenient to assume that the same material extends to regions outside the absorber slab of thickness  $\tau$ . Since  $\alpha$  and  $\beta$  depend only on the properties inside the slab, this assumption leads to no loss in generality. If the flux varies linearly from the center to the edge of the mesh cell,

$$\phi_1 = (\phi_{-1} + \phi_1)/2$$
 and  $J_1 = (D/h)(\phi_{-1} - \phi_1)$ 

The solution to the diffusion equation within the source-free absorber consists of a symmetric (cosh kx) part and an asymmetric (sinh kx) part with respect to the centerline. For the symmetric solution,  $\phi_l = \phi_r$ ,  $J_l = J_r$ ,  $\phi_l = C \cosh k(\tau - h)/2$ , and  $\phi_{-1} = C \cosh k(\tau + h)/2$  so that after some manipulation

$$\alpha = \frac{J_1 + J_r}{\phi_1 + \phi_r} = \frac{J_1}{\phi_1} = \frac{2D(\phi_{-1} - \phi_1)}{h(\phi_{-1} + \phi_1)} = \frac{2D[\sinh(k\tau/2)\sinh(kh/2)]}{h[\cosh(k\tau/2)\cosh(kh/2)]} = \frac{2D}{h}[\tanh(k\tau/2)\tanh(kh/2)]$$

Similarly, for the asymmetric solution,  $J_1 = -J_r$ ,  $\phi_1 = -\phi_r$ ,  $\phi_1 = A \sinh k(\tau - h)/2$ ,  $\phi_{-1} = A \sinh k(\tau + h)/2$  so that

$$\beta = \frac{J_1 - J_r}{\phi_1 - \phi_r} = \frac{J_1}{\phi_1} = \frac{2D(\phi_{-1} - \phi_1)}{h(\phi_{-1} + \phi_1)} = \frac{2D[\cosh(k\tau/2)\sinh(kh/2)]}{h[\sinh(k\tau/2)\cosh(kh/2)]} = \frac{2D}{h}\frac{\tanh(kh/2)}{\tanh(k\tau/2)} \quad .$$

The ratio of these equations gives

$$\frac{\alpha}{\beta} = \tanh^2(k\tau/2)$$

from which it follows that

$$k = (2 / \tau) \tanh^{-1} (\alpha / \beta)^{1/2} = (1 / \tau) \ln \left[ \frac{\beta^{1/2} + \alpha^{1/2}}{\beta^{1/2} - \alpha^{1/2}} \right] .$$

The expression for the effective diffusion coefficient is obtained by adding the equations for  $\alpha$  and  $\beta$ .

$$D = \frac{h}{2}(\alpha + \beta) \frac{[1 + \cosh kh] \tanh k\tau}{2\sinh kh} = D_{eff}$$

An expression for the effective macroscopic absorption cross section is obtained by writing the diffusion equation for the control slab in finite difference form and solving for  $\Sigma_a$ . Thus,

$$\Sigma_{a} = D \frac{d^{2}\phi}{dx^{2}} / \phi = \frac{D}{h^{2}} \left[ \frac{\phi_{n+1}}{\phi_{n}} - 2 + \frac{\phi_{n-1}}{\phi_{n}} \right] = \frac{2D}{h^{2}} [\cosh kh - 1] = \Sigma_{a-eff}$$

where

$$\begin{split} \varphi_n &= C \cosh kx_n \\ \varphi_{n+1} &= C \cosh k(x_n+h) \\ \varphi_{n-1} &= C \cosh k(x_n-h) \end{split}$$

These equations for k, D, and  $\Sigma_a$  determine the effective diffusion parameters in terms of the blackness coefficients ( $\alpha$  and  $\beta$ ) and the mesh interval size h for the case of mesh-centered fluxes.

The same procedures can be used to find the effective diffusion parameters for diffusion codes which evaluate fluxes on mesh boundaries. The results for k and  $\Sigma_a$  are the same as those given above. However, the expression for the effective diffusion coefficient becomes

$$D = \frac{h}{2}(\alpha + \beta) \frac{\tanh k\tau}{\sinh kh} = D_{eff} .$$

For greatest accuracy the effective diffusion parameters should be evaluated using the spectrum-weighted blackness coefficients  $\triangleleft(P_5)$  and  $\triangleleft(P_5)$ .