CONF-8410173--6

# BLACKNESS COEFFICIENTS, EFFECTIVE DIFFUSION PARAMETERS, AND CONTROL ROD WORTHS FOR THERMAL REACTORS - METHODS

CONF-8410173--6

M. M. Bretscher Argonne National Laboratory Argonne, Illinois 60439

DE85 005058

## ABSTRACT

Simple diffusion theory cannot be used to evaluate control rod worths in thermal neutron reactors because of the strongly absorbing character of the control material. However, reliable control rod worths can be obtained within the framework of diffusion theory if the control material is characterized by a set of mesh-dependent effective diffusion parameters.

For thin slab absorbers the effective diffusion parameters can be expressed as functions of a suitably-defined 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 presented.

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 discussed.

## INTRODUCTION

In strongly absorbing media the neutron flux is a rapidly varying function of position. This gives rise to steep flux gradients and under these circumstances Fick's law of diffusion is invalid. Thus, normal diffusion theory cannot be used to evaluate control rod worths in thermal neutron reactors. However, higher order methods may be used to determine effective diffusion parameters for the control material. With these modified parameters diffusion, theory may be used to accurately calculate control rod worths.

For control materials in the shape of thin sheets, whose thickness is very small relative to the transverse dimensions, a pair of blackness coefficients may be defined and evaluated to a high-order approximation. Effective diffusion parameters for the absorber slab are determined from these blackness coefficients. On the other hand, for control elements which cannot be described in terms of a one-dimensional slab geometry, a different method may be used to determine the effective diffusion parameters for the lumped absorber. Both of these methods are discussed in this paper.



### EFFECTIVE DIFFUSION PARAMETERS FOR THIN SLAB ABSORBERS

For the case of thin absorber slabs effective diffusion parameter can be obtained in terms of two "blackness coefficients" defined by the equations

$$\alpha = \frac{J_{\ell} + J_{r}}{\phi_{\ell} + \phi_{r}} , \qquad \beta = \frac{J_{\ell} - J_{r}}{\phi_{\ell} - \phi_{r}} .$$

Here  $\phi_{\ell}$ ,  $\phi_{r}$ ,  $J_{\ell}$ , and  $J_{r}$  are the asymptotic neutron fluxes and neutron currents into the slab evaluated on the left-hand and right-hand surfaces of the absorber. Because of this definition, the blackness coefficients depend only on the properties of the absorber slab. This section deals with the evaluation of  $\alpha$  and  $\beta$  and the corresponding effective diffusion parameters.

### Blackness Theory Assumptions

Blackness theory provides a method, based on the one-dimensional transport equation, for evaluating  $\alpha$  and  $\beta$ . From the outset it is well to state the assumptions upon which blackness theory depends.

1. The control slab is assumed to be of infinite lateral extent.

2. There are no neutron sources within the control slab due to fission, n2n, or scattering reactions 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 slabs.

5. Blackness coefficients evaluated for infinite slabs are applicable to finite slabs whose width-to-thickness ratio is very large.

Because of the first two assumptions, the one-dimensional monoenergetic Boltzmann transport equation may be solved within the slab to determine the surface fluxes and currents. The fourth assumption is probably violated at locations just outside the absorber slab. As a result, the flux shape determined using blackness-modified diffusion parameters is likely to be erroneous in the immediate vicinity of the control slab. The last assumption is necessary because quantities analogous to a and  $\beta$  for finite slabs do not exist. However, the assumption is expected to provide a good approximation.

#### Reflection and Transmission Coefficients

In order to account for both scattering and absorption events within the control slab, the blackness coefficients will be expressed in terms of the neutron reflection and transmission coefficients introduced by Maynard.<sup>1</sup> Consider a slab of control material of thickness  $\tau$  and bounded by vacuum.

The angular flux of neutrons incident on the left boundary of the slab is taken to be of the form  $\mu^n$  where n is an integer and  $\mu$  is the cosine of the angle between the flux direction and the normal to the slab. No neutrons enter the slab from the right. For isotropic scattering the angular flux,  $\psi_n(x,\mu)$ , within the slab satisfies the monoenergetic one-dimensional Boltzmann transport equation,

$$\mu \frac{\partial}{\partial x} \psi_n(x,\mu) + \Sigma_t \psi_n(x,\mu) = \frac{\Sigma_s}{2} \int_{-1}^{1} \psi_n(x,\mu') d\mu',$$

subject to the boundary conditions

$$ψ_n(0, μ) = μ^n, μ>0$$
  
 $ψ_n(τ, μ) = 0, μ<0$ 

The reflection and transmission coefficients are defined as

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

 $R_{mn}$  and  $T_{mn}$  are the reflected and transmitted contributions to the outgoing m<sup>th</sup> moments due to the incoming flux. They are defined to be always positive.

With a  $\mu^n$  source distribution, the tranport code ONEDANT<sup>2</sup> can be used to solve the monoenergetic one-dimensional Boltzmann equation for the surface angular fluxes  $\psi_n(0,\mu)$  and  $\psi_n(\tau,\mu)$  using an angular quadrature of 24 (S<sub>24</sub>) and double P<sub>N</sub> quadrature constants. The equations for the reflection and transmission coefficients may then be numerically integrated by Gauss-Legendre quadrature methods<sup>3</sup> to obtain R<sub>mn</sub> and T<sub>mn</sub>.

For the special case of a pure absorber ( $\Sigma_s = 0$ )  $R_{mn}$  is zero and  $T_{mn}$  can be expressed analytically. For this case the transmitted angular flux is just the product of the incident flux and the probability of a neutron passing through the slab without absorption. Thus,

$$\psi_{n}(\tau,\mu) = \mu^{n} e^{-\Sigma_{a}\tau/\mu}, \mu > 0$$
  
= 0,  $\mu < 0$ .

Thus,

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

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

### Matching Boundary Conditions

Before we can express the blackness coefficients  $\alpha$  and  $\beta$  in terms of the reflection and transmission coefficients, it is necessary to consider matching conditions imposed at the surfaces of the absorber slab. Consider the three-region slab configuration shown below.



Three-Region Slab Configuration

The angular fluxes incident on Region II from Regions I and III must be continuous at the boundaries. Therefore,

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

The moments of the distributions leaving Region II are determined from the incident destributions by means of the reflection and transmission coefficients.

The boundary fluxes in Regions I and III are expanded into a power series over the full range of  $\mu(-1 \text{ to } 1)$ .

$$\psi_{I}(0,\mu) = \sum_{n=0}^{L} A_{n} \mu^{n}$$
$$\psi_{III}(\tau,\mu) = \sum_{n=0}^{L} B_{n} \mu^{n}$$

Using these expansions, which are equivalent to the  $P_L$  approximation, Maynard<sup>1</sup> has shown that the angular flux continuity requirement leads to the matching conditions

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

and

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

provided region II is a source-free region which scatters neutrons isotropically. It turns out that only odd values of m need be considered with  $m_{max} = L$ .

To obtain analytical expressions for the blackness coefficients the angular fluxes on the surfaces of the absorber plate are expanded in a Legendre series. Thus, in the  $P_L$  approximation

$$\psi(x,\mu) \approx \frac{1}{2} \sum_{n=0}^{L} (2n+1) \psi_n(x) P_n(\mu)$$

. .

where  $\psi_n(x)$  is the nth spherical harmonic moment corresponding to the onedimensional monoenergetic Boltzmann transport equation. They have been evaluated in Ref. (4). Although the higher order moments are more complicated,  $\psi_0(x)$  and  $\psi_1(x)$  are just the neutron flux and neutron current, respectively.

We now evaluate the angular fluxes on the left-hand and right-hand surfaces of the absorber plate in the  $P_1$  approximation.

$$\begin{split} \psi_{g} &\equiv \psi_{I}(0,\mu) = \sum_{n=0}^{L=1} A_{n}\mu^{n} = A_{0} + A_{1}\mu \\ &= \frac{1}{2} \sum_{n=0}^{L=1} (2n+1)\psi_{n}(0)P_{n}(\mu) = \frac{1}{2}\psi_{0} \div \frac{3}{2}\psi_{1}\mu = \frac{1}{2}\phi_{g} + \frac{3}{2}J_{g}\mu \\ \psi_{r} &\equiv \psi_{III}(\tau,\mu) = B_{0} + B_{1}\mu = \frac{1}{2}\phi_{r} - \frac{3}{2}J_{r}\mu \end{split}$$
  
Hence,  $A_{0} = \frac{1}{2}\phi_{g}$ ,  $A_{1} = \frac{3}{2}J_{g}$ ,  $B_{0} = \frac{1}{2}\phi_{r}$ ,  $B_{1} = -\frac{3}{2}J_{r}$ .

If these results are substituted into the matching equations (for L = 1), one obtains:

$$\frac{1}{2} \left(\frac{1}{2} - R_{10}\right) \phi_{\ell} - \frac{1}{2} T_{10} \phi_{r} - \frac{3}{2} \left(\frac{1}{3} + R_{11}\right) J_{\ell} - \frac{3}{2} T_{11} J_{r} = 0$$

$$\frac{1}{2} \left(\frac{1}{2} - R_{10}\right) \phi_{r} - \frac{1}{2} T_{10} \phi_{\ell} - \frac{3}{2} \left(\frac{1}{3} + R_{11}\right) J_{r} - \frac{3}{2} T_{11} J_{\ell} = 0 ,$$

From these equations it follows that

$$\alpha \equiv \frac{J_{2} + J_{r}}{\phi_{\ell} + \phi_{r}} = \frac{[1 - 2R_{10} - 2T_{10}]}{2[1 + 3R_{11} + 3T_{11}]}$$
$$\beta \equiv \frac{J_{\ell} - J_{r}}{\phi_{\ell} - \phi_{r}} = \frac{[1 - 2R_{10} + 2T_{10}]}{2[1 + 3R_{11} - 3T_{11}]}$$

Note that the blackness coefficients are functions only of the properties of the absorber slab ( $\Sigma_a$ ,  $\Sigma_s$ ,  $\tau$ ).

Although the algebra is tedious, the same methods may be used to evaluate  $\alpha$  and  $\beta$  in higher orders of approximation. In Ref. (4) the blackness coefficients have been evaluated in the P<sub>1</sub>, P<sub>3</sub>, and P<sub>5</sub> approximations.

It was pointed out earlier that for a purely absorbing slab ( $\Sigma_s = 0$ ),  $R_{mn} = 0$  and  $T_{mn} = E_{m+n+2}$ . Thus, in the P<sub>1</sub> approximation,

$$\alpha_{0} = \frac{1 - 2E_{3} (\Sigma_{a}\tau)}{2 [1 + 3E_{4} (\Sigma_{a}\tau)]}$$
  
$$\beta_{0} = \frac{1 + 2E_{3} (\Sigma_{a}\tau)}{2 [1 - 3E_{4} (\Sigma_{a}\tau)]}$$

where the subscript on  $\alpha$  and  $\beta$  is a reminder that these equations apply only to the zero scattering case. Although without mathematical justification, these results may be multiplied by 0.4692/0.5 in order to force agreement with the correct result for a perfectly black absorber ( $\Sigma_a \rightarrow \infty$ ). We will call these modified values "dirty blackness" (DB) coefficients. They are given by the equations

> $\alpha_{0} (DB) = 0.4692 \frac{\left[1 - 2E_{3} (\Sigma_{a}\tau)\right]}{\left[1 + 3E_{4} (\Sigma_{a}\tau)\right]}$  $\beta_{0} (DB) = 0.4692 \frac{\left[1 + 2E_{3} (\Sigma_{a}\tau)\right]}{\left[1 - 3E_{4} (\Sigma_{a}\tau)\right]}.$

This dirty blackness approximation works remarkably well for those energy groups for which  $\Sigma_s \ll \Sigma_a$ . For high energy groups the absorption cross section is usually small enough so that normal diffusion theory can be used making blackness theory unnecessary.

Broad-group blackness coefficients are best obtained by weighting the fine-group values. Thus,

$$\langle \alpha \rangle = \frac{\langle J_{\underline{\ell}} + J_{\underline{r}} \rangle}{\langle \phi_{\underline{\ell}} + \phi_{\underline{r}} \rangle} = \frac{\int_{\Delta u} \alpha(u) [\phi_{\underline{\ell}}(u) + \phi_{\underline{r}}(u)] du}{\int_{\Delta u} [\phi_{\underline{\ell}}(u) + \phi_{\underline{r}}(u)] du}$$
$$\langle \beta \rangle = \frac{\langle J_{\underline{\ell}} - J_{\underline{r}} \rangle}{\langle \phi_{\underline{\ell}} - \phi_{\underline{r}} \rangle} = \frac{\int_{\Delta u} \beta(u) [\phi_{\underline{\ell}}(u) - \phi_{\underline{r}}(u)] du}{\int_{\Delta u} [\phi_{\underline{\ell}}(u) - \phi_{\underline{r}}(u)] du}$$

where  $\Delta u$  is the lethargy range of the broad group. Because the same surface flux combinations appear in both the numerator and denominator in the expressions for  $\langle \alpha \rangle$  and  $\langle \beta \rangle$ , highly precise values of  $\phi_{g}$  and  $\phi_{T}$  are not necessary. These fine-group surface fluxes used for weighting may be obtained from a one-dimensional P<sub>1</sub>, Sg transport calculation using ONEDANT<sup>2</sup> with cross sections generated by EPRI-CELL<sup>5</sup> or MC<sup>2</sup>-II.<sup>6</sup> Numerical methods are then used to determine  $\langle \alpha \rangle$  and  $\langle \beta \rangle$  for each of the broad-groups.

### **Control Slab 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, they will be expressed in such a way as to contain an explicit dependence on the mesh interval size, h. This allows one to use a very coarse mesh in the absorber for the diffusion calculations. We will derive equations for the effective values of D and  $\Sigma_a$  for use in those diffusion codes, such as DIF3D,<sup>7</sup> which evaluate fluxes at the center of mesh intervals. For codes which evaluate fluxes on mesh interval boundaries see Ref. (4) for the corresponding effective diffusion parameters.

Consider the diagram below



Control Slab

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 of generality. If we assume that the flux varies linearly from the center to the edge of the mesh cell, it is easy to show that

$$\phi_{g} = \frac{1}{2} (\phi_{-1} + \phi_{1}) \qquad J_{g} = \frac{D}{h} (\phi_{-1} - \phi_{1}) .$$

For the symmetric solution to the diffusion equation,  $J_{\ell} = J_r$ ,  $\phi_{\ell} = \phi_r$ ,  $\phi_{\tau} = C \cosh k (\tau - h)/2$ , and  $\phi_{-1} = C \cosh k (\tau + h)/2$  so that

$$\alpha = \frac{J_{\ell} + J_{r}}{\phi_{\ell} + \phi_{r}} = \frac{J_{\ell}}{\phi_{\ell}} = \frac{2D}{h} \frac{(\phi_{-1} - \phi_{1})}{(\phi_{-1} + \phi_{1})} = \cdots =$$
$$= \frac{2D}{h} [\sinh (k\tau/2) \sinh (kh/2)] / [\cosh (k\tau/2) \cosh (kh/2)]$$

Similarly, for the asymmetric solution

$$\beta = \frac{2D}{h} \left[ \cosh \left( \frac{k\tau}{2} \right) \sinh \left( \frac{kh}{2} \right) \right] / \left[ \sinh \left( \frac{k\tau}{2} \right) \cosh \left( \frac{kh}{2} \right) \right].$$

The ratio of these two equations gives

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

from which it follows that

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

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

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

Finally, an exp ssion for the effective macroscopic absorption cross section can be obtained by writing the diffusion equation,

$$D \frac{d^2 \phi}{dx^2} - \Sigma_a \phi = 0,$$

in the finite difference form and solving for  $\Sigma_a$ . Thus,

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

where

$$\phi_n = C \cosh kx_n$$
  
$$\phi_{n+1} = C \cosh k(x_n + h)$$
  
$$\phi_{n-1} = C \cosh k(x_n - h)$$

The above equations for k, D, and  $\Sigma_a$  determine the effective diffusion parameters in terms of the blackness coefficients and the mesh interval size, h.

### MULTI-DIMENSIONAL CONTROL RODS

It has just been shown that control rod worths can be calculated using blackness theory for that special class of control elements that can be approximated by a one-dimensional slab treatment. For this class of problems, a pair of blackness coefficients was evaluated which depended only on the characteristics of the control material and from which mesh-dependent effective diffusion parameters were determined. In the more general case, however, where the thickness of the lumped absorber is not negligible relative to the transverse dimensions, quantities analogous to the  $\alpha$  and  $\beta$  blackness coefficients do not exist and other methods are needed to determine effective diffusion parameters. Analytical expressions for the effective diffusion parameters cannot be obtained for two-dimensional and three-dimensional control rods. For these cases an iterative technique is needed to determine  $D_{eff}$  and  $\Sigma_{a_{eff}}$ . The assumption is made that effective diffusion parameters for the strong absorber can be found which depend primarily on the cross sections of the absorber, its dimensions, and the mesh spacing used in diffusion theory to describe the region, but do not depend on the environment outside the lumped absorber.

To determine the effective diffusion parameters a characteristic control cell with reflecting boundary conditions is defined. This cell explicitly models the lumped absorber, its immediate environment, and a surrounding fuel region. For this cell high-order transport or Monte Carlo calculations are performed to determine for each energy group the capture rate in the homogenized control region (absorber lump and immediate environment) relative to the fission rate in the surrounding fuel region. If the reaction rate ratio is determined from transport calculations, it may be necessary to divide the absorber into several nested regions and to generate appropriate cross sections for each region.

The same cell is used for diffusion-theory calculations choosing the same mesh structure which will be used later for global diffusion calculations. Beginning with the highest energy group, these diffusion-theory calculations are repeated using different sets of  $\Sigma_a$  and D values for the homogenized control region. For each case and for each energy group the capture rate in the homogenized control region is determined relative to the fission rate in the surrounding fuel region. Effective diffusion parameters are those values of  $\Sigma_a$  and D for the homogenized control region which produce the same reaction rate ratios as those obtained from the high-order transport or Monte Carlo calculations.

Control rod worths are determined by performing global diffusion calculations with and without the control rod inserted using these group-dependent values for  $\Sigma_{a_{eff}}$  and  $D_{eff}$ . This procedure has been used by the University of Michigan to calculate the worths of the shim-safety rods in the Ford Nuclear Reactor.<sup>8</sup>

#### CONCLUSIONS

To calculate control rod worths within the framework of diffusion theory it is necessary to determine effective diffusion parameters for the strongly absorbing control material. If the control rod can be represented by a set of thin slab absorbers, effective diffusion parameters can be determined in terms of a pair of blackness coefficients and the mesh interval with. This method can be expected to yield reliable eigenvalues provided the P5 blackness coefficients are calculated from good, self-shielded, cross section data.

If the geometry of the control rods does not lend itself to a thin slab approximation,  $\alpha$  and  $\beta$  blackness coefficients do not exist. Other methods must then be used to determine effective diffusion parameters for the control material. One such method is to define a representative control cell and to determine by a Monte Carlo or high-order transport calculation the capture rate in the absorber relative to the fission rate in a nearby fuel region for each energy group. For the same cell, D and  $\Sigma_a$  of the control material are adjusted so that a diffusion-theory calculation gives the same values for the group-dependent reaction rate ratios.

#### ACKNOWLEDGEMENT

Contributions to this study from E. M. Gelbard are gratefully acknowledged. It was he who showed how mesh-dependent effective diffusion parameters can be expressed in terms of the blackness coefficients.

## REFERENCES

- C. W. Maynard, "Blackness Theory and Coefficients for Slab Geometry," Nucl. Sci. Eng. <u>6</u>, 174 (1959). Also, C. W. Maynard, "Blackness Theory for Slabs," in <u>Naval Reactors Physics Handbook</u>, Vol. I, A. Radkowsky, Editor, pp. 409-448, U.S. AEC (1964).
- 2. R. D. O'Dell, F. W. Brinkley, and D. R. Marr, "User's Manual for ONEDANT: A Code Package for One-Dimensional, Diffusion-Accelerated, Neutral-Particle Transport," LA-9184~M (February 1982).
- 3. F. B. Hildebrand, <u>Introduction to Numerical Analysis</u>, McGraw-Hill Book Company, Inc., 1956, see Chapter 8.
- M. M. Bretscher, "Blackness Coefficients, Effective Diffusion Parameters, and Control Rod Worths for Thermal Reactors," ANL/RERTR/TM-5 (September 1984).
- 5. B. A. Zolotar, et al., "EPRI-CELL Description," Advanced Recycle Methodology Program System Documentation, Part II, Chapter 5, Electric Power Research Institute (September 1977). EPRI-CELL code supplied to Argonne National Laboratory by Electric Power Research Institute, Palo Alto, California (1977).
- 6. H. Henryson II, B. J. Toppel, and C. G. Stenberg, "MC<sup>2</sup>-2: A Code to Calculate Fast Neutron Spectra and Multigroup Cross Sections," ANL-8144 (June 1976).
- 7. K. L. Derstine, "DIF3D: A Code to Solve One, Two, and Three Dimensional Finite Difference Theory Problems," ANL-82-64 (April 1984).
- D. K. Wehe, C. R. Diumm, J. S. King, W. R. Martin, and J. C. Lee, "Operating Experience, Measurements, and Analysis of the LEU Whole Core Demonstration at the FNR," Proceedings of the International Meeting on Reduced Enrichment for Research and Test Reactors," 24-27 October, 1983, Tokai, Japan (May 1984).