UNCLASSIFIED

OAK RIDGE NATIONAL LABORATORY

Operated By

UNION CARBIDE NUCLEAR COMPANY

POST OFFICE BOX P
OAK RIDGE, TENNESSEE ORNL
CENTRAL FILES NUMBER

CF-56-3-170

"External Transmittal Authorized"

COPY NO. 32

DATE: March 1, 1956
SUBJECT: NEUTRON SELF-SHIELDING OF A PLANE
ABSORBING FOIL
TO: Listed Distribution
FROM: Joel Bengston

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

NOTICE

This document contains information of a preliminary nature and was prepared primarily for internal use at the Oak Ridge National Laboratory. It is subject to revision or correction and therefore does not represent a final report.

UNCLASSIFIED

715 001

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

NEUTRON SELF-SHIELDING OF A PLANE ABSORBING FOIL

Table of Contents

	Page
Abstract	3
I. Introduction	4
II. The New Double Spherical Harmonic Method	7
III. The Plane Foil Problem	19
IV. Direct Comparison of Conventional and New Spherical Harmonic Methods in Self-Shielding Problems	30
V. A Modified Serber-Wilson Method for the Plane Foil Problem	36
IV. Acknowledgements	42
App. I. The Milne Problem Without Capture in Double P_1 Approximation	43
App. II. Formulas for Use of Double P_2 Approximation . . .	46

- A B S T R A C T -

The flux depression in a plane foil of pure absorber placed in an infinite medium is calculated by a number of approximate methods.

It is found that procedures based on analytic iteration of the integral form of the transport equation cannot easily be made to yield dependable results. The new double spherical harmonic method developed by Yvon is combined with an exact treatment of neutron transmission through the foil to give a quite accurate answer for the flux depression. It is demonstrated numerically that the accuracy of the double P_1 approximation is comparable to that of the ordinary P_5 method, although it is equivalent to the less accurate P_3 method in complexity. A simple formula for the flux depression has been derived by a modification of the Serber-Wilson method and found to give a result which is never more than 3% greater than the correct value.

I. Introduction

The principal problem investigated in this report is that of the flux depression caused by a plane absorbing foil placed in an infinite medium containing a spatially uniform source of neutrons. The discussion is limited to a steady state, one velocity problem with isotropic scattering. Since this apparently simple problem has as yet no analytic solution in closed form, several approximate methods are used in this report to attack it. The resulting recommendations for methods of calculation are naturally of interest for direct application to experimental situations of which the postulated conditions are a reasonably good representation. However, the relative success and simplicity of the different methods in this problem should also be of interest as a criterion for the choice of method to be used to attack other or more complicated problems.

The method found capable of the greatest accuracy in this investigation is based on Yvon's recent modification of the conventional spherical harmonic method of solving the transport equation. The modification is the use of two different spherical harmonic expansions for the angular ranges 0 to 90° and 90° to 180°, thus allowing for the physically necessary discontinuity at 90° in the neutron angular distribution at or near a boundary (e.g., in the Milne problem). Since this method is of more general interest, its development is outlined in Section II of this report in some detail, with formulas given for the two lowest orders of approximation. These are the double P_1 and double P_2 approximations, which are equivalent in complexity to the conventional P_3 and P_5 approximations. The results obtained via Yvon's

method in the Milne problem are also reproduced in part from Yvon's report and compared with the less accurate results obtained via the conventional spherical harmonic method. It should be noted, however, that this double spherical harmonic method has as yet been worked out only for plane slab geometry.

Section III of this report is concerned with attempts to obtain an accurate solution of the foil problem. The one velocity transport equation with isotropic scattering can be transformed into an integral equation for the flux, and a solution of the foil problem was attempted by direct iteration of the inhomogeneous (source) term. It was found impossible to integrate analytically the term quadratic in the scattering cross-section, and use of just the first two terms is found to give a result which can be in error by a factor of 4 or 5 if the ratio of scattering to total cross-section is near unity. In the case of the transport equation modified by the representation of the foil as a negative source (a method due to Skyrme), the lowest order of approximation is again found to be of little value and repeated iteration is exactly analogous in complexity to the case of the unmodified transport equation.

The most accurate solution of the foil problem was obtained by a combination of the Yvon double spherical harmonic method with the exact exponential attenuation formula used to carry the solution through the foil. This procedure was used in the two lowest orders of approximation, and the results checked by substitution in the integral equation for the flux and performance of one iteration.

In Section IV, a direct comparison between the double and ordinary spherical harmonic methods is undertaken for the foil problem and also a two region lattice. In accord with expectation, the double P_1 method was found to be superior to the ordinary P_3 method and at least comparable in accuracy to the P_5 method, which is considerably more complex numerically.

In Section V, a simple approximate formula for the flux depression in a foil is developed by a modification of the Serber-Wilson method. This formula has been compared numerically with the more accurate double P_1 calculation for several foil thicknesses and a wide range of absorptive properties of the outer medium, and found to give a result which is always greater than the correct value, but never more than 3% greater. The absence of scattering in the foil makes the Serber-Wilson formulation especially simple in this specific problem, but the fact that it gives here answers of accuracy approaching that of the conventional P_3 method should make it of interest for other applications.

In self-shielding problems, we are usually interested in the behavior of the neutron flux at and near a boundary between two media of quite different properties. It is well known that the usual diffusion theory is inadequate near boundaries, but the lower orders of approximation in the conventional spherical harmonics method also have a fundamental defect in their inability to represent the angular distribution of neutrons near a boundary.

We will restrict ourselves to one velocity problems in plane geometry and assume isotropic scattering. The time-independent transport equation can then be written:

$$\mu \frac{\partial \psi(x, \mu)}{\partial x} + \frac{1}{\lambda} \psi(x, \mu) = \frac{c(x)}{2\lambda} \int_{-1}^1 \psi(x, \mu') d\mu' + \frac{S(x)}{2} \quad (1)$$

where μ is the cosine of the angle between the velocity vector and the X axis, λ is the neutron mean free path, c is the number of emergent neutrons per collision, S is the source strength of neutrons, and $\psi(x, \mu) d\mu$ is the total path length per second of the neutrons in a unit volume centered at x whose velocity vectors have direction cosines between μ and $\mu + d\mu$.

The conventional spherical harmonic method¹ consists of expanding the angular distribution of path length, $\psi(x, \mu)$, in a finite number of spherical harmonics:

$$\psi(x, \mu) = \sum_{l=0}^L \frac{(2l+1)}{2} \psi_l(x) P_l(\mu), \quad -1 \leq \mu \leq 1 \quad (2)$$

1. J. C. Mark, The Spherical Harmonic Method:

I. General Theory, CRT-340
 II. Applications, MT-97

The use of this relationship and the orthogonality properties of the Legendre functions reduces the transport equation to a set of $L + 1$ simultaneous linear differential equations for the coefficients $\psi_l(x)$.

Now consider a problem in which a strongly absorptive medium ($\sigma_{\text{scatt}} \ll \sigma_{\text{abs}}$) of thickness $2a$, is centered at $x = 0$ and separates two regions of low absorption cross section. Neutrons will be thermalized for the most part in the good scattering and moderating media, and to a negligible extent in the strong absorber. Since the strong absorber scatters few neutrons, the neutron angular distributions at either edge of the foil can be related simply by the exponential attenuation law:

$$\psi(a, \mu) \approx \psi(-a, \mu) e^{-2a/\mu\lambda}, \quad \mu > 0, \quad (3)$$

then as $\mu \rightarrow 0$ from the positive direction, $\psi(a, \mu) \rightarrow 0$, except for the small contribution due to scattering in the absorber. But if we consider neutrons entering the absorber at grazing incidence, the angular distribution $\psi(a, \mu = 0 - \epsilon)$ should remain finite as $\epsilon \rightarrow 0$. There is then a sharp discontinuity in $\psi(x, \mu)$ at $\mu = 0$. To reproduce accurately this abrupt discontinuity by using the expansion in Eq. (2) would require a very large number of spherical harmonics.

It would then seem preferable to use an expansion which will allow a discontinuity in angular distribution to appear even in the lowest orders of approximation. This has been done by J. Yvon² of the French atomic energy program. Yvon has suggested using two spherical harmonic expansions, each

2. Unpublished manuscript on Milne problem, which has been translated and given limited distribution at ORNL by W. K. Ergen.

valid in half the angular range:

$$\begin{aligned}\psi(x, \mu) &= \sum_{\ell=0}^L (2\ell + 1) P_{\ell}(2\mu - 1) \psi_{\ell}(x) \quad 0 < \mu < 1 \\ &= \sum_{\ell=0}^L (2\ell + 1) P_{\ell}(2\mu + 1) X_{\ell}(x) \quad -1 < \mu < 0\end{aligned}\quad (4)$$

Sykes³ had earlier made an equivalent improvement in the Wick-Chandrasekhar "discrete ray" method of solving the Milne problem, which involves the use of Gauss' approximate formula for numerical integration to approximate the integral on the right-hand side of Eq. (1). Sykes suggested the use of Gauss' formula twice, i.e., once for each half of the angular range, and in this way obtained solutions to the Milne problem which were decidedly more accurate than solutions of the same order of approximation using the conventional Wick method. Sykes' modification of the Wick method will not be used here, since the Wick and spherical harmonic methods are essentially equivalent, but the Wick method is more tedious numerically, particularly in multi-media problems.

The expansion coefficients have been chosen in Eq. (4) in such manner that

$$\begin{aligned}\psi_{\ell}(x) &= \int_0^1 \psi(x, \mu) P_{\ell}(2\mu - 1) d\mu \\ X_{\ell}(x) &= \int_{-1}^0 \psi(x, \mu) P_{\ell}(2\mu + 1) d\mu\end{aligned}\quad (5)$$

The integral on the right-hand side of Eq. (1), which is conveniently termed the "neutron flux", can then be written:

$$\rho(x) \equiv \int_{-1}^1 \psi(x, \mu) d\mu = \psi_0(x) + X_0(x) \quad (6)$$

3. Sykes, Monthly Notes of the Royal Astronomical Society, 3, 377 (1951).

Equations relating the harmonic components of the angular distribution can now be obtained by multiplying Eq. (1) by $P_m(2\mu - 1)$ and integrating over $0 \leq \mu \leq 1$,

$$\int_0^1 \mu \frac{\partial \psi}{\partial x} P_m(2\mu - 1) d\mu + \frac{1}{\lambda} \psi_m(x) = \left[\frac{c}{2\lambda} \rho(x) + \frac{S(x)}{2} \right] \delta_{0,m} \quad (7)$$

The integral on the left hand side can be evaluated by expanding the spatial derivative of the angular distribution in harmonics:

$$\begin{aligned} \int_0^1 \mu \frac{\partial \psi}{\partial x} P_m(2\mu - 1) d\mu &= \sum_{\ell=0}^{\infty} (2\ell + 1) \frac{d\psi_{\ell}}{dx} \int_0^1 \mu P_{\ell}(2\mu - 1) P_m(2\mu - 1) d\mu \\ &= \sum_{\ell=0}^{\infty} (2\ell + 1) \frac{d\psi_{\ell}}{dx} \left\{ \frac{1}{4} \int_{-1}^1 \gamma P_{\ell}(\gamma) P_m(\gamma) d\gamma + \frac{1}{4} \int_{-1}^1 P_{\ell}(\gamma) P_m(\gamma) d\gamma \right\} \end{aligned} \quad (7.1)$$

where $\gamma = 2\mu - 1$. Now use the well-known property of Legendre functions,

$$\mu P_{\ell}(\mu) = \frac{\ell}{2\ell + 1} P_{\ell-1}(\mu) + \frac{\ell + 1}{2\ell + 1} P_{\ell+1}(\mu) \quad (8a)$$

in the first integral on the left above, and the orthogonality relationship,

$$\int_{-1}^1 P_{\ell}(\mu) P_m(\mu) d\mu = \frac{2}{2\ell + 1} \delta_{\ell,m}$$

in both integrals, and thus obtain,

$$\begin{aligned} \int_0^1 \mu \frac{\partial \psi}{\partial x} P_m(2\mu - 1) d\mu &= \sum_{\ell=0}^{\infty} \frac{1}{4} \frac{d\psi_{\ell}}{dx} \left\{ \frac{2}{2m + 1} \left[\ell \delta_{\ell-1,m} + (\ell + 1) \delta_{\ell+1,m} \right] \right. \\ &\quad \left. + 2 \delta_{\ell,m} \right\} \\ &= \frac{1}{2} \left\{ \frac{m}{2m + 1} \frac{d\psi_{m-1}}{dx} + \frac{d\psi_m}{dx} + \frac{m + 1}{2m + 1} \frac{d\psi_{m+1}}{dx} \right\} \end{aligned} \quad (7.2)$$

Similarly, equations containing the X_ℓ 's may be obtained by multiplying Eq. (1) by $P_m(2\mu + 1)$ and integrating over $-1 \leq \mu \leq 0$,

$$\int_{-1}^0 \mu \frac{\partial \psi}{\partial x} P_m(2\mu + 1) d\mu + \frac{1}{\lambda} X_m(x) = \left[\frac{c}{2\lambda} \rho(x) + \frac{S(x)}{2} \right] \delta_{0,m} \quad (9)$$

Again we evaluate the remaining integral by expanding in harmonics:

$$\begin{aligned} \int_{-1}^0 \mu \frac{\partial \psi}{\partial x} P_m(2\mu + 1) d\mu &= \sum_{\ell=0}^{\infty} (2\ell + 1) \frac{dX_\ell}{dx} \int_{-1}^0 \mu P_\ell(2\mu + 1) P_m(2\mu + 1) d\mu \\ &= \sum_{\ell=0}^{\infty} (2\ell + 1) \frac{dX_\ell}{dx} \left\{ \frac{1}{4} \int_{-1}^1 \nu P_\ell(\nu) P_m(\nu) d\nu \right. \\ &\quad \left. - \frac{1}{4} \int_{-1}^1 P_\ell(\nu) P_m(\nu) d\nu \right\} \\ &= \frac{1}{2} \left\{ \frac{m}{2m+1} \frac{dX_{m-1}}{dx} - \frac{dX_m}{dx} + \frac{m+1}{2m+1} \frac{dX_{m+1}}{dx} \right\} \end{aligned} \quad (9.2)$$

where $\nu = 2\mu + 1$, and the last step was made by comparison of Eqs. (7.1) and (7.2).

The final equations are then:

$$\begin{aligned} m \frac{d\psi_{m-1}}{dx} + (2m+1) \frac{d\psi_m}{dx} + (m+1) \frac{d\psi_{m+1}}{dx} + \frac{2(2m+1)}{\lambda} \psi_m(x) \\ = \left[\frac{c}{\lambda} (\psi_0 + X_0) + S(x) \right] \delta_{0,m} \end{aligned} \quad (10a)$$

and

$$\begin{aligned} m \frac{dX_{m-1}}{dx} - (2m+1) \frac{dX_m}{dx} + (m+1) \frac{dX_{m+1}}{dx} + \frac{2(2m+1)}{\lambda} X_m \\ = \left[\frac{c}{\lambda} (\psi_0 + X_0) + S(x) \right] \delta_{0,m} \end{aligned} \quad (10b)$$

These equations may be solved in the "double P_L approximation" by assuming that $\psi_m = X_m = 0$ for all $m \geq L + 1$, and obtaining in this way $2(L + 1)$ equations from (10 ab). Note that the X_m 's and ψ_m 's are linked only by the scattering terms in the $m = 0$ equations.

To obtain solution to Eqs. (10 ab) in the special case of no sources, it is sufficient to substitute,

$$\begin{aligned}\psi_m(x) &= A_m e^{\gamma x/\lambda} \\ X_m(x) &= B_m e^{\gamma x/\lambda}\end{aligned}\tag{11 ab}$$

obtaining the equations,

$$\begin{aligned}m\gamma A_{m-1} + (2m + 1)(2 + \gamma)A_m + (m + 1)\gamma A_{m+1} &= c(A_0 + B_0)\delta_{0,m} \\ m\gamma B_{m-1} + (2m + 1)(2 - \gamma)B_m + (m + 1)\gamma B_{m+1} &= c(A_0 + B_0)\delta_{0,m}\end{aligned}\tag{12 ab}$$

Since this is a homogeneous set of linear equations, the condition for the existence of a solution is the vanishing of the determinant of order $2(L + 1)$ formed from the coefficients of the A_m and B_m :

$$\begin{vmatrix}(\gamma+2-c) & -c & \gamma & 0 & 0 & 0 \\ -c & (2-c-\gamma) & 0 & \gamma & 0 & 0 \\ \gamma & 0 & 3(2+\gamma) & 0 & 2\gamma & 0 \\ 0 & \gamma & 0 & 3(2-\gamma) & 0 & 2\gamma \\ 0 & 0 & 2\gamma & 0 & 5(2+\gamma) & 0 \\ 0 & 0 & 0 & 2\gamma & 0 & 5(2-\gamma)\end{vmatrix} = 0\tag{13}$$

The symmetric form of this determinant requires that the roots γ are real, and are solutions of a polynomial of order $L + 1$ in γ^2 .

4. The proof of this statement would be similar to that indicated on pages 92-3 of Kourganoff, Basic Methods in Transfer Problems. Oxford University Press, 1952.

The lowest order of approximation which seems worthwhile as an improvement over diffusion theory is the double P_1 approximation.

Equations (12 ab) become for this case:

$$\begin{array}{rclcl}
 (\nu+2-c)A_0 & -c B_0 & +\nu A_1 & = 0 & \\
 -cA_0 & +(2-c-\nu)B_0 & +\nu B_1 & = 0 & \\
 \nu A_0 & & +3(2+\nu)A_1 & = 0 & \\
 & \nu B_0 & +3(2-\nu)B_1 & = 0 &
 \end{array}
 \left. \begin{array}{l} \\ \\ \\ \end{array} \right\} \begin{array}{l} m = 0 \\ \\ m = 1 \end{array} \quad (14)$$

It then follows that $A_1 = -\frac{\nu}{3(2+\nu)} A_0$; $B_1 = -\frac{\nu}{3(2-\nu)} B_0$

$$B_0 = \frac{2\nu^2 + 12\nu - 3\nu c - 6c + 12}{3c(2+\nu)} A_0 \quad (15)$$

$$A_0 = \frac{2\nu^2 - 12\nu + 3\nu c - 6c + 12}{3c(2-\nu)} B_0$$

Continuation of the last two of Eqs. (15) gives the determinant of Eq. (13),

$$\nu^4 - 12\nu^2(2-c) + 36(1-c) = 0 \quad (16a)$$

which, on putting $1-c \equiv \alpha$, may be solved to give

$$\nu^2 = 6 \left\{ (1+\alpha) \pm \sqrt{1+\alpha+\alpha^2} \right\} \quad (16b)$$

For small values of α , it is useful for numerical purposes to expand the square root in the above equation, giving the two solutions,

$$\nu_1^2 = 3\alpha \left(1 - \frac{3}{4}\alpha + \frac{3}{8}\alpha^2 - \frac{3}{64}\alpha^3 + \dots \right) \quad (17 \text{ ab})$$

$$\nu_2^2 = 12 \left(1 + \frac{3}{4}\alpha + \frac{3}{16}\alpha^2 - \frac{3}{32}\alpha^3 + \dots \right)$$

The lower root here, as in the conventional P_3 spherical harmonic approximation,

may be identified with the asymptotic solution to the transport equation, for which the exponent satisfies

$$\frac{\text{arth } \nu}{\nu} = \frac{1}{1 - \alpha} \quad , \quad (18a)$$

which, for small values of α , may be expanded,

$$\nu^2 = 3\alpha \left(1 - \frac{4}{5} \alpha + \frac{4}{175} \alpha^2 + \dots \right) \quad (18b)$$

Then, for small α , the relative inaccuracy of the double P_1 value of ν_1^2 , is of the order of $\alpha/20$; the relative inaccuracy in the P_3 value of ν_1^2 , however, is of the order of α^3 . Indeed, plotting the three values of ν , as in Fig. 1, shows that the root given by the P_3 approximation is always more accurate than the corresponding root from the double P_1 approximation. The error of the double P_1 approximation for the root is about twice that of the P_3 root for $\alpha \gtrsim 1/2$; for $\alpha = 1$, the error assumes its maximum value of about 27%, as compared with about 16% for the P_3 case. It then seems likely that the double P_1 approximation may give a poor representation of the solution far from boundaries where the asymptotic solution should take over, but this would be serious only for media with large α . However, the primary reason for the introduction of the double spherical harmonic method is its more successful representation of conditions within a few mean free paths of a boundary. The problems investigated in this report will deal primarily with neutron distributions at and near boundaries.

Yvon has applied this new spherical harmonic method to the Milne problem without capture. In this case the exact results have been obtained via the

15

Fig. 1 - Comparison of Lowest $|\gamma|$ in Single and Double Spherical Harmonic Methods with Exact Asymptotic Value

$\alpha = \frac{\sum a}{\sum 1}$

ORNL-IR-DWG.-13144

UNCLASSIFIED

-15-

715 015

Wiener-Hopf method⁵, and the results of use of the conventional spherical harmonic method are also well known⁶. In the Milne problem, we consider a semi-infinite medium which scatters neutrons isotropically without capture or energy change. This medium occupies all space to the right of the $x = 0$ plane, and let the region to the left of $x = 0$ be a vacuum. We also impose the condition of a steady current at infinity of strength j in the negative x direction. We wish to find the neutron distribution in the medium and the angular distribution of neutrons leaving the medium at $x = 0$. It is evident that the correct boundary condition to impose on the solution at $x = 0$ is

$$\psi(0, \mu) = 0 \text{ for all } \mu > 0 \quad (19)$$

while Placzek's paper, Ref. 5, tells us that

$$\lim_{\epsilon \rightarrow 0} \psi(x = 0, \mu = 0 - \epsilon) = 0.5, \quad (20)$$

so that there is an abrupt discontinuity in the angular distribution at $\mu = 0$. Neither the exact boundary condition, Eq. (19), nor the discontinuity can be reproduced in the conventional spherical harmonic method with a finite number of spherical harmonics. There are two approximate boundary conditions which are commonly used as substitutes for Eq. (19):

(a) Marshak's boundary conditions. If Eq. (19) is true, it is evident that

$$\int_0^1 P_L(\mu) \psi(0, \mu) d\mu = 0 \quad (21)$$

for all L . In the P_L approximation, where L is odd, there are a total of $L + 1$ constants in the solution to be determined from the boundary conditions,

5. Placzek and Seidel, Phys. Rev. 72, 550 (1947)
 Placzek, P.R. 72, 556 (1947)
 J. C. Mark, P.R. 72, 558 (1947).

6. See, e.g., Weinberg and Noderer, declassified ORNL Report, CF-51-5-98, Vol. 1.

but $\frac{L+1}{2}$ of these are determined by the boundary conditions at infinity, leaving $\frac{L+1}{2}$ to be determined at $x = 0$. Since the particular case in which $\ell = 1$ in Eq. (21) corresponds to the physically desirable condition of no current entering the medium from the vacuum, it is customary to use Eq. (21) for odd values of ℓ only to determine the constants in the solution.

(b) Mark's boundary conditions. It can be shown⁷ that replacing the vacuum at the left of $x = 0$ by a fictitious purely absorptive medium in which the spherical harmonic expansion is also used is equivalent to the boundary condition

$$\psi(0, \mu_i) = 0 \quad (22)$$

where μ_i are the positive roots of $P_{L+1}(\mu_i) = 0$.

Since both of these boundary conditions are approximate ones, approaching the true case only as the order of the approximation becomes very large, results using these boundary conditions should be inferior to those using an approximation method such that the boundary conditions can be fitted exactly even in the lower orders of approximation. Yvon's new double spherical harmonic method is capable of satisfying the boundary conditions in any order, as can be seen from Eq. (4), simply by making all $\psi_\ell(0) = 0$. It then follows that the new spherical harmonic method should give better results than the old in equivalent orders of approximation. It is shown explicitly in Table 1 that this is true in the lowest order of approximation which is an improvement over diffusion theory. This is the P_3 approximation in the case of the conventional, and the double P_1 approximation in the case of the Yvon method.

7. B. Davison, Transport Theory of Neutron, IIT-18, pp. 107-9.

Table I. Comparison of Spherical Harmonic Solutions
to the Exact Solution for the Milne Problem

Quantity	P_3 , Mark Boundary Condition	P_3 Marshak	P_1^2	Exact
Extrapolation length in mean free paths	0.6949	0.7051	0.7113	0.7104
Error in extrapolation length	- .0155	- .0053	+ .0009	
Maximum error in $\psi_0(x)$	4%	4.4%	1.8%	
Maximum error in the angular distribution of neutrons entering vacuum at $x = 0$	23%	17%	7.2%	

The double P_1 approximation for the Milne problem is worked out explicitly in Appendix I. The next two orders of approximation in the new method have also been carried out by Yvon for this problem, and again yield more accurate results than corresponding orders in the conventional spherical harmonic expansion. Thus, the Mark and Marshak boundary conditions used with the conventional P_5 approximation give 0.7039 and 0.7082 mean free paths respectively for the extrapolation length, compared with 0.71056 in the double P_2 approximation.

III. The Plane Foil Problem

The principal problem investigated in this report is finding the flux depression due to a purely absorbing foil of thickness $2a$ embedded in an infinite medium in which there is a uniform source of neutrons. The most important quantity to be found in this problem is the self-shielding factor, which gives the ratio of the average value of the flux in the foil to that which would exist if the foil were not present, i.e.,

$$f = \frac{\langle \rho \rangle_{\text{Foil}}}{\rho(\infty)} \quad (23)$$

For illustrative purposes, it was decided to consider a specific case in which the thickness of the absorbing foil was $2a = 0.295$ mean free paths and the outer medium had a very small absorption cross-section, $\Sigma_a / \Sigma_{\text{total}} = .00146$, and a uniform source of neutrons. In this case the self-shielding factor predicted by the conventional P_1 approximation to transport theory is

$$f(P_1) = 0.047 .$$

Other estimates can be obtained by making use of the integral equation for the flux. If we measure dimensions in units of the mean free path, Eq. (1) can be transformed into the integral equation⁸,

$$\rho(x) = \frac{1}{2} \int_{-\infty}^{\infty} E_1 |x - x'| \left\{ c(x') \rho(x') + \lambda(x') S(x') \right\} dx' \quad (24)$$

where

$$E_n(z) = \int_1^{\infty} \frac{e^{-wz}}{w^n} dw \quad (25)$$

8. See Placzek and Seidel, Ref. 5 above, Section III, for method of derivation.

In principle, this integral equation can be solved by successive iteration to any desired accuracy, but in practice this will be found difficult if not impossible to do analytically. To start the solution of the foil problem, let

$$\begin{aligned} S(x) &= 0, \text{ for } |x| < a \\ &= S_o, \text{ for } |x| > a, \end{aligned} \quad (26)$$

and let subscripts i and o be used to designate inner (foil) and outer media respectively. Make use of the known asymptotic value of the flux to write,

$$\rho(x) = \frac{\lambda_o S_o}{1 - c_o} + \phi(x) \quad (27)$$

so that $\phi(x) \rightarrow 0$ as $x \rightarrow \pm \infty$. The integral equation then becomes:

$$\phi(x) = \frac{1}{2} \int_{-\infty}^{\infty} c(x') \phi(x') E_1 |x - x'| dx' + g(x) \quad (28a)$$

where

$$g(x) = -\frac{1}{2} (1 - c_i) \frac{\lambda_o S_o}{1 - c_o} \int_{-a}^a E_1 |x - x'| dx' \quad (28b)$$

For $|x| < a$,

$$\begin{aligned} \int_{-a}^a E_1 |x - x'| dx' &= \int_{-a}^x dx' \int_1^{\infty} \frac{e^{-w(x-x')}}{w} dw + \int_x^a dx' \int_1^{\infty} \frac{e^{-w(x'-x)}}{w} dw \\ &= \int_1^{\infty} \frac{dw}{w^2} \left\{ 1 - e^{-w(x+a)} + 1 - e^{-w(a-x)} \right\} \\ &= 2 - \int_1^{\infty} \frac{e^{-wa}}{w^2} (e^{wx} + e^{-wx}) dw \end{aligned} \quad (28c)$$

For $x > a$,

$$\begin{aligned} \int_{-a}^a E_0 |x - x'| dx' &= \int_{-a}^a dx' \int_1^{\infty} \frac{e^{-w(x-x')}}{w} dw \\ &= \int_1^{\infty} \frac{e^{-wx}}{w^2} (e^{wa} - e^{-wa}) dw. \end{aligned} \quad (28d)$$

It will be assumed henceforth that $c_i = 0$. The lowest order of approximation to the solution evidently corresponds to using $g(x)$ to represent the deviation of the flux from its asymptotic value (note that this would be exact if $c_0 = 0$ also). In this way one obtains for the average value in the foil,

$$\langle g(x) \rangle_{\text{Foil}} = \left(\frac{S}{\Sigma_{1a}} \right)_0 \left[1 - \frac{1}{4a} \left\{ 1 - 2 E_3(2a) \right\} \right]. \quad (29)$$

Since $\rho(\infty) = S/\Sigma_a$, substitution of Eq. (29) in (27) and then in (23) gives,

$$f(c=0) = \frac{1}{4a} \left\{ 1 - 2 E_3(2a) \right\}. \quad (30)$$

This is the same result obtained by Bartels in an unpublished KAPL report by an equivalent first collision method, although the quantity f is erroneously defined in that report as being the ratio of the average value of the flux in the foil to that at the edge, rather than to the value at infinity.⁹ The numerical value obtained by this method for the specific illustrative case chosen ($2a = 0.295$) was

$$f(c_0 = 0) = 0.670.$$

Since this is an order of magnitude larger than the P_1 result, it was decided to iterate this result. The next order of approximation consists of putting

9. This discrepancy was first observed by R. R. Bate (private communication).

$\phi(x) = g(x)$ under the integral sign on the righthand side of Eq. (28a).

Making use of the symmetry of solutions about $x = 0$, this gives,

$$\phi_1 (|x| < a) - g(x) = \frac{c_0}{2} \int_a^\infty dx' g(x') \left\{ E_1(x' + x) + E_1(x' - x) \right\} dx' \quad (31)$$

Using (28b) and (28d) for $g(x)$ gives,

$$\begin{aligned} \phi_1 (|x| < a) - g(x) &= \frac{c_0 \lambda_0 S_0}{4(1 - c_0)} \int_a^\infty dx' \int_1^\infty \frac{e^{-wx'}}{w^2} (e^{wa} - e^{-wa}) dw \\ &\quad \cdot \left\{ \int_1^\infty \frac{e^{-v(x'+x)}}{v} dv + \int_1^\infty \frac{e^{-v(x'-x)}}{v} dv \right\} \quad (32) \\ &= - \frac{c_0 S_0}{4 \sum_{a0}} \int_1^\infty \frac{dw}{w^2} (e^{wa} - e^{-wa}) \int_1^\infty \frac{dv}{v} (e^{vx} + e^{-vx}) \frac{e^{-(w+v)a}}{w+v} \cdot \end{aligned}$$

Next find the average of this quantity in the foil,

$$\begin{aligned} \phi_1 - g >_{\text{Foil}} &= \frac{1}{a} \int_0^a (\phi_1 - g) dx \\ &= - \frac{c_0}{4a} \left(\frac{S_0}{\sum_a} \right) \int_1^\infty \frac{dw}{w^2} (1 - e^{-2aw}) \int_1^\infty \frac{dv}{v^2} (1 - e^{-2av}) \frac{1}{v+w} \cdot \end{aligned} \quad (33)$$

Substituting

$$\frac{1}{v+w} = \int_0^\infty dx e^{-x(v+w)},$$

we obtain

$$\begin{aligned} - \frac{4a}{c_0} \left(\frac{\sum_a}{S} \right) < \phi_1 - g >_{\text{Foil}} &= \int_0^\infty dx \left\{ \int_1^\infty \frac{dw}{w^2} e^{-wx} (1 - e^{-2wa}) \right\}^2 \\ &= \int_0^\infty dx \left\{ E_2(x) - E_2(x + 2a) \right\}^2 \\ &= J_{22} - 2G'_{22}(2a) + \int_{2a}^\infty dx \left[E_2(x) \right]^2 \quad (34) \end{aligned}$$

where the first two quantities are defined in Eqs. (37.15) and (37.29) of Kourganoff.¹⁰ To evaluate the remaining integral, use Eq. (37.18) of Kourganoff:-

$$E_2^2(x) = \frac{2}{3} e^{-x} E_2(x) + \frac{1}{3} \frac{d}{dx} \left[x E_2^2(x) \right],$$

and integrate using Eq. (37.14) of Kourganoff:-

$$\int_{2a}^{\infty} dx \left[E_2(x) \right]^2 = -\frac{2a}{3} E_2^2(2a) - \frac{2}{3} \left[e^{-2a} E_1(2a) - e^{-2a} E_2(2a) - E_1(4a) \right]$$

getting G'_{22} from Eq. (37.39) and J_{22} from Table V of Kourganoff, we eventually obtain:

$$\begin{aligned} \langle \phi_1 - g \rangle_{\text{Foil}} = & -\frac{c_0}{4a} \left(\frac{s}{\sum_a} \right)_0 \left\{ \frac{2}{3} (1 - \ln 2) + 2 M_3(2a) \right. \\ & - 2 E_3(2a) - \frac{2a}{3} E_2^2(2a) + \frac{2}{3} E_1(4a) \\ & \left. + \frac{2}{3} e^{-2a} \left[E_2(2a) - E_1(2a) \right] \right\} \end{aligned} \quad (35)$$

where

$$M_n(Z) = \int_1^{\infty} \frac{e^{-Zt}}{t^n} \frac{\ln(1+t)}{t} dt \quad (35.1)$$

is obtainable from recurrence relations and tables in Kourganoff.

Equation (35) was evaluated numerically for $2a = 0.295$, $c_0 = .99854$, and this result added to that of Eq. (29), giving

$$f(c_0 = 0, \text{ once iterated}) = 0.604,$$

which is about 10% lower than the uniterated result. Further iteration was attempted and abandoned because the integrals in the next iteration (c_0^2 terms) could not be reduced to tabulated functions. This method then yields only

10. Kourganoff, Basic Methods in Transfer Problems, Oxford University Press, 1952.

an upper bound to the correct solution for f , and since $c \simeq 1$, many more terms might be necessary for a good approximation.

A third approximate method of solution, due to Skyrme,¹¹ is to alter the transport equation, representing the absorbing properties of the foil by a negative source term. The integral equation, Eq. (24) has the solution $\rho(x) = \lambda S_0 / (1 - c)$ for a uniform infinite medium in which there is a source strength of S_0 neutrons/cm³/sec. Now replace scattering medium and the source S_0 in the region $|x| < b$ by a sink term, $-\Sigma'_a \rho(x)$, where Σ'_a is the absorption cross-section due to the foil. The integral equation then becomes,

$$\begin{aligned} \rho(x) = & \frac{1}{2} \int_{-\infty}^{\infty} E_1 |x - x'| \left\{ c \rho(x') + \lambda S_0 \right\} dx' \\ & - \frac{1}{2} \int_{-b}^b E_1 |x - x'| \left\{ c \rho(x') + \left[S_0 + \Sigma'_a \rho(x') \right] \right\} dx', \end{aligned} \quad (36)$$

then replace $\rho(x')$ in the integrals on the right hand side by its unperturbed value corresponding to a uniform infinite medium, obtaining

$$\rho(x) \cong \frac{\lambda S_0}{1 - c} - \frac{\lambda S_0}{2(1 - c)} (1 + \lambda \Sigma'_a) \int_{-b}^b E_1 |x - x'| dx', \quad (37)$$

and the integral to be evaluated here is evidently given by Eqs. (28c,d).

The quantity b here, however, is measured in mean free paths of the outer medium. In our numerical example, the actual foil thickness was .0106 cm, the total cross section of the outer medium 0.3423 cm^{-1} , so that $2b = .003478$ mean free paths, and $\lambda \Sigma'_a = (0.295)/(.003478) = 84.83$. Averaging the value of Eq. (37) over the foil, and using the result of Eq. (29), we obtain

11. Skyrme, Reduction in Neutron Density Caused by an Absorbing Disc, MS-91.

$$f(\text{Skyrme}) = 0.018$$

in the lowest order of approximation. This result could be iterated once, using the method leading up to Eq. (35), but this has not been done.

It was decided instead to abandon primary emphasis on iterative methods, relying instead on Yvon's double spherical harmonic approximations coupled with an exact treatment of the flux in the foil. It was found, however, that solutions obtained by Yvon's method could easily be iterated once analytically, and this was used as a criterion of their accuracy.

The angular distributions at the two boundaries of the foil ($x = \pm a$) are connected by

$$\psi(a, \mu > 0) = \psi(-a, \mu > 0) e^{-2a/\mu} : \quad (38)$$

Since $\mu = 0$ in the foil region. The lefthand side can be represented by an expansion as in Eq. (4):-

$$\psi(a, \mu > 0) = \sum_{\ell=0}^L (2\ell+1) P_{\ell}(2\mu-1) \psi_{\ell}(a), \quad (38.1)$$

and a similar expansion holds for the lefthand side in terms of the $\psi_{\ell}(-a)$, but the symmetry of the problem allows us to write

$$\psi(-a, \mu > 0) = \psi(a, -\mu) = \sum_{\ell=0}^L (2\ell+1) P_{\ell}(1-2\mu) X_{\ell}(a), \quad (38.2)$$

where Eq. (4) has again been used. Substituting Eqs. (38.1) and (38.2) in Eq. (38), we obtain an expression containing only the components of the angular distribution at one edge of the foil,

$$\sum_{\ell=0}^L (2\ell+1) \psi_{\ell}(a) P_{\ell}(2\mu-1) = \sum_{\ell=0}^L (2\ell+1) (-)^{\ell} P_{\ell}(2\mu-1) X_{\ell}(a) e^{-2a/\mu}. \quad (38.3)$$

Algebraic equations linking the flux components can now be obtained by multiplying Eq. (38.3) by successive powers of μ and integrating over $0 \leq \mu \leq 1$. This will be done explicitly here for the double P_2 approximation. The first equation, from direct integration of (38.3), with $w \equiv \frac{1}{\mu}$ on the righthand side:

$$\begin{aligned} \psi_0(a) = \int_0^1 \psi(-a, \mu > 0) e^{-2a/\mu} d\mu = \int_1^\infty \frac{dw}{w^2} e^{-2aw} \left\{ X_0(a) - 3 \left(\frac{2}{w} - 1 \right) X_1(a) \right. \\ \left. + 5 \left(\frac{6}{w^2} - \frac{6}{w} + 1 \right) X_2(a) \right\} = \left[X_0 + 3 X_1 + 5 X_2 \right]_a E_2(2a) \\ - 6 \left[X_1 + 5 X_2 \right]_a E_3(2a) + 30 X_2(a) E_4(2a) . \end{aligned} \quad (39.1)$$

The next equation is obtained by multiplying (38.3) by μ and integrating:

$$\begin{aligned} \frac{1}{2} \left[\psi_0 + \psi_1 \right]_a = \left[X_0 + 3 X_1 + 5 X_2 \right]_a E_3(2a) \\ - 6 \left[X_1 + 5 X_2 \right]_a E_4(2a) + 30 X_2(a) E_5(2a) . \end{aligned} \quad (39.2)$$

and on multiplication by μ^2 ,

$$\begin{aligned} \left[\frac{1}{3} \psi_0 + \frac{1}{2} \psi_1 + \frac{1}{6} \psi_2 \right]_a = \left[X_0 + 3 X_1 + 5 X_2 \right]_a E_4(2a) \\ - 6 \left[X_1 + 5 X_2 \right]_a E_5(2a) + 30 X_2(a) E_6(2a) . \end{aligned} \quad (39.3)$$

In the region $x \geq a$, the double spherical harmonic expansions of Eq. (4) are valid, with

$$\begin{aligned}\psi_{\ell}(x) &= \sum_{i=1}^{L+1} A_{\ell i} e^{-\nu_i(x-a)} + \frac{S}{2 \sum_a} \delta_{\ell,0} \\ X_{\ell}(x) &= \sum_{i=1}^{L+1} B_{\ell i} e^{-\nu_i(x-a)} + \frac{S}{2 \sum_a} \delta_{\ell,0}\end{aligned}\quad (40)$$

The ν_i and A_i , B_i for the double P_1 method are given in Eqs. (15) and (16) and the double P_2 quantities in Appendix II. The negative subscripts in the above equations indicate that the negative value of ν should be used in the equations relating the coefficients (e.g., Eq. (15)). In the double P_L approximation, there are just $L + 1$ arbitrary coefficients in Eqs. (40), which can be determined exactly (in terms of $S/\sum_a$) from the $L + 1$ equations of the form of Eqs. (39).

The double spherical harmonic calculation as described has been carried out for the foil, and the flux exterior to the foil was obtained from Eqs. (6) and (40). To obtain the average value of the flux in the foil, however, it is most convenient to start from the generalization of Eq. (38),

$$\psi(x, \mu > 0) = \psi(-a, \mu) e^{-(a+x)/\mu}, \quad -a < x < a. \quad (41)$$

Next use Eq. (5a) to give $\psi_0(x)$, and integrate over μ as in deriving Eq. (39.1), again using the double P_2 approximations,

$$\psi_0(x) = \int_0^1 \psi(x, \mu > 0) d\mu = \int_1^{\infty} \frac{dw}{w^2} \sum_{\ell=0}^2 (2\ell+1) X_{\ell}(a) P_{\ell}\left(1 - \frac{2}{w}\right) e^{-(a+x)w},$$

and average over the foil,

$$\langle \psi_0 \rangle_{\text{Foil}} = \frac{1}{2a} \int_{-a}^a \psi_0(x) dx = \frac{1}{2a} \int_1^{\infty} \frac{dw}{w^3} \sum_{\ell=0}^2 (2\ell+1) X_{\ell}(a) P_{\ell}\left(1 - \frac{2}{w}\right) \left[1 - e^{-2wa}\right].$$

Since symmetry requires that $\langle \psi_0 \rangle = \langle X_0 \rangle = (1/2) \langle \rho \rangle$, we have from Eq. (39.2)

$$\begin{aligned} \langle \rho \rangle_{\text{Foil}} = \frac{1}{a} & \left\{ \left[X_0 + 3 X_1 + 5 X_2 \right]_a \left[\frac{1}{2} - E_3(2a) \right] - 6 \left[X_1 + 5 X_2 \right]_a \left[\frac{1}{3} - E_4(2a) \right] \right. \\ & \left. + 30 X_2(a) \left[\frac{1}{4} - E_5(2a) \right] \right\} . \end{aligned} \quad (42)$$

Substituting the results of the double P_1 and double P_2 solutions of Eqs. (39) and (40) in Eq. (42) gave, for our illustrative problem,

$$f(\text{double } P_1) = 0.12485$$

$$f(\text{double } P_2) = 0.12506$$

Since higher order approximations get increasingly more difficult numerically, it was decided to test the above results by an iteration in the integral equation for the flux, Eq. (40). The form of the flux corresponding to the above solutions, is, from Eq. (40),

$$\rho(x) = \frac{S}{\sum_a} + \sum_{i=1}^{L+1} F_i e^{-\gamma_i(x-a)}, \quad x \geq a, \quad (43a)$$

where

$$F_i = A_{oi} + B_{oi}.$$

We can then use Eq. (28) to iterate the deviation of the flux from its asymptotic value, the first iterate being

$$\begin{aligned} \phi_1(|x| < a) - g(x) &= \frac{c_0}{2} \int_a^\infty dx' \sum_{i=1}^{L+1} F_i e^{-\gamma_i(x'-a)} \left\{ E_1(x' + x) + E_1(x' - x) \right\} \\ &= \frac{c_0}{2} \sum_{i=1}^{L+1} F_i e^{\gamma_i a} \int_a^\infty e^{-\gamma_i x'} dx' \int_1^\infty \frac{dw}{w} e^{-wx'} (e^{-wx} + e^{wx}) \\ &= \frac{c_0}{2} \sum_{i=1}^{L+1} F_i \int_1^\infty \frac{dw e^{-wa}}{w(w + \gamma_i)} (e^{wx} + e^{-wx}) . \end{aligned} \quad (44)$$

Averaging this result over the foil, we obtain

$$\begin{aligned} \langle \phi_1 - g \rangle_{\text{Foil}} &= \frac{c_o}{2a} \sum_{i=1}^{L+1} F_i \int_1^{\infty} \frac{dw}{w^2(w + \gamma_i)} (1 - e^{-2wa}) \\ &= \frac{c_o}{2a} \sum_{i=1}^{L+1} \frac{F_i}{\gamma_i} \left[1 - \frac{\ln(1 + \gamma_i)}{\gamma_i} + Q(\gamma_i, 2a) - E_2(2a) \right] \end{aligned} \quad (45a)$$

where

$$Q(\gamma, Z) = \int_1^{\infty} \frac{dw e^{-\gamma Z}}{w(w + \gamma)} = \frac{1}{\gamma} \left[E_1(Z) - e^{\gamma Z} E_1(\{1 + \gamma\}Z) \right]. \quad (45b)$$

For $\gamma \ll 1$ it may be more convenient to expand,

$$Q(\gamma, Z) = \sum_{n=0}^{\infty} (-\gamma)^n E_{2+n}(Z). \quad (45c)$$

Then use of Eqs. (27), (29) and (45) will yield a once iterated average value of the flux in the foil, and the results for the double P_1 and double P_2 solutions of the illustrative problem are:

$$f(\text{double } P_1, \text{ once iterated}) = 0.12504$$

$$f(\text{double } P_2, \text{ once iterated}) = 0.12511$$

On the basis of these and the uniterated results, it was decided that the correct answer to the problem, to four significant figures, is $f = 0.1251$.

IV. Direct Comparison of Conventional and New Spherical Harmonic Methods in Self-Shielding Problems

An accurate value of the self-shielding factor, f , of a plane foil in an infinite medium having been obtained by the methods discussed above, it was felt desirable to use this "exact" value as a standard of comparison to evaluate the relative accuracy of the conventional spherical harmonic method and Yvon's new method. For this purpose the spherical harmonic expansions were used within the foil as well as outside. One justification for this lies in the fact that, in the conventional spherical harmonics case, the use of Eq. (38) in the foil will not lead to an unambiguous set of equations of the type of Eqs. (39). Indeed, the use of the conventional expansion, Eq. (2), in Eq. (38), multiplication by $P_m(\mu)$ and integration over μ will give $L + 1$ equations linking the $\psi_e(a)$, while there are only $(L + 1)/2$ arbitrary constants which require determination in the odd spherical harmonic approximations. The ambiguity in the proper choice of equations carrying solutions through the foil is then exactly analogous to that arising in the choice of Marshak's boundary conditions in the Milne problem, and it again seems that the accuracy of the solution should suffer from this ambiguity.

The primary justification for using the spherical harmonic expansions within the foil is our interest in obtaining an estimate of the error in cases in which the scattering cross section in the foil is not negligible, so that the "exact" relation, Eq. (38), cannot be used. It is also fortunate that using the spherical harmonic expansions in the foil makes the solutions less accurate, so that the error can be found more easily.

The foil problem was thus done in double P_1 and conventional P_3 and P_5 approximations, with the harmonic expansion used in the foil in all cases. The results for these and the previously discussed calculations are summarized in Table II. From them it can be seen that the errors in the calculation of f are:

double P_1 , 0.2%

conventional P_5 , 0.8%

conventional P_3 , 1.4%

all results being too high. The double P_1 method is then seen to be superior, not only to the P_3 approximation, which is of the same order of numerical complexity, but also to the P_5 approximation, which is much more difficult to use (e.g., there are six simultaneous equations to solve instead of four). On the other hand, the accuracy of the P_3 method is probably sufficient for many purposes, and is certainly much better than the other methods which are in error by factors of 4 or 5.

In Table II are also listed the results obtained by using Eqs. (44) and (45a) to iterate the spherical harmonic solutions once. It is seen that, in each case where the spherical harmonic expansion was used in the foil, the iterated result for either f or $\rho(a)$ is further from the correct answer than the uniterated one, but the deviation from the correct answer is of opposite sign. It is evident, then, that a single iteration of an approximate result need not improve and can decrease its accuracy. This is not unexpected, since each iteration makes an overall improvement in the function iterated, but the value of the function at a given point or in a small region of space (e.g., the foil region) can oscillate on successive iterations, a definite

32

Table II. Calculated Values of Flux for Plane Foil in Infinite Medium Problem. $2a = 0.295$, $= \sum_a / \sum_{\text{tot}} = .00146$ (outside)
All fluxes in units of $(S/\sum_a)_0$.

Method	$\rho(0)$	$\rho(a)$	$\rho(a)$ once Iterated	$\langle \rho(x) \rangle$ Foil	$\langle \rho(x) \rangle$ Foil once Iterated	$\frac{\langle \rho \rangle}{\rho(a)}$	$\frac{\langle \rho \rangle}{\rho(a)}$ once Iterated
Double P_2 , exact equation in foil	.12100	.13561	.13558	.12506	.12511	.9222	.9228
Double P_1 , exact equation in foil	.12079	.13549	.13545	.12485	.12504	.9215	.9231
Double P_1 in both media	.12152	.13297	.13352	.12528	.12328	.9422	.9233
P_5 in both media	.12280	.13234	.13055	.12595	.12064	.9517	.9241
P_3 in both media	.12426	.13158	.12725	.12669	.11754	.9628	.9237
Method of Bartels (solution for $C = 0$ outside)	.6447	.7368	.6595	.6698	.6043	.9091	.9163
Standard P_1 , both media				.0475			
Lowest approx. in Skyrme method				.0177			
Modified Serber-Wilson method				.12626			

improvement being necessary only after a large number of iterations. However, the difference between the uniterated value of f and its first iterate can be regarded as a measure of the extent to which the solutions interior to and exterior to the foil are compatible as approximations to the exact solution of the transport equation. This is because $c = 0$ in the foil, so that the iterated value of f is actually a weighted average of the flux outside the foil (the weighting function being an integral of an E function). Indeed, it is seen from Table II that the difference between the iterated and uniterated results is roughly proportional to the known error of the uniterated value of f . This is essentially the justification for the use of iteration as a measure of the accuracy of the double P_2 calculation (with exact equation used in foil) which has been used as the "exact" calculation relative to which these errors are measured.

A similar comparison of regular and double spherical harmonic methods has been undertaken for an infinite plane lattice, consisting of central absorbing regions of half-thickness 1.089 mean free paths in which $\alpha = \Sigma_a / \Sigma_1 = 0.547$ sandwiched between moderating regions of half-thickness 2.786 mean free paths with $\alpha \approx .000821$; a constant source of neutrons was assumed in the moderator region, with none in the absorber regions. The calculation was undertaken in the double P_1 approximation, and also in the conventional P_3 , P_5 and P_7 approximations. Since the exact value of the flux was not known for such a lattice, the P_7 calculation was arbitrarily taken as the accurate standard. The differences between the other results and the P_7 result for the flux were calculated. The difference in percent is plotted in Fig. 2 as a function of position through the unit cell. From

34

Fig. 2 - Comparison of Spherical Harmonic Calculations for a Plane Lattice with P_7 Calculation

ORNL-IR-DWG.-13145

UNCLASSIFIED

-34-

715 034

Fig. 2 it can be seen that the P_3 solution varies the most from the P_7 , with a maximum deviation of about 2.8%. The maximum deviation of the double P_1 flux is about 1.25% and that of the P_5 about 1%.

The fact that the P_5 deviation curve is like the P_3 with a reduced amplitude, and the double P_1 is similar to the other two with opposite sign leads one to suspect that the exact result actually lies between the P_7 result (represented by the X axis) and the double P_1 calculation. It is then probably more than safe to say that the accuracy of the double P_1 method in the lattice problem is at least comparable to that of the P_5 calculation. It also may be noted from the figure that, since the fluxes oscillate about the correct value, the error in any self-shielding factor or thermal utilization calculated from these fluxes would be of the order of half the maximum errors quoted, i.e., of the same order as the errors in the plane slab problem. It is then evident that for calculations in which an error of one to two percent is allowable, the conventional P_3 method is satisfactory, but the double P_1 method is certainly preferable, being no more difficult and considerably more accurate.

V. A Modified Serber-Wilson Method
for the Plane Foil Problem

The Serber-Wilson method was developed to patch up diffusion theory by the use of integral boundary conditions to circumvent the known failure of the "asymptotic" diffusion theory solutions near boundaries. The Serber formulation¹² involves using the diffusion theory form for the solution, but replacing the customary diffusion theory requirement of continuity of the flux at boundaries by the requirement that the solution satisfy the exact integral equation at the center of the system. The condition of continuity of current at boundaries is equivalent to an integral condition (conservation of neutrons) and therefore was left unchanged. The use of the Serber-Wilson method in thermal utilization calculations has been suggested by A. M. Henry.¹³

In the case of a plane absorbing foil embedded in an infinite medium, two factors make possible a very simple solution by a modified Serber-Wilson method. First, no assumption need be made as to the shape of the flux in the inner medium, since there is no scattering therein. Secondly, the integral obtained by putting the diffusion theory solution for the exterior medium on the righthand side of the integral equation, Eq. (24) can easily be evaluated in terms of tabulated functions for any point within the foil, not just the center. If we assume that the flux in the outer medium is of the form,

$$\rho(x > a) = \frac{S}{\Sigma_a} + B e^{-\lambda(x-a)} \quad (46)$$

12. Originated in unpublished Los Alamos reports. Described by Davison, Transport Theory of Neutrons, LT-18.

13. A. M. Henry, unpublished ANL report.

Then Eqs. (27), (29) and (45a) enable us to write for the average value of the flux in the non-scattering foil of thickness $2a$,

$$\langle \rho \rangle_{\text{Foil}} = \frac{[1 - 2 E_3(2a)]}{4a} \frac{S}{\Sigma_a} + \frac{cB}{2a\gamma} \left[1 - \ln \frac{1+\gamma}{\gamma} + Q(\gamma, 2a) - E_2(2a) \right]. \quad (47)$$

To obtain another equation containing B , we will use a neutron balance condition. Since we are measuring distance in units of mean free path, the net absorption of neutrons/cm²/sec in the righthand half of the foil is

$$\int_0^a \rho(x) dx = a \langle \rho \rangle_{\text{Foil}}. \quad (48a)$$

The net production of neutrons/cm²/sec in the righthand moderator region is

$$\int_a^\infty (\lambda S - \alpha \rho) dx = -\alpha B \int_0^\infty e^{-\gamma y} dy = -\frac{\alpha}{\gamma} B. \quad (48b)$$

Since these two must be equal,

$$B = -\frac{\gamma a}{\alpha} \langle \rho \rangle_{\text{Foil}}. \quad (48c)$$

Combining Eqs. (47) and (48c) gives,

$$\langle \rho \rangle_{\text{Foil}} = \frac{\frac{[1 - 2 E_3(2a)]}{4a} \frac{S}{\Sigma_a}}{1 + \frac{c}{2\alpha} \left[1 - \frac{\ln(1+\gamma)}{\gamma} + Q(\gamma, 2a) - E_2(2a) \right]} \quad (49)$$

where, as before

$$Q(\gamma, 2a) = \frac{1}{\gamma} \left[E_1(2a) - e^{2a\gamma} E_1(\{1+\gamma\}2a) \right], \quad (45b')$$

and the expansion in Eq. (45c) is convenient for $\gamma \ll 1$. Equation (49) reduces to Eq. (30) when $c = 0$, and is therefore exact in this limit.

This method was used for the specific foil problem treated elsewhere in this report, giving

$$f(\text{Serber-Wilson}) = 0.12626 ,$$

which is $\sim 0.9\%$ high, and better than the P_3 result. The success in this case prompted a brief survey to explore the accuracy of this formula. For this purpose, the self-shielding factor was found as a function of α from Eq. (49) and by use of the double P_1 method. This was done for three foil thicknesses, $2a = 0.295, 1.0, \text{ and } 2.0$ mean free paths. For each thickness, the difference as a function of α had a maximum in the vicinity of $\alpha = 0.1$ to 0.3 . In this region a few double P_2 calculations were done and it was finally ascertained that the maximum error of Eq. (49) was certainly less than 3% in all three cases. Moreover, the modified Serber-Wilson calculation always gives a value of f which is too high. This situation is analogous to the fact that Serber-Wilson criticality calculations always give too low a critical radius,¹² and can be explained by comparing the behavior of the exact and Serber-Wilson solutions for the flux near the foil boundary. The exact solution drops sharply in the moderator near the foil, due to non-asymptotic terms which are not present in the Serber-Wilson solution, Eq. (46). The Serber-Wilson solution near the foil being too high, its use in the integral equation makes the flux in the foil thus obtained too high, since nearby points count most strongly in determining the flux.

Since the values of the self-shielding factor, $f(\alpha, a)$, were found by double P_1 calculation for $0 < \alpha \leq 1$ and for three choices of a , in the course of investigating the accuracy of Eq. (49), these values are plotted in Fig. 3, to indicate the variation of f with the two parameters. The

Fig. 3 - Self-Shielding Factor, f , as a Function of $\alpha = \Sigma_a / \Sigma$ in Outer Medium for Three Foil Thicknesses

curves are seen to be relatively flat for $\alpha \gtrsim 1/2$, the value of f for $\alpha = 1/2$ being only 10 to 15% lower than that for $\alpha = 1$. This may well explain the success reported by the KAPL group in using the $\alpha = 1$ result to fit experiment. In view of the simplicity of the modified Serber-Wilson calculation of f , however, it would seem preferable to the $\alpha = 1$ approximation for use in all but the crudest calculations.

Also found by double spherical harmonic methods, in the course of this investigation of the Serber-Wilson method, was the ratio of the average value of the flux in the foil to that at its edge, as a function of x and foil thickness. This was done since it had already been noted in the $2a = 0.295$ case that the value of this quantity obtained for $\alpha = .00146$ by the double P_2 method was less than 2% different from the value for $\alpha = 1$, obtained from Eqs. (28) and (29),¹⁴

$$\left. \frac{\langle \rho \rangle_{\text{Foil}}}{\rho(a)} \right|_{c=0} = \frac{1 - 2 E_3(2a)}{2a [1 + E_2(2a)]} \quad (50)$$

Table III. Ratio of Average Value of Flux in Foil to that at the Edge as a Function of Foil Thickness ($2a$) and Ratio of Absorption to Total Cross Section of Outer Medium (α)

$\alpha \backslash 2a$	0.295	1.0	2.0
.00146	.922	.726	.506
.01	.920	.724	.502
.1	.917	.709	.484
1.	.909	.680	.453

14. Eq. (50) was first obtained by R. R. Bate by another method.

The fact that the interior flux distribution is approximately independent of the nature of the external medium was recognized in the earliest lattice calculations of Placzek and collaborators at Montreal.¹⁵ The validity of Eq. (50) as a useful approximation would certainly be generally useful, so the value of this ratio was obtained for $2a = 0.295, 1.0, \text{ and } 2.0$, and various values of α , and some of these values may be found in Table III. It is seen that even for the thickest foil considered, the result given by Eq. (50) is within about 10% of the correct one for all values of α .

The approximate correctness of Eq. (50) suggests a possible variation in the application of the Serber-Wilson method to self-shielding problems in spherical and cylindrical geometry. In these cases, if the total mean free path is different in the two media, the kernel in the integral form of the transport equation is a complicated function of more than one variable, except for the point at the center of symmetry of the problem (this is why Serber chose the center point to apply his condition). For this reason, it is unlikely that the modification and simplification of the Serber-Wilson method made above for plane geometry can be extended to the other cases. However, an improvement in the conventional Serber-Wilson method as applied to the problem may be possible if, instead of using diffusion theory to determine the constants in the interior medium, the ratio of the average value of the flux in the foil to that in the center (a quantity analogous to that in Eq. (50)) is calculated from the integral equation for the special case of $\alpha = 1$, assuming that the neutron mean free paths are equal in the two media. This ratio should, in analogy with Eq. (50), be approximately

15. A. M. Weinberg, private communication.

correct independent of the nature of the outer medium. Moreover, the ratio $\langle \rho \rangle \text{ foil}/\rho(0)$ is just what will enter into the analogue of Eq. (48c) if we replace Eq. (47) by one giving the flux at the origin. The self-shielding factor defined as in Eq. (23) will then again be expressible in a simple equation of the form of Eq. (47).

Acknowledgements

Almost all of the numerical calculations in this report were performed by Miss Ann Forbes of the ANP Physics group, for whose efficiency and accuracy I am indeed grateful.

Appendix I

THE MILNE PROBLEM WITHOUT CAPTURE IN THE DOUBLE P_1 APPROXIMATION

If we use the double P_1 approximation in a non-capturing medium, Eqs. (10-16) are valid with $c = 1 - \alpha = 1$. The roots from Eq. (16b) are:

$$\nu^2 = 0, 12. \quad (A1)$$

We discard the exponentially increasing solution, since we know that the diffusion theory solution is valid asymptotically. For the root $\nu_- = -\sqrt{12}$, Eq. (15) gives:

$$A_1 = -\frac{\sqrt{3}}{3(\sqrt{3}-1)} A_{0-}$$

$$B_{0-} = \frac{3\sqrt{3}-5}{\sqrt{3}-1} A_{0-} \quad (A2)$$

$$B_{1-} = \frac{9-5\sqrt{3}}{6} A_{0-}$$

The $\nu^2 = 0$ root corresponds to a solution of the form

$$\psi_i = a_i x + \alpha_i$$

$$X_i = b_i x + \beta_i \quad (A3)$$

Putting these in Eq. (10) with $S = 0$ and measuring distance in units of mean free paths gives:

$$a_0 = b_0$$

$$a_1 = b_1 = 0$$

$$\alpha_1 = \beta_1 = -\frac{1}{6} a_0 \quad (A4)$$

$$\alpha_0 = \beta_0 - a_0$$

The total solutions are then:

$$\begin{aligned}
 \psi_0 &= A_0 e^{-\sqrt{12}x} + a_0 x + (\beta_0 - a_0) \\
 x_0 &= \frac{3\sqrt{3} - 5}{\sqrt{3} - 1} A_0 e^{-\sqrt{12}x} + a_0 x + \beta_0 \\
 \psi_1 &= -\frac{\sqrt{3}}{3(\sqrt{3} - 1)} A_0 e^{-\sqrt{12}x} - \frac{a_0}{6} \\
 x_1 &= \frac{9 - 5\sqrt{3}}{6} A_0 e^{-\sqrt{12}x} - \frac{a_0}{6}
 \end{aligned} \tag{A5}$$

The boundary condition to apply at $x = 0$ is $\psi_0(0) = \psi_1(0) = 0$,

$$\begin{aligned}
 \therefore \beta_0 &= a_0 - A_0 \\
 A_0 &= -\frac{\sqrt{3} - 1}{2\sqrt{3}} a_0 \\
 \beta_0 &= \frac{3\sqrt{3} - 1}{2\sqrt{3}} a_0
 \end{aligned} \tag{A6}$$

Then the flux is

$$\begin{aligned}
 \rho(x) &= \psi_0 + x_0 \\
 &= 2 a_0 \left[x + \frac{2\sqrt{3} - 1}{2\sqrt{3}} - \left(1 - \frac{\sqrt{3}}{2}\right) e^{-\sqrt{12}x} \right] \\
 &= 2 a_0 \left[x + 0.71132 - 0.13397 e^{-3.46410x} \right]
 \end{aligned} \tag{A7}$$

The extrapolation length is therefore

$$\lambda_{\text{ext}} = 1 - \frac{1}{2\sqrt{3}} = 0.711325 \tag{A8}$$

The coefficient a_0 can be determined in terms of the current, $-j$, in the X direction:

$$\int_{-1}^1 \mu \psi(x, \mu) d\mu = -j = \frac{1}{2} (x_1 - x_0 + \psi_1 + \psi_0) = -\frac{2}{3} a_0 \quad (A9)$$

$$\therefore a_0 = \frac{3}{2} j$$

The angular distribution at $x = 0$ is:

$$\psi(0, \mu < 0) = 2\sqrt{3} (2 - \sqrt{3}) j [1 - \sqrt{3}\mu] \quad (A10)$$

This result is that obtained by Fermi nearly 20 years previously by use of the P_1 approximation with what we now call Mark's boundary condition, which leads, however, to an extrapolation length of $1/\sqrt{3} = 0.5773$.

Appendix II

FORMULAS FOR DOUBLE P_2 APPROXIMATION

In the double P_2 approximation, there are six equations of the form of Eq. (12) above, and the determinant for ν , Eq. (13), leads to the equation

$$\nu^6 - \nu^4 (84 - 24c) + \nu^2 (420 - \frac{860}{3}c) - 400(1 - c) = 0. \quad (A16a)$$

When $\alpha = 1 - c \ll 1$, the cubic can be iterated for the lowest root by collecting the terms in α on one side, obtaining

$$\nu^2 = 3\alpha \frac{1 - \frac{43}{60}\nu^2 + \frac{3}{50}\nu^4}{1 - \frac{9}{20}\nu^2 + \frac{3}{400}\nu^4} \quad (A16b)$$

$$\simeq 3\alpha (1 - \frac{4}{5}\alpha + \dots)$$

To obtain the other roots, divide Eq. (A16a) by ν^2 and rearrange, again collecting terms in α together:

$$\nu^4 - 60\nu^2 + \frac{400}{3} - \alpha(24\nu^2 - \frac{860}{3} + \frac{400}{\nu^2}) = 0. \quad (A16c)$$

$$\therefore \nu^2 = 30 \pm 10\sqrt{\frac{23}{3} + \alpha(\frac{6}{25}\nu^2 - \frac{43}{15} + \frac{4}{\nu^2})}$$

which can also be iterated conveniently for small α .

The equations of the form of (15) are:

$$\begin{aligned} A_1 &= -\frac{5\gamma(2+\gamma)}{60+60\gamma+11\gamma^2} A_0 & B_1 &= -\frac{5\gamma(2-\gamma)}{60-60\gamma+11\gamma^2} B_0 \\ A_2 &= \frac{2\gamma^2}{60+60\gamma+11\gamma^2} A_0 & B_2 &= \frac{2\gamma^2}{60-60\gamma+11\gamma^2} B_0 \end{aligned}$$

$$(1-\alpha) A_0 = \left\{ 1 - \gamma + \alpha - \frac{5\gamma^2(2-\gamma)}{60-60\gamma+11\gamma^2} \right\} B_0$$

or

$$(1-\alpha) B_0 = \left\{ 1 + \gamma + \alpha - \frac{5\gamma^2(2+\gamma)}{60+60\gamma+11\gamma^2} \right\} A_0$$

of which the first or second is preferable for numerical use depending upon whether γ is negative or positive.

1-49

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK