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Letters to the Editors

A Criticism of the Use of Diffusion Theory for the Study of Thermal Neutrons in Beryllium*

The diffusion approximation is a convenient and simple method often used to study the behavior of neutrons in matter. As with any approximation used in physics, reasonable care must be exercised to insure that the range of validity is not exceeded; also, since many general results are available from more accurate treatments of the Boltzmann equation, it is incumbent upon the user of a simple approximation to compare his results with known theory. If these cautions are not observed it is easy to lose touch with reality. The purpose of this note is to point out that Grover and Kothari[1] in a recent paper in this journal (hereafter denoted by 'GK') have used the diffusion approximation in a situation where it is invalid. They were concerned with the calculation of the thermal diffusion length and asymptotic spectrum in beryllium poisoned with various amounts of absorber. They neglected the fact that the total cross section below the Bragg cutoff is so small that diffusion theory fails for relatively modest amounts of absorber. They also reported that they calculated values of the reciprocal of the diffusion length, κ, that violate the requirement that κ be less than the minimum of the total cross section[2,3,4].

If one assumes that the transport approximation is a valid method for treating anisotropic scattering (and this is not a trivial point[5]) the eigenvalue equation for κ in transport theory is

$$\phi(E) = \frac{1}{2\kappa} \ln \frac{\Sigma_{tr}(E) + \kappa}{\Sigma_{tr}(E) - \kappa} \int_0^\infty \Sigma(E' \to E)\, \phi(E')\, dE'. \qquad (1)$$

The symbols here have their usual meanings, and it should be remembered that $\Sigma_{tr} = \Sigma_s(1 - \overline{\cos\theta}) + \Sigma_a$. Since the asymptotic distribution must be a non-singular everywhere-positive function it is obvious that κ, if it exists[2,3], must be less than the minimum $\Sigma_{tr}(E)$. Equation (1), which in Bethe's B_1 approximation[6], can be solved by the introduction of an auxiliary eigenvalue in much the same way that GK solve the diffusion-theory eigenvalue equation; and, indeed, it is just the approach taken by Honeck[7] in studying the same problem for other moderators.

To derive the diffusion approximation one expands the logarithm terms in powers of κ/Σ_{tr}; after trivial manipulation one obtains

$$\Sigma_{tr}\left(1 - \frac{1}{3}\left(\frac{\kappa}{\Sigma_{tr}}\right)^2 - \frac{4}{45}\left(\frac{\kappa}{\Sigma_{tr}}\right)^4 - \frac{44}{945}\left(\frac{\kappa}{\Sigma_{tr}}\right)^6 \ldots\right)\phi(E) = \int \Sigma(E' \to E)\, \phi(E')\, dE'. \qquad (2)$$

(Explicit indication of the energy dependence of Σ_{tr} has been omitted.)

The expansion is valid for all energies only if $(\kappa/\Sigma_{tr})^2 < 1$ for all energies, this being compatable with the limit on κ mentioned above. The diffusion equation results from dropping all except the first two terms on the right. One notes that for the diffusion approximation to be valid at all energies $(\kappa/\Sigma_{tr})^2$ must be small at all energies. As noted by Davison[8], it is the spatial dependence of the flux that determines the validity of the transport equation, the amount of absorption entering implicitly. (This means that it is possible to have a situation for which the diffusion approximation is adequate for the fundamental, but invalid for higher modes.) Therefore, the validity of diffusion theory must be examined after its application.

The above paragraphs contain previously stated and presumably well-known results; they are repeated here only to set the stage for displaying the reasons why it is felt that the GK results are of doubtful validity. Below the Bragg cutoff the transport cross section of beryllium drops to a value of about 0.7 barns (the value was read from the curve in the GK paper.) To this, one must add the absorption cross section at this energy to find the minimum value of the total-transport cross section. Assuming that the values of σ_a quoted by GK are at an energy of 300k and that the cross section has a $1/v$ dependence one can then calculate $(\Sigma_{tr})_{min}$, the upper limit on κ for each absorber concentration. One can then compare these limiting values with the results given by GK (the most convenient way is via the expansion of κ^2 in powers of Σ_a that they give.) Such a comparison shows that the limits on κ is exceeded in the GK calculation if the added σ_a is of the order of 0.042 barns. Thus, only their 'no-absorption' case, and their case with σ_a = 0.01 barns, give results that are compatable with the general transport-theory result. This is because they have implicitly used an expansion of the logarithm in Eq. (1) where it is not applicable, and because in this case there is an enhancement of the flux in the low cross-section

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[2] M. NELKIN, "Neutron Thermalization a la Mode," *Proc. BNL Conf. Neutron Thermalization,* Vol. **IV,** RF1-20, BNL-719 (c-32), (1962).

[3] N. CORNGOLD, "Some Transient Phenomena in Thermalization I, Theory," *Nucl. Sci. Eng.*, **19,** 80-90, (1964).

[4] N. CORNGOLD and P. MICHAEL, "Some Transient Phenomena in Thermalization II, Implications for Experiment," *Nucl. Sci. Eng.*, **19,** 91-94, (1964).

[5] G. RAKAVY and Y. YEIVEN, "The Transport Approximation of the Energy-Dependent Boltzmann Equation," *Nucl. Sci. Eng.*, **15,** 158-160, (1963).

[6] H. A. BETHE, USAEC Report AECD 2105, (1948); also H. A. BETHE, L. TONKS and H. HURWITZ, Jr., *Phys. Rev.*, **80,** 11 (1950).

[7] H. C. HONECK, "On the Calculation of Thermal Neutron Diffusion Parameters," *Proc. BNL Conf. Neutron Thermalization,* Vol. **IV,** 1186-1210, BNL 719 (c-32), (1962).

[8] B. DAVISON and J. B. SYKES, *Neutron Transport Theory,* Oxford (1957); p. 95.

region, it is impossible to claim that this region of the energy scale is unimportant. One should also note that for σ_a = 0.01 barns, the smallest value used by GK, $(\kappa/\Sigma_{tr})^2$ is of the order of 0.3 just below the Bragg cutoff. Hence, even for this small absorption, which is about what exists in natural beryllium, there is some doubt as to the validity of diffusion theory.

The GK paper presents values of diffusion parameters that are based upon the calculated dependence of κ^2 on Σ_a. Since the calculations are based upon an invalid application of diffusion theory one must conclude that the derived parameters have little to do with reality and an agreement with experiment is most likely fortuitous.

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Comments on Michael's Criticism of the Use of Diffusion Theory for the Study of Thermal Neutrons in Beryllium

In the preceding letter, Michael[1] has criticized our earlier paper[2] for using diffusion theory for the study of thermal neutrons in beryllium. There are two main points in his letter: a) he suggests an alternative approach to the problem—that of 'transport approximation,' and b) puts forward arguments to show that our use of diffusion theory was not justified.

Let us consider the first point first. According to Eqs. (1) or (2) of his letter, even the equilibrium neutron energy distribution will not be Maxwellian for the case $\Sigma_a = 0$ (we use the notation of (Ref. 1)), except in the special case of completely isotropic scattering, when $\Sigma_{tr}(E)$ is the same as $\Sigma_s(E)$. The two equations are quite inappropriate for multi-velocity problems and all conclusions that have been drawn from them are unreliable. The difficulty has arisen because Michael has applied the result of Rakavy and Yeiven's paper[3] to a case where it is not applicable. 'If these cautions are not observed it is easy to loose touch with reality.' Further to quote Davison[4], ' . . . the approximation (transport approximation) leads in general to rather poor results, as we might expect.' We feel that the suggestion by Michael, that one should solve his Eq. (1) by introducing an auxiliary eigenvalue, is not seriously meant.

In spite of the above, the point raised by him concerning the validity of using diffusion theory in the case of poisoned beryllium moderator is significant and needs some clarification.

It is well known that diffusion theory is a poor approximation for neutrons with energy just below the Bragg cutoff energy, because of their very low scattering cross section. However, since these neutrons form only a small fraction of the total number of neutrons (Table I), one expects κ^2 calculated on the basis of diffusion theory to be essentially correct. According to diffusion theory

$$\kappa^2 = 3\int \Sigma_a(E)\ \phi_0(E)\ dE \Big/ \int \frac{\phi_0(E)\ dE}{\Sigma_{tr}(E)} , \tag{1}$$

TABLE I

Ratio, R, of Neutron Flux Below the Bragg Cut-off to the Total Neutron Flux

Absorption cross-section $\Sigma_a(E)$ [a] cm^{-1}	R
($\times 10^{-2}$)	($\times 10^{-2}$)
0.12	2.5
0.50	3.5
0.84	4.4
1.20	6.5

[a] ($\Sigma_a(E)$ corresponds to velocity = 2.22×10^5 cm/sec.)

where $\phi_0(E)$ is the asymptotic flux (large distances). If the diffusion theory breaks down in a small range of energy (below the Bragg cut-off), $\phi_0(E)$ will be in error in that energy range, but since κ^2 is defined as an integral over the entire energy spectrum, the error in κ^2 will be small. Thus, there does not seem to be any ground for taking such a pessimistic view as Michael does—"the derived parameters have little to do with reality and agreement with experiment is most likely fortuitous." One can very well consider this agreement as corroborating the fact that diffusion theory works, even for cases where neutrons in a small energy range do not fulfill the conditions demanded by the diffusion theory.

No one will dispute that the use of diffusion theory should not be pressed too far and that more elaborate transport-theory calculations should be done (anyway, not on the lines suggested by Michael but rather as done by Honeck[5].) It is, however, worthwhile to remember that there are other important approximations involved in all present-day calculations, for example, the use of a particular lattice model in calculating the scattering kernels, the use of incoherent approximation, expansion of highly angle-dependent kernels in terms of a few Legendre polynomials, etc. In view of these and because of its great simplicity, the use of diffusion theory need not be abandoned. On the other hand, it does have a distinct advantage in that the sharp peaks in the transport cross-section can be explicitly taken into account.

The one oversight in our paper[2] has been our failure to state explicitly that the limit set on κ^2 by diffusion theory

$$\kappa^2 \leqslant 3\Sigma_{tr}(E).\ (\Sigma_a(E) + \Sigma_s(E))\Big|_{\min} \tag{2}$$

will not be valid for large Σ_a, for the simple reason that when the diffusion length becomes of the order of the average scattering mean free path, the theory itself will break down. Since the various parameters occurring in diffusion theory are quantities averaged over the equilibrium neutron-energy distribution, the validity of the theory should be judged by the criterion as to whether the average absorption mean free path far exceeds the average value of scattering mean free path. In other words, the condition for the validity of diffusion theory is[6-8]

$$\overline{\Sigma}_a \ll \overline{\Sigma}_s . \tag{3}$$

[1]PAUL MICHAEL, *Nucl. Sci. Eng.*, this issue, p. 93.
[2]P. S. GROVER and L. S. KOTHARI, *Nucl. Sci. Eng.*, **22**, 366 (1965).
[3]G. RAKAVY and Y. YEIVEN, *Nucl. Sci. Eng.*, **15**, 158 (1963).
[4]B. DAVISON and J. B. SYKES, *Neutron Transport Theory*, Oxford (1957), p. 241.
[5]HENRY HONECK, Brookhaven Conf. on Neutron Thermalization (1962).
[6]A. M. WEINBERG and L. C. NODERER, Report No. ORNL 51-5-98 (1951).
[7]A. M. WEINBERG and E. P. WIGNER, *The Physical Theory of Neutron Chain Reactors*, Chicago (1958); p. 191.
[8]A. D. GALANIN, *Thermal Reactor Theory*, Pergamon Press (1960); p. 15.