just the ones for which diffusion theory is best, for it describes the flux near the surface quite poorly for the two sources considered, but with an (area normalized) angular and spatial distribution between those of the two actual fluxes (all observations are consistent with diffusion theory being best for a source closer to the isotropic of the two). Thus, the very data used by Pomraning to demonstrate that his method is "superior" indicate that it compares worst when the variational principle should be at its best.

When any calculational method applied to a restricted set of situations makes some arbitrary gross quantity remarkably more accurate than the detailed distributions or any theoretical reason would suggest, the accuracy must be suspected of being fortuitous before it is accepted as very general.

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The Treatment of Boundary Terms in a Variational Principle Characterizing Transport Theory

In a recent note[1] Amster has presented a variational treatment of the diffusion theory boundary conditions that is purported to be more correct than a variational treatment by Pomraning and Clark (hereafter referred to as the PC treatment)[2]. His main argument for this position is the belief that his procedure is more straightforward and less arbitrary. In this note I would like to point out that the treatment of the diffusion theory (or higher order P_N) boundary conditions is, by necessity, arbitrary (even within the framework of the variational method), and further that Amster's treatment and the PC treatment are different in their aims.

Considering the first point, it is clear that the treatment of the P_N boundary conditions must be arbitrary. No finite expansion in full range polynomials can represent exactly the transport theory fluxes at the system boundaries since these fluxes are, in general, discontinuous in angle. The boundary conditions of Mark and Marshak (see Ref. 3 for a discussion) arise from completely different considerations and are a manifestation of this arbitrariness. In the PC treatment, which was an attempt to improve upon the boundary conditions of Mark and Marshak, the transport equation was characterized by a variational principle, including appropriate boundary terms in the functional. The use of a Legendre polynomial in angle trial function led to the usual P_N equations together with a set of nonlinear equations whose solution yielded a new set of boundary conditions applicable to all problems. Amster used the same functional to characterize the transport equation, but employed the classical Ritz method to determine the arbitrary constants in the general solution to a particular problem. Since this procedure leads to a set of linear equations with a unique solution, Amster argues that his procedure contains no arbitrariness and hence is basically more correct. There is an arbitrariness within the variational method, however, which Amster failed to consider and which strongly affects the result obtained by the Ritz method (as well as the result obtained by the PC treatment). This is an arbitrariness in the boundary terms of the functional itself. Consider a system with a free surface (no entering neutrons) at the left hand face, $z = a$. An appropriate functional is

$$F[\phi, \phi^*] = \int_a^\infty dz \int_{-1}^1 d\mu [\phi^* H\phi - S\phi^* - T\phi] +$$
$$+ \int_0^1 d\mu\, \mu \phi^*(a, \mu)\phi(a, \mu) +$$
$$+ \int_0^1 d\mu \alpha(\mu)\phi^2(a, \mu) +$$
$$+ \int_{-1}^0 d\mu \beta(\mu)\phi^{*2}(a, \phi) , \qquad (1)$$

where $\alpha(\mu)$ and $\beta(\mu)$ are *completely arbitrary* functions. The notation in Eq. (1) follows that in Ref. 2. The choice for these two functions will strongly affect the approximate solution found by the Ritz method. The main point to be emphasized is that the treatment of the P_N boundary conditions by the variational method is, unfortunately, arbitrary and it is difficult, if not impossible, to remove this arbitrariness.

The second main point to be made is that the results of Amster's treatment and the PC treatment are of a completely different nature. In the PC treatment the variational method is used to develop an approximate theory in the usual sense

[1] H. AMSTER, "A More Straightforward Use of Variational Principles with Boundary Conditions," *Nucl. Sci. Eng.*, this issue, p. 255.

[2] G. C. POMRANING and M. CLARK, Jr., *Nucl. Sci. Eng.*, **16**, 147-154 (1963).

[3] B. DAVISON and J. B. SYKES, *Neutron Transport Theory*, The Clarendon Press, Oxford, (1957).

of deriving a set of differential equations together with associated boundary conditions. Amster, on the other hand, is suggesting a method to determine the constants in the general solution of the set of differential equations applied to a specific problem. That is, Amster requires the general solution of the diffusion equation for the particular problem at hand before applying his boundary considerations. From a practical point of view (such as developing a computer code), this procedure is rather difficult to use in that the boundary conditions (in the usual sense) at a free surface depend upon the details of the problem under consideration. While in principle Amster's method is applicable to any problem, each problem requires recourse to the variational method. Further, in a realistic situation such as a multigroup, multiregion problem, it is certainly impractical to obtain the general solution of the diffusion equation and then use the Ritz method to determine the arbitrary constants.

In answer to the six specific questions which Amster raises in his letter, the following comments seem appropriate.

1) Linear restrictions were placed on the flux components at each boundary because this is the most general boundary condition compatible with the physics of the problem. That is, neutron transport theory is linear and hence we prescribed the appropriate number of general linear combinations of the flux components at the boundaries of the system as the boundary conditions on our approximate theory. The variational method was used to determine the coefficients in the linear combinations. Note that the linear restrictions were placed on the flux components and not their variations. The latter linear combinations were derived from the former. As pointed out by both Amster and Federighi[4], no stationary point of the reduced functional exists if arbitrary boundary variations are allowed. Hence, in deriving an approximate theory, it is necessary to restrict the variations at the boundaries in some manner. The linear restriction is clearly the most natural.

2) The arbitrariness in the variational treatment of the P_N boundary conditions has already been discussed. More specific to Amster's question, it is often the case that physical grounds are used to discard extraneous mathematical solutions. This is the situation in the PC treatment and the extraneous solutions are easily discarded.

3) It seems most reasonable for the diffusion theory linear extrapolation distance to be independent of the problem. This is precisely the situation with the Mark and Marshak boundary conditions as well as in the PC treatment. This should be attributed to the gross inability of the diffusion theory angular distribution to represent the free surface boundary condition. In higher order P_N theories, the Mark, Marshak, and PC treatments do lead to a linear extrapolation distance dependent upon the problem under consideration. However, the boundary conditions themselves (i.e., the linear combination coefficients on the flux components at a free surface) remain independent of the problem, as they indeed should in a useful and proper P_N theory. It might also be noted that the use of an asymptotic distribution as the trial function in the PC method[5] leads to an asymptotic diffusion theory together with a linear extrapolation distance dependent upon the composition of the medium. An asymptotic distribution is, by its very nature, too crude to yield a dependence on the size of the system.

4) Amster's suggestion that one use the results from the exact solution of the Milne problem to develop boundary conditions for the P_N approximation is, in fact, what is usually done in the diffusion theory case. That is, one generally uses a linear extrapolation distance of $0.7104\ \lambda_{tr}$ in preference to the values from a Mark or Marshak treatment. In higher order P_N approximations, however, this procedure is not feasible. For example, in the P_3 case two linear combinations involving four constants are the appropriate boundary conditions. One constant could be established by demanding proper asymptotic behavior for the Milne problem, but it is not clear what the other three conditions should be. Further, in the limit as N (the order of the approximation) approaches infinity, one has no assurance with this procedure that the resulting boundary conditions will yield exact results for all problems. One does have this assurance, however, with the Mark, Marshak, and PC boundary conditions.

5) Because of its simplicity, a low order P_N approximation, in particular diffusion theory, can only hope to predict accurately the asymptotic flux distribution. For the Milne problem the linear extrapolation distance is a direct measure of the asymptotic flux. As pointed out in Ref. 5, the capture fraction was used for comparison purposes only because the magnitude of the asymptotic flux from an exact calculation is not readily available in the literature. For low absorption systems the flux is almost entirely in the asymptotic distribution and hence, for these systems, the capture fraction comparison gives a good indication of the accuracy of the asumptotic distribution. With regard to Amster's point that only the value of the functional is estimated accurately by a variational principle, the following statement must be made.

[4] F. FEDERIGHI, *Nucleonik*, 6, 277-285 (1964).

[5] G. C. POMRANING, *Nucl. Sci. Eng.*, 21, 62-78 (1965).

There are two distinct manners in which to use the variational method. The first, as Amster points out, is to accurately estimate a single quantity, namely the exact value of the functional. The second, which is the essence of the PC treatment, is to characterize a physical theory with a variational principle from which an approximate theory can be derived. For example, Hamilton's principle in classical mechanics completely characterizes the equations of motion. Yet Hamilton's functional (the time integral of the Lagrangian) does not, in general, reduce to a quantity of interest when evaluated with the exact solution of these equations.

6) As previously pointed out, the PC treatment and that of Amster are different in their aims and arise from different uses of the variational method. There is no reason, nor does it make any sense, to try to "extend the PC treatment to the general direct (Ritz) method."

Two further points should be made. First, with reference to the specific example in Amster's paper, it is clear that his method for this (rather unrealistic) problem yields a result superior to the PC treatment. This is not surprising in that Amster is treating a specific problem whereas the PC method is developing an approximate theory. That is, in using the variational method to develop a theory which is presumably applicable to a wide range of problems, it is to be expected that for certain problems this theory will be less accurate than a method such as Amster's which uses the variational method to treat a particular situation. For other problems, however, the PC treatment is the better of the two. For example, in the treatment of the Milne problem Amster's method yields a linear extrapolation distance of $\frac{2}{3}\lambda_{tr}$ and is clearly inferior to the PC treatment in the prediction of the flux distribution. Even more interesting is the application of Amster's method to a purely scattering slab of halfthickness $1/\sqrt{2}$ mean free paths. If the source is not symmetric about the midplane, any other treatment of the boundary conditions is (literally) infinitely better than the Ritz method. Amster attributes the failure of his suggested method in this case to the inadequacy of diffusion theory. This explanation does not seem sufficient. If the source is symmetric about the midplane, Amster's method yields a linear extrapolation distance of $\frac{2}{3}\lambda_{tr}$, a qualitatively correct answer. However, if the source contains an *arbitrarily small* amount of asymmetry, the solution by Amster's method is divergent. Thus the mathematics displays a discontinuity which does not exist in the physical problem. Although diffusion theory may not be adequate to quantitatively describe this problem, it should be capable of giving a qualitative picture of the physics involved.

The final point to be made is that the PC boundary conditions can be derived on physical grounds without reference to the variational method. As an example, consider the diffusion theory treatment of a free surface at the left hand boundary of a slab system, $z = a$. The transport theory boundary condition is

$$\phi(a, \mu) = 0, \quad 0 < \mu \leq 1. \tag{2}$$

It is clear that the diffusion theory flux expansion

$$\phi(z, \mu) = \frac{1}{2}\phi(z) + \frac{3}{2}J(z)\mu \tag{3}$$

cannot satisfy Eq. (2) exactly (except in the trivial case $\phi(a) = J(a) = 0$). As an approximation we can demand, however, that the importance-weighted, integrated current entering the system vanish, i.e.,

$$\int_0^1 d\mu\,\mu\phi(a, \mu)\phi^*(a, \mu) = 0, \tag{4}$$

where $\phi^*(z, \mu)$ is the neutron importance (adjoint). It is easily shown[2] that ϕ and ϕ^* are related by

$$\phi^*(z, \mu) = \phi(z, -\mu)\,. \tag{5}$$

As pointed out by Federighi[4], this equation relating the direct and adjoint fluxes need not be used in deriving the importance-weighted boundary conditions. However, we choose to use it here to simplify the discussion. Using Eqs. (3) and (5) in Eq. (4), we find

$$\frac{\phi(a)}{J(a)} = \frac{3}{\sqrt{2}}\,. \tag{6}$$

Further, the use of Fick's law of diffusion

$$J(z) = -\frac{\lambda_{tr}}{3}\frac{d\phi(z)}{dz} \tag{7}$$

yields for d, the linear extrapolation distance,

$$d \equiv \frac{\phi(a)}{\dfrac{d\phi(a)}{dz}} = 0.7071\,\lambda_{tr}\,. \tag{8}$$

This 'importance weighting' technique has been used by Federighi[4] in deriving free surface boundary conditions for the P_N approximation up to $N = 15$.

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