# Letters to the Editors

## On the Linear Extrapolation Distance

The standard practice used in computing the thermal worth of a control element within an assembly by diffusion (P-1) theory is to replace the element by an internal boundary condition and carry the diffusion calculation up to the point at which this boundary condition is applied. Generally one of two conditions is used. The first of these states that the scalar flux vanishes at a distance $z_0$ past the assembly–control interface. $z_0$ is referred to as the extrapolated endpoint. The second condition states that at the assembly–control interface the flux and its gradient satisfy $-(1/\varphi)\mathbf{n}\cdot\nabla\varphi = 1/d$, where $\mathbf{n}$ is a unit normal vector pointing into the control region. $d$ is referred to as the linear extrapolation distance. This latter condition is the more natural of the two since it is applied at the actual assembly–control interface, and for this reason is the one most generally used. In this letter we restrict ourselves to a discussion of the linear extrapolation distance and suggest two simple methods of improving upon the value of $d$ presently being used in thermal control worth calculations.

If the control element is black, i.e., all neutrons impinging upon it are absorbed, the P-1 value of the linear extrapolation distance, $d$, using a Marshak (no return current) boundary condition is $0.6667\ \lambda_{tr}$, where $\lambda_{tr}$ is the transport mean free path. However, an exact transport solution for a semi-infinite halfspace bounded by a vacuum with a source at infinity, i.e., the Milne problem, gives $d$ equal to $0.7104\ \lambda_{tr}$ for a pure isotropic scatterer.[1] Accordingly, the P-1 result of $0.6667\ \lambda_{tr}$ is often replaced by the transport result of $0.7104\ \lambda_{tr}$ as the value of $d$ used in conjunction with diffusion theory. Further, two corrections are frequently applied to the transport value of $0.7104\ \lambda_{tr}$. The first of these accounts for the variation of the Milne value of $d$ with $c$, the mean number of secondaries per collision. In the limit $c = 0$, i.e., a pure absorber, the linear extrapolation distance in the Milne problem is $1.0000\ \lambda_{tr}$. The value of $d$ for intermediate values of $c$ can be obtained from the tabulation of Case, deHoffmann, and Placzek (*1*). Secondly, the linear extrapolation distance varies with the curvature of the control element. In the limit of a black cylinder with an infinite curvature (zero radius), transport theory gives $1.3333\ \lambda_{tr}$ as the value of $d$. For cylinders of finite curvature $d$ can be estimated from the plot of $d$ versus radius given by Weinberg and Wigner (*2*).

All of the above remarks are based on a Milne-type solution, i.e., a medium with the source of neutrons at infinity. If one is using few-group diffusion theory to compute the thermal worth of a control element, the slowing down source to the thermal group is not at infinity, but can better be represented as spatially constant in the vicinity of the control element. The semi-infinite halfspace with a spatially constant source can be treated exactly by transport theory and should yield a more realistic linear extrapolation distance for the control worth calculation than does the Milne analysis.

According to Davison (*3*), the asymptotic solution for the scalar flux within a semi-infinite halfspace occupying $z > 0$ and containing a spatially constant source of magnitude $S$ is

$$\varphi(z) = \frac{S}{\Sigma(1-c)}\left\{1 - \frac{1}{c}\left[\frac{2(1-c)(1-\nu^2)}{c-(1-\nu^2)}\right]^{1/2} \cdot e^{-\nu\Sigma(z+z_0)}\right\}, \tag{1}$$

where $\Sigma$ is the macroscopic collision cross section, $c$ is the mean number of secondaries per collision, $z_0$ is the extrapolated endpoint in the Milne problem and is tabulated by Case *et al.* (*1*), and $\nu$ is the asymptotic eigenvalue of the Boltzmann equation, given by

$$\frac{2\nu}{c} = \ln\left(\frac{1+\nu}{1-\nu}\right). \tag{2}$$

From Eq. (1) the linear extrapolation distance for the constant source problem is easily found to be

$$\frac{d}{\lambda_{tr}} = \frac{1}{\nu}\left\{c\left[\frac{c-(1-\nu^2)}{2(1-c)(1-\nu^2)}\right]^{1/2} e^{\nu\Sigma z_0} - 1\right\}. \tag{3}$$

Table I compares numerical values computed from Eq. (3) with the corresponding Milne (source at infinity) values as tabulated by Case *et al.* (*1*). We note that for a pure absorber, i.e., $c = 0$, Eq. (3) gives an infinite extrapolation distance, which, when used with diffusion theory, would yield zero control worth. This is obviously an incorrect limit and is a manifestation of the inadequacy of any asymptotic theory, such as diffusion theory, for strongly absorbing systems.

Since $(1 - c) \ll 1$ is the region of practical interest, an expansion of Eq. (3) in powers of $(1 - c)$ is useful. Correct to order $(1 - c)$ we find

$$d/\lambda_{tr} = 0.7104[1 + 0.5340(1-c)^{1/2} + 1.1523(1-c) + 0(1-c)^{3/2}], \tag{4}$$

whereas the Milne result gives

$$d/\lambda_{tr} = 0.7104[1 + 0.4953(1-c) + 0(1-c)^2]. \tag{5}$$

Because of the incorrect limiting behavior for a purely absorbing system, one is led to consider an alternate method of improving upon the Milne value of $d$. Again we consider the semi-infinite constant source problem and equate the exit current from the halfspace according to exact transport

[1] For isotropic scattering, $\lambda_{tr} \equiv 1/\Sigma$.

TABLE I

LINEAR EXTRAPOLATION DISTANCE, $d$, AS A FUNCTION OF THE MEAN NUMBER OF SECONDARIES PER COLLISION, $c$, FOR THE SEMI-INFINITE HALFSPACE

| $c$ | $d/\lambda_{tr}$-Milne source | $d/\lambda_{tr}$-Constant source |
|---|---|---|
| 0 | 1.000 | $\infty$ |
| ⋮ | ⋮ | ⋮ |
| 0.5 | 0.920 | 3.602 |
| 0.6 | 0.875 | 2.272 |
| 0.7 | 0.830 | 1.610 |
| 0.8 | 0.787 | 1.219 |
| 0.9 | 0.747 | 0.959 |
| 1.0 | 0.710 | 0.710 |

TABLE II

LINEAR EXTRAPOLATION DISTANCE, $d$, REQUIRED TO GIVE EXACT TRANSPORT LEAKAGE FROM A SEMI-INFINITE HALFSPACE WITH A SPATIALLY CONSTANT SOURCE

| $c$ | $d/\lambda_{tr}$; $D = 1/3\Sigma$ | $d/\lambda_{tr}$; $D = (1-c)/\nu^2\Sigma$ |
|---|---|---|
| 0.0 | 0.756 | 3.000 |
| 0.1 | 0.755 | 2.676 |
| 0.2 | 0.753 | 2.361 |
| 0.3 | 0.751 | 2.012 |
| 0.4 | 0.749 | 1.747 |
| 0.5 | 0.746 | 1.517 |
| 0.6 | 0.743 | 1.312 |
| 0.7 | 0.739 | 1.141 |
| 0.8 | 0.735 | 1.001 |
| 0.9 | 0.729 | 0.874 |
| 1.0 | 0.710 | 0.710 |

analysis to the diffusion theory result in terms of an unknown linear extrapolation distance, $d$. This equality can then be solved for $d$. Using this value of $d$ to compute the thermal absorption of a control slab by diffusion theory will then give an exact transport result if the assembly is large and the slowing down source to the thermal group is spatially constant in the vicinity of the control element. If these two conditions are only approximately satisfied, as is the actual situation, one would still expect the result to be more accurate than that obtained using the Milne value for $d$.

The diffusion theory result for the leakage, $L$, from a semi-infinite halfspace with a spatially constant source of magnitude $S$ and isotropic scattering is

$$L = \frac{S/\Sigma}{\sqrt{(1-c)/D\Sigma}\,[1+\sqrt{(1-c)/D\Sigma}\,(\Sigma d)]}. \quad (6)$$

whereas the transport result for this problem is easily found from the analysis of Davison (*3*) to be

$$L = \frac{S}{\Sigma c}\left[\frac{1}{\nu} - I(c)\right], \quad (7)$$

where $D$ is the diffusion coefficient and $I(c)$ is tabulated by Case *et al.* (*1*). Equating Eqs. (6) and (7) and solving for $d$ gives[1]

$$\frac{d}{\lambda_{tr}} = \frac{c}{[(1/\nu) - I(c)][(1-c)/D\Sigma]} - \frac{1}{\sqrt{(1-c)/D\Sigma}}. \quad (8)$$

To use Eq. (8) to compute $d$, one must know $D$ as a function of $c$. The two most widely used diffusion theories are classical (P-1) diffusion theory with $D = 1/3\Sigma$ and asymptotic (transport) diffusion theory with $D = (1-c)/\nu^2\Sigma$. Table II gives numerical values of $d$ as a function of $c$ according to Eq. (8) for these two choices of $D$.

For $(1-c) \ll 1$ and $D = 1/3\Sigma$, Eq. (8) can be expanded as

$$d/\lambda_{tr} = 0.7104[1 + 0.0926(1-c)^{1/2} - 1.5573(1-c) + 0(1-c)^{3/2}]. \quad (9)$$

A similar expansion for $D = (1-c)/\nu^2\Sigma$ yields

$$d/\lambda_{tr} = 0.7104[1 + 0.4178(1-c)^{1/2} - 0.7573(1-c) + 0(1-c)^{3/2}]. \quad (10)$$

REFERENCES

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## On the Existence of Tributyl Phosphate Monohydrate

Tributyl phosphate (TBP) has found wide utility in the processing of heavy metal ores and spent fuel elements by solvent extraction. Wallace Davis has reported a study of the nitric acid–TBP system in which equilibrium distribution data are used to obtain a quantitative description of the extraction process (*1*). In common with earlier work (cited in ref. *1*), Davis' description assumes the existence of the complex TBP·$H_2O$. A second article by Davis (*2a*) expresses some doubt as to whether the complex is actually formed; a third article (*2b*) implies that free TBP and TBP·$H_2O$ are simply not distinguishable thermodynamically (Equation 7).

Olander and Benedict have recently reported the use of mass transfer data on the TBP—$H_2O$ system to indicate the nonexistence of TBP·$H_2O$ (*3*). The latter authors compare the mass transfer rates of water entering the organic phase with "ordinary" systems in which they claim no complexing between water and solvent takes place. The "ordinary"