Letters to the Editor

Comments on "A New Definition of the Cell Diffusion Coefficient"

In two recent papers, Gelbard[1] and Köhler[2] have discussed the definition of the cell diffusion coefficient from different viewpoints, with the first author criticizing and the second author effectively rejecting Benoist's long-known formula[3] for regular lattices.

The problem was, however, thoroughly examined by Bonalumi in an even earlier paper,[4] where all the apparent contradictions between different "versions" had been cleared, and, in addition, a consistent formulation for nonuniform lattices had been proposed.

Since Ref. 4 does not seem to be widely noticed, it is the purpose of this Letter to bring to attention at least one basic point raised in that reference, i.e., the necessity of a conceptually sharp distinction between the groupwise leakage term and the energy-integrated order-B^2 term in the "cell balance." The following derivation is basically the same as in a hard to find report by Berna,[5] and, for the sake of simplicity, is offered in a multivelocity formalism for a buckled source problem.

Define: the vector flux ψ, the cross-section-like operator $\hat{\Sigma}$ such that

$$\hat{\Sigma} f = \Sigma(E) f(E,\boldsymbol{\Omega}) - \int_{(4\pi)} d\Omega' \int_0^\infty \Sigma_s(E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}) f(E',\boldsymbol{\Omega}') dE' \ , \tag{1}$$

the (isotropic) source

$$\frac{q(\boldsymbol{r},E)}{4\pi} \exp(i\boldsymbol{B}\cdot\boldsymbol{r}) \ ,$$

the Boltzmann operator H such that

$$Hf = \boldsymbol{\Omega}\cdot\boldsymbol{\nabla} f + \hat{\Sigma} f \ . \tag{2}$$

The associated transport equation reads

$$H\psi = \frac{q}{4\pi} \exp(i\boldsymbol{B}\cdot\boldsymbol{r}) \ \ ; \tag{3}$$

if x is an axis directed as $\boldsymbol{B}$, the ansatz $\psi = f \exp(i\boldsymbol{B}\cdot\boldsymbol{r})$ gives

$$Hf + i\boldsymbol{\Omega}\cdot\boldsymbol{B} f = \frac{q}{4\pi} \Rightarrow Hf + iB\Omega_x f = \frac{q}{4\pi} \ . \tag{4}$$

If the origin of x is in the cell center $\boldsymbol{r}_0$, one can expand

$$\exp(i\boldsymbol{B}\cdot\boldsymbol{r}) = \exp(i\boldsymbol{B}\cdot\boldsymbol{r}_0) \left(1 + iBx - \frac{B^2x^2}{2} + \ldots\right) \tag{5}$$

and other expansions are, with obvious symbols and mutual relationships,

$$f = \sum_{n=0}^{\infty} (-iB)^n f_n = f_0 - iBf_1 - B^2 f_2 + \ldots \tag{6}$$

$$\phi = \int_{(4\pi)} \psi \, d\Omega = \exp(i\boldsymbol{B}\cdot\boldsymbol{r}) \left[F_0 - iBF_1 - B^2F_2 + \ldots\right] \tag{7}$$

$$\boldsymbol{J} = \int_{(4\pi)} \boldsymbol{\Omega}\psi \, d\Omega = \exp(i\boldsymbol{B}\cdot\boldsymbol{r})\boldsymbol{g} \ \ , \tag{8}$$

$$\boldsymbol{g} = \boldsymbol{j}_0 - iB\boldsymbol{j}_1 + B^2\boldsymbol{j}_2 + \ldots \ . \tag{9}$$

Such expansions applied to Eq. (4) give:

$$Hf_0 = \frac{q}{4\pi}, \text{ infinite lattice problem} \tag{10}$$

$$Hf_{i+1} = \Omega_x f_i, \text{ all } i \geq 0 \tag{11}$$

and, upon integration over $d\Omega$:

$$\operatorname{div} \boldsymbol{j}_0 + \hat{\Sigma} F_0 = q \tag{10$'$}$$

$$\operatorname{div} \boldsymbol{j}_{i+1} + \hat{\Sigma} F_{i+1} = j_{ix}, \text{ all } i \geq 0 \ . \tag{11$'$}$$

Note the following important equations:

$$\operatorname{div} \boldsymbol{J} = \exp(i\boldsymbol{B}\cdot\boldsymbol{r}) \left(\operatorname{div} \boldsymbol{g} + iBg_x\right) \tag{12}$$

$$\boldsymbol{j}_0 \equiv 0 \text{ on the cell boundary surface} \tag{13}$$

$$\int_{\text{(cell)}} \operatorname{div} \boldsymbol{j}_i \, dV = 0, \text{ all } i \geq 0 \text{ (for lattice periodicity)} \ . \tag{14}$$

The following basic identity is easily established

$$\int_{\text{(cell)}} \left(xj_{0x} + \frac{x^2}{2} \operatorname{div} \boldsymbol{j}_0\right) dV \equiv \frac{1}{2} \int_{\text{(cell)}} \operatorname{div} \left(x^2\boldsymbol{j}_0\right) dV = 0 \tag{15}$$

because of Green's theorem and Eq. (13); with the convention that all volume integrals cover the unit cell, it is possible to prove, because of Eqs. (10′), (11′), and (15), the following equation:

$$\int \hat{\Sigma} \left(xF_1 - \frac{x^2}{2} F_0\right) dV = \int \left\{x(j_{0x} - \operatorname{div} \boldsymbol{j}_1) - \frac{x^2}{2} (q - \operatorname{div} \boldsymbol{j}_0)\right\} dV$$

$$= - \int \left(x \operatorname{div} \boldsymbol{j}_1 + \frac{qx^2}{2}\right) dV \ . \tag{16}$$

We are at last in a position to write down the individual terms contributing to the actual cell balance; "net removal," "leakage," and "source" terms [arbitrarily premultiplied by $\exp(-i\boldsymbol{B}\cdot\boldsymbol{r}_0)$] are:

$$\hat{A} = \exp(-i\boldsymbol{B}\cdot\boldsymbol{r}_0) \int \hat{\Sigma} \phi \, dV \tag{17}$$

$$\mathcal{L} = \exp(-i\boldsymbol{B}\cdot\boldsymbol{r}_0) \int \operatorname{div} \boldsymbol{J} \, dV \tag{18}$$

$$S = \exp(-i\boldsymbol{B}\cdot\boldsymbol{r}_0) \int q \exp(i\boldsymbol{B}\cdot\boldsymbol{r}) dV \ . \tag{19}$$

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[1] E. M. GELBARD, *Nucl. Sci. Eng.*, **54**, 327 (1974).

[2] P. KÖHLER, *Nucl. Sci. Eng.*, **57**, 333 (1975).

[3] P. BENOIST, "Théorie du coefficient de diffusion des neutrons dans un réseau comportant des cavités," CEA-R-2278, Centre d'Etudes Nucléaires, Saclay (1964).

[4] R. A. BONALUMI, *Energ. Nucl.*, **21**, 231 (1974).

[5] PH. BERNA, "Recherche d'une définition cohérente du coefficient de diffusion," SPM-1123, Centre d'Etudes Nucléaires, Saclay (1970).

If the cell, q, and $\hat{\Sigma}$ are symmetric about $\boldsymbol{r}_0$, use of antisymmetry of xF_0, F_1, and of Eq. (16) into Eq. (17), use of Eq. (15) and repeated application of Eq. (14) into Eq. (18) and antisymmetry of xq in Eq. (19) lead to the following:

$$\hat{A} = \int \hat{\Sigma} F_0 \, dV - B^2 \int \left(\hat{\Sigma} F_2 + x \operatorname{div} \boldsymbol{j}_1 + \frac{qx^2}{2} \right) dV + 0\,(B^4) \tag{17$'$}$$

$$\mathcal{L} = B^2 \int (j_{1x} + x \operatorname{div} \boldsymbol{j}_1) \, dV + 0\,(B^4) \tag{18$'$}$$

$$S = \int q \, dV - B^2 \int \frac{x^2}{2} q \, dV + 0\,(B^4) \quad . \tag{19$'$}$$

One can check that because of Eqs. (10′), (11′), and (14), the cell balance is respected; through order B^2, all coefficients of $\mathcal{L} + \hat{A} - S$ do vanish.

It is also convenient to calculate

$$G = \exp(-i\boldsymbol{B} \cdot \boldsymbol{r}_0) \int \phi \, dV$$

$$= \int F_0 \, dV + B^2 \int \left(-F_2 + xF_1 - \frac{x^2}{2} F_0 \right) dV + 0\,(B^4) \quad , \tag{20}$$

and, through order B^2, with self-explanatory symbols, to let

$$\hat{A} = A_0 + A_2 B^2 \tag{21}$$

$$\mathcal{L} = \mathcal{L}_2 B^2 \tag{22}$$

$$S = S_0 + S_2 B^2 \tag{23}$$

$$G = G_0 + G_2 B^2 \quad . \tag{24}$$

(We note that $A_0 - S_0 = A_2 + \mathcal{L}_2 - S_2 = 0$.)

Now the homogenized removal cross section $\tilde{\Sigma}$ and diffusion coefficient $\tilde{D}$ should be such that, whichever definition one takes for the "homogenized flux":

$$\frac{\tilde{\Sigma}}{\tilde{\Sigma} + \tilde{D} B^2} = \frac{\hat{A}}{S} \Rightarrow \tilde{\Sigma} S = \hat{A} \, (\tilde{\Sigma} + \tilde{D} B^2) \tag{25}$$

so that if one lets

$$\tilde{\Sigma} = \Sigma_0 + \Sigma_2 B^2 \tag{26}$$

$$\tilde{D} = D_0 + D_2 B^2 \tag{27}$$

and equates order-B^2 terms in Eq. (25), zero order gives $S_0 = A_0$ as obvious, one gets

$$D_0 = \Sigma_0 \frac{S_2 - A_2}{A_0} \quad . \tag{28}$$

Equation (28) says that D_0 is uniquely defined provided Σ_0 is defined. In a uniform lattice, it is irrelevant which normalization is chosen for Σ_0; if we take the usual one, advocated by Gelbard although inapplicable in nonuniform lattices,[4] i.e.,

$$\Sigma_0 = \frac{A_0}{G_0} \tag{29}$$

then becomes

$$D_0 = \frac{S_2 - A_2}{G_0} = \frac{\mathcal{L}_2}{G_0} = \frac{\int (j_{1x} + x \operatorname{div} \boldsymbol{j}_1) \, dV}{\int F_0 \, dV} \quad , \tag{30}$$

which proves Benoist right, as expected from Eq. (18′), but also proves Köhler wrong. The reason is that Köhler's D takes into account nonleakage B^2 terms related to A^2 and S_2, and arbitrarily introduced by Köhler's definitions of homogenized source and absorption rate, which do not reproduce S and $\hat{A}$.

The situation is only slightly different as far as the definition of a diffusion area L^2 is concerned; no matter what normalization is used for Σ_0, the purpose of such a removal cross section is to reproduce $\hat{A}$. If the homogenized flux ϕ_{hom} is calculated as

$$\phi_{\text{hom}} = \frac{S_0/V}{\Sigma_0 (1 + B^2 L^2)} \exp(i\boldsymbol{B} \cdot \boldsymbol{r}) \quad , \tag{31}$$

one must impose

$$\exp(-i\boldsymbol{B} \cdot \boldsymbol{r}_0) \int \Sigma_0 \, \phi_{\text{hom}} \, dV = \hat{A}$$

so that

$$A_0 + A_2 B^2 = \frac{S_0 \left(1 - B^2 \left\langle \frac{x^2}{2} \right\rangle \right)}{1 + B^2 L^2} + 0\,(B^4) \quad ,$$

where

$$\left\langle \frac{x^2}{2} \right\rangle = \frac{1}{V} \int \frac{x^2}{2} \, dV \quad .$$

Equating order-B^2 terms yields

$$L^2 = -\frac{A_2}{A_0} - \left\langle \frac{x^2}{2} \right\rangle = \frac{\int (\hat{\Sigma} F_2 + x \operatorname{div} \boldsymbol{j}_1) \, dV}{\int \hat{\Sigma} F_0 \, dV} + \int \frac{x^2}{2} \left(\frac{q}{S_0} - \frac{1}{V} \right) dV \quad .$$

But Eq. (11′) for $i = 1$ gives, as correctly stated by Köhler,

$$\int \hat{\Sigma} F_2 \, dV = \int j_{1x} \, dV$$

so that

$$L^2 = \frac{D_0}{\Sigma_0} + \int \frac{x^2}{2} \left(\frac{q}{S_0} - \frac{1}{V} \right) dV \xrightarrow[\text{uniform}]{\text{if } q} \frac{D_0}{\Sigma_0} \quad .$$

Therefore, corrections to D_0/Σ_0 do arise in connection with nonuniformity of the source, but basically the Benoist equation is confirmed. One thing, instead, is worth recalling, which was first pointed out by Benoist[3] himself: the term containing $x \operatorname{div} \boldsymbol{j}_1$ (Benoist's "absorption correction") is such that, in a few-group criticality calculation, it cancels out when all the groupwise L^2's are summed up to yield a migration area. This is particularly well displayed if we transform a part of the absorption correction following Carter.[6] The absorption correction is:

$$\int x \operatorname{div} \boldsymbol{j}_1 dV = \int x (j_{0x} - \hat{\Sigma} F_1) \, dV$$

and because of Eqs. (15) and (10′):

$$\int x \operatorname{div} \boldsymbol{j}_1 \, dV = \int \frac{x^2}{2} (\hat{\Sigma} F_0 - q) \, dV - \int x \hat{\Sigma} F_1 dV \quad ,$$

displaying that what is removed for one group takes the role of a source in another (particularly so in a criticality calculation, where q can be included altogether in $\hat{\Sigma} F_0$ upon properly redefining $\hat{\Sigma}$); one may conclude that, as far as the overall neutron leakage is concerned, Benoist's absorption correction is inactive, but this is not true at the level of any single energy group, where current continuity requires use of the complete "Benoist" D.

Of necessity, the foregoing discussion ignores two other, perhaps more fundamental questions:

1. How should Σ_0 be normalized?
2. How meaningful is the definition of uniform-lattice constants such as Σ_0, D_0 in a nonuniform lattice, and how can one remedy the situation?

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[6] C. CARTER, unpublished paper as quoted by D. C. Leslie, "The Calculation of Leakage and of Flux Distributions in Systems with Superimposed Buckling," AEEW-M.292, U.K. Atomic Energy Authority, Winfrith (1964).

In the writer's opinion, the answer is given in Ref. 4, Secs. 3 and 4, regardless of whether the interstitial ("moderator") region is dealt with by diffusion or transport theory.

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Comments on "Systems with Stochastic Parameters"

In a recent paper, Karmeshu and Bansal[1] have considered the response of the point model reactor kinetics equations to a random parametric reactivity excitation. They make the statement that their results differ from those of Williams[2] because he assumed that no correlation exists between reactivity and neutron density. It is the purpose of this Letter to point out the reason for the neglect of this correlation in Williams' paper and to emphasize the importance of this particular problem.

The reasoning outlined here follows closely that of Gray and Caughey.[3] We consider the point model reactor kinetics equations with one group of delayed neutrons in the form

$$\frac{dN(t)}{dt} = \frac{1}{l}\left[\rho(t) - \beta\right]N(t) + \lambda C(t) + S(t) \tag{1}$$

$$\frac{dC(t)}{dt} = -\lambda C(t) + \frac{\beta}{l} N(t) \tag{2}$$

$$\rho(t) = \rho_0 + \Delta(t) \quad \text{and} \quad S(t) = S_0 + \mathcal{J}(t) \quad .$$

Now $\Delta(t)$ and $\mathcal{J}(t)$ can be considered either as Gaussian, physical white noise sources or, alternatively, as derivatives of a Wiener process such that

$$\Delta(t) = \frac{\delta W}{\delta t} \quad \text{and} \quad \mathcal{J}(t) = \frac{\delta V}{\delta t} \quad , \tag{3}$$

where δW and δV are jump processes. Equations (1) and (2) with the excitation given by Eq. (3) can be interpreted in a discrete sense by assuming that, at the start of each time interval, δt, the system receives a random impulse that sends it from state P_1 to P_2 instantaneously due to the action of the term $(\delta WN + \delta V)/l$. From this stage the system moves according to the term $[(\rho_0 - \beta)N/l + \lambda C + S_0]\delta t$ until the end of the time interval when it is a state P_3. The process is then repeated indefinitely, with impulses followed by steady motion in successive time intervals δt. This type of behavior is characteristic of Brownian motion, shot noise, or neutron emission from fission. In this case, N and δW are uncorrelated.

The other situation arises when δW and δV are a continuous process such that $\delta W/\delta t$ is a mathematical approximation for a Gaussian process with a very short correlation time. In this case N and δW are correlated.

Thus, when we formulate the Fokker-Planck equation and are required to evaluate the limit

$$A_1 = \lim_{\delta t \to 0} \frac{\langle \delta N \rangle}{\delta t} \quad , \tag{4}$$

then for Wiener impulses we obtain

$$A_1 = \frac{1}{l}(\rho_0 - \beta)N + \lambda C + S_0 \quad , \tag{5}$$

whereas for the Gaussian continuous process we obtain

$$A_1 = \frac{1}{l}\left(\rho_0 - \beta + \frac{\sigma_{11}^2}{l}\right) + \lambda C + S_0 \quad , \tag{6}$$

where

$$\langle \delta W \rangle = 0 \tag{7}$$

and

$$\langle (\delta W)^2 \rangle = 2\sigma_{11}^2 \delta t \quad . \tag{8}$$

When these and the other coefficients are inserted into the Fokker-Planck equation, it can be readily shown[4] that the corresponding first moment equations are:

Wiener Process

$$\frac{d\langle N \rangle}{dt} = \frac{1}{l}(\rho_0 - \beta)\langle N \rangle + \lambda \langle C \rangle + S_0 \tag{9}$$

Gaussian Process

$$\frac{d\langle N \rangle}{dt} = \frac{1}{l}\left(\rho_0 - \beta + \frac{\sigma_{11}^2}{l}\right)\langle N \rangle + \lambda \langle C \rangle + S_0 \quad . \tag{10}$$

Williams[2] obtained Eq. (9), and Karmeshu and Bansal have obtained the solution of Eq. (10) where $D = \rho_0^2\sigma_{11}^2$ and not $D = \sigma_{11}^2$ as suggested. It might also be mentioned that the solution of Eq. (10) was obtained by Williams[5] by the renormalization technique [see Eq. (8.10) of that paper].

Now we must discuss which equation is the correct one. There is no doubt that, if we wish $\Delta(t)$ to simulate the effects of random neutron injection from fission, Eq. (9) must be correct. This follows from the fact that Eq. (9) is the exact moment equation of the zero power probability balance equation. On the other hand, when the reactivity perturbation is due to random vibration or some other *mechanical* cause, it seems physically more realistic to adopt the Gaussian assumption and employ Eq. (10). From the practical point of view it does seem that an experimental investigation of these two types of stochastic perturbation would be useful. Initial indications from the work of Akcasu[6] on boiling water reactors suggest that its effect is not insignificant.

Finally, it must be pointed out that the technique described by Karmeshu and Bansal for calculating the first moments has no material advantage, other than conciseness over the iteration technique discussed by Bourret[7,8] in his earlier works. In addition, all the results quoted by Karmeshu and Bansal for the first moments can be obtained directly from Sec. 8 of the paper by Williams.[5]

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[8] R. C. BOURRET, *Can. J. Phys.*, **43**, 619 (1965).