## Letters to the Editor

## A Defense of Benoist's Corrected Diffusion Coefficient

Various approaches to the problem of homogenization of heterogeneous lattice cells by Benoist,<sup>1</sup> Deniz,<sup>2</sup> Gelbard,<sup>3</sup> and Larsen<sup>4</sup> have appeared in the literature over the years that have led to a variety of definitions of lattice cell diffusion coefficient. These diffusion coefficients were derived using different techniques, and it was with the purpose of unifying these derivations that the present author<sup>5</sup> applied what is now generally known as the buckling method to a uniform array of heterogeneous lattice cells. In Ref. 5, it is shown how the diffusion coefficients of Refs. 1 through 4 arise very naturally from a single equation, that being the neutron balance equation for a single lattice cell. This equation is derived using an assumed form  $\exp(iBx)$  for the macroscopic variation in fluxes between cells where B is the geometric buckling. This assumed form contains the assumption that we are considering cells in an asymptotic region, i.e., far from any cells of a different type or from the core edge. Thus, this neutron balance equation [Eq. (5) of Ref. 5] is valid for all the cells in the asymptotic region in that it gives (correct to order  $B^2$ ) the relative cell reaction rates and eigenvalue. This eigenvalue is the same as that of the original transport equation from which Eq. (1)was derived, to order  $B^2$ . All expansions in Ref. 5 are curtailed at order  $B^2$ , and no claim is made to reproduce the transport equation eigenvalue exactly as it seems to have been understood by Chiang and Dorning<sup>6</sup> and Rao and Lee,<sup>7</sup> but only to order  $B^2$ .

Complete details of how this neutron balance equation can be manipulated to cast it into the different forms that explicitly contain the various diffusion coefficients<sup>1-4</sup> are contained in Ref. 5, so it will suffice here to write it as

$$(DB^2 + \overline{\Sigma}_a)\overline{\phi}_0 = \frac{\nu\overline{\Sigma}_f}{k_{eff}}\overline{\phi}_0 \quad , \tag{1}$$

where  $\overline{\Sigma}_a$  and  $\nu \overline{\Sigma}_f$  are the smeared cross sections, which generally depend on  $B^2$  since they are smeared with the buckled lattice flux. The corresponding cross sections independent of B

are being smeared using the infinite lattice flux only for the Deniz-Gelbard and Larsen definitions of D.

An alternative approach to homogenization is the asymptotic method.<sup>4,8,9</sup> The method has been used to produce an actual differential diffusion equation for the macroscopic flux shape in the asymptotic region of the lattice with Deniz-Gelbard/Larsen diffusion coefficients. That is, we get an equation of the form

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$$\frac{-Dd^2A}{dx^2} + \overline{\Sigma}_a A = \frac{\nu \overline{\Sigma}_f A}{k_{eff}} \quad , \tag{2}$$

where A(x) represents the macroscopic variation of the flux. Taking  $A \equiv \exp(iBx)$  reproduces Eq. (1). Indeed, Ref. 8 establishes the general result that the buckling method generates the dispersion law for the asymptotic diffusion equation and that therefore the two methods are equivalent.

This very brief resumé of the buckling and asymptotic methods is necessary to set the scene for the main purpose of this Letter, which is to remove some confusion that obviously still exists as to the relative standing and merits of the different diffusion coefficients as expounded in the recent paper of Rao and Lee.7 First, Rao and Lee7 state that Larsen and Hughes<sup>8</sup> argue that the Benoist diffusion coefficients (corrected or uncorrected) are not suitable for use in diffusion theory calculations. This is quite untrue. Reference 8 merely points out that the methods by which Benoist diffusion coefficients were originally derived differs substantially from the buckling and asymptotic methods. Hughes<sup>5</sup> clearly explains the way that either of these diffusion coefficients, when used with the corresponding smeared cross sections, can be used to give the neutron balance equation with the correct (to order  $B^2$ ) lattice eigenvalue. Rao and Lee<sup>7</sup> themselves show how the asymptotic method can be used to produce one equation of the form (2) for the Benoist uncorrected diffusion coefficient  $D^{BU}$  [Eq. (33) of Ref. 7], which is entirely equivalent to Eq. (8) of Ref. 5.

As for the Benoist corrected diffusion coefficient  $(D^{BC})$ , Rao and Lee<sup>7</sup> derive the corresponding neutron balance equation [Eq. (41) of Ref. 7], which is equivalent to Eq. (10) of Ref. 5, explicitly using an expansion of the cell flux in terms of the macroscopic variation across the whole lattice. This, they argue, is an inconsistency, which gives rise to the wellknown double valuedness of  $D^{BC}$  (depending on where the center of the lattice cell is defined),<sup>3,5</sup> and makes it "clear that  $D^{BC}$  is not a candidate for diffusion theory calculations." In answer to the first point, Ref. 5 shows quite clearly that the macroscopic variation is included in the derivation of *all* the

<sup>&</sup>lt;sup>1</sup>P. BENOIST, "Theorie du Coefficient du Diffusion des Neutrons dans un Reseau Comportant des Cavites," CEA-R-2278, Centre d'Etudes Nucléaires de Saclay (1964).

<sup>&</sup>lt;sup>2</sup>V. DENIZ, Nucl. Sci. Eng., 28, 397 (1967).

<sup>&</sup>lt;sup>3</sup>E. M. GELBARD, Nucl. Sci. Eng., 54, 327 (1974).

<sup>&</sup>lt;sup>4</sup>E. W. LARSEN, Nucl. Sci. Eng., **60**, 357 (1976).

<sup>&</sup>lt;sup>5</sup>R. P. HUGHES, Nucl. Sci. Eng., 67, 85 (1978).

<sup>&</sup>lt;sup>6</sup>REN-TAI CHIANG and J. J. DORNING, *Trans. Am. Nucl. Soc.*, **33**, 779 (1979).

<sup>&</sup>lt;sup>7</sup>J. V. MÜRALIDHAR RAO and S. M. LEE, *Nucl. Sci. Eng.*, **82**, 71 (1982).

<sup>&</sup>lt;sup>8</sup>E. W. LARSEN and R. P. HUGHES, *Nucl. Sci. Eng.*, **67**, 85 (1978). <sup>9</sup>E. W. LARSEN, *Ann. Nucl. Energy*, **7**, 249 (1980).

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different diffusion coefficients (a unified derivation), and in this sense all the diffusion coefficients are on the same footing. There is no inconsistency in the derivation of  $D^{BC}$ . Further, the fact that it is double valued, depending on the cell definition, should be of no concern. Indeed, since  $D^{BC}$  gives the actual (correct to order  $B^2$ ) cell leakage rate, we should be surprised if its value did not depend on the definition of the cell. Although  $D^{BC}$  is "space dependent" in this sense, it does not mean that we have not homogenized the cell, but merely that the homogenization is different for different definitions of the cell. This does not rule out  $D^{BC}$  as a candidate for diffusion theory calculations but does require us to state which region or cell whose reaction rates we want to preserve. It seems to be necessary to restate here that only  $D^{BC}$  (and the corresponding cross sections) will preserve the cell reaction rates. Rao and  $\text{Lee}^7$  favor the use of  $D^{BU}$  because the prescription is single valued and preserves the cell reaction rates in the least-squares sense described by Köhler.<sup>5,10</sup> It is by no means obvious that this has any advantage over the other diffusion coefficient definitions.

In conclusion then, we must say that there is no basis at all for the rejection by Rao and Lee<sup>7</sup> of Benoist's corrected diffusion coefficient in favor of Benoist's uncorrected diffusion coefficient (together with the corresponding smeared cross sections). Indeed, in order to reproduce the correct (to order  $B^2$ ) reaction rates within a cell deep in a lattice array, we must use the Benoist corrected prescription for that cell as already stated.<sup>5</sup>

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<sup>10</sup>P. KÖHLER, Nucl. Sci. Eng., 57, 333 (1975).

## Response to "A Defense of Benoist's Corrected Diffusion Coefficient"

The arguments of Hughes<sup>1</sup> in favor of the Benoist corrected diffusion coefficient have been analyzed, and we stand by what we concluded in our earlier work<sup>2</sup> regarding this coefficient. We further clarify our stand in the following comments, which have been made with reference to Hughes's arguments.<sup>1</sup>

1. Hughes has stated,<sup>1</sup> "This eigenvalue is the same as that of the original transport equation from which Eq. (1) was derived, to order  $B^2$ . All expansions in Ref. 5 [our Ref. 3] are curtailed at order  $B^2$ , and no claim is made to reproduce the transport equation eigenvalue exactly as it seems to have been understood by Chiang and Dorning and Rao and Lee, but only to order  $B^2$ ."

We point out that in Sec. II of Ref. 3, Hughes has stated,

<sup>3</sup>R. P. HUGHES, Nucl. Sci. Eng., 67, 85 (1978).

"When used with the correctly smeared cell cross sections, the resulting diffusion equation will have the same eigenvalue  $k_{eff}^{-11}$  as the original transport equation, Eq. (1)." Perhaps he implied here that the eigenvalues are the same but only to order  $B^2$ . However, our contention<sup>2</sup> was more fundamental in that in all the homogenization methods discussed in Refs. 2 and 3, only the asymptotic approximation to the transport eigenvalue is preserved to order  $B^2$ . To us, it is still not evident that preserving to the second order the asymptotic approximation  $k_{asymptotic}$  of the transport eigenvalue  $k_{eff}$  implies preserving to the second order the transport eigenvalue itself, irrespective of the outer boundary conditions. In other words, do the coefficients of the following series,

$$k_{asymptotic}^{-1} = k_{\infty}^{-1} (1 + \epsilon k_1 + \epsilon^2 k_2 + \dots)$$
  
$$k_{eff}^{-1} = k_{\infty}^{-1} (1 + \epsilon k_1' + \epsilon^2 k_2' + \dots)$$

match irrespective of the outer boundary conditions?

2. Hughes has written<sup>1</sup> "Rao and Lee state that Larsen and Hughes argue that the Benoist diffusion coefficients are not suitable for use in diffusion theory calculations. This is quite untrue."

Our statement was made with reference to the following remarks made by Larsen and Hughes in Ref. 4.

- a. "However, a careful look at Benoist's analysis shows that his method and the class of physical problems to which it applies differ considerably from the methods and problems considered above."
- b. "The above derivation shows that Benoist's method is not one in which a homogenized diffusion equation is derived directly from a perturbation expansion of the neutron transport equation about an infinite critical medium, as in the asymptotic and buckling methods. Rather, a diffusion equation is hypothesized, and physical arguments are used to determine its coefficients. However, Gelbard has shown that the numerical value of these coefficients differs, depending on how one chooses to define a cell. In addition, no proof has been published that relates the solution of Benoist's diffusion equation to the exact solution of the transport equation."
- c. "In sum, the Benoist (and related) methods do not clearly apply to near-critical systems, and their methodology, although based on a perturbation expansion, differs substantially from that of the buckling and asymptotic methods."

If the above remarks do not imply that the Benoist diffusion coefficients are not suitable for diffusion theory calculations approximating the original transport problem, and are not on the same footing as the Larsen or the Deniz-Gelbard diffusion coefficients, then we do not understand the need for the above referred comments in a lengthy discussion on Benoist's method under Sec. VII.F of Ref. 4. It was these remarks that led us to attempt to derive the Benoist diffusion equation using the asymptotic method, and we found this to be possible<sup>2</sup> for the case of the Benoist uncorrected diffusion coefficient  $D^{BU}$  but not for the Benoist corrected diffusion coefficient  $D^{BC}$ .

3. Hughes has further stated,<sup>1</sup> "Rao and Lee themselves show how the asymptotic method can be used to produce one

<sup>&</sup>lt;sup>1</sup>R. P. HUGHES, Nucl. Sci. Eng., 83, 408 (1983).

<sup>&</sup>lt;sup>2</sup>J. V. MURALIDHAR RAO and S. M. LEE, *Nucl. Sci. Eng.*, **82**, 71 (1982).

<sup>&</sup>lt;sup>4</sup>E. W. LARSEN and R. P. HUGHES, Nucl. Sci., Eng., 73, 274 (1980).