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Letters to the Editors

Calculation of Disadvantage Factors for Small Cells

The calculation of the disadvantage factor for small reactor cells has been discussed by several authors[1,2,4,5,7,9] who did not come to the same conclusion. The point that caused confusion is the behavior of the disadvantage factor in case the moderator's thickness in mean free paths goes to zero: does it decrease monotonically with decreasing thickness of the moderator or not? The aim of the present paper is to show that the disadvantage factor does not decrease monotonically with decreasing moderator thickness (keeping size and composition of the fuel rod constant), but has a logarithmic singularity in its first derivative that causes it to increase from a certain point. (For slab lattices the disadvantage factor itself has already this logarithmic singularity).

It was shown by Newmarch[1] that serious errors may arise from the Wigner-Seitz (WS) cylindrical-cell approximation combined with a reflective outer boundary when transport theory is used for calculations on small lattice cells. This was confirmed by Thie[2] who studied six, arbitrarily chosen, tightly packed square lattices with a low-density moderator (H_2O). He came to the conclusion that the use of P_3, S_4, or S_8 together with the WS approximation and the reflective-boundary condition may lead to gross overestimates of the disadvantage factor if the thickness of the moderator in mean free paths is less than 0.5. From all the methods he investigated, Amouyal's[3] approximation gave best agreement with the Monte Carlo (MC) calculations which he performed for three of the six lattices in the actual xy geometry. To improve the transport calculations and still retain the WS model, Clendenin[4] proposed to replace the reflective boundary conditions in the P_3 approximation by the following requirements: zero current and zero flux gradient at the cell boundary together with a third requirement whose choice was found to have little influence on the results. Honeck[5], on the other hand, suggested an isotropic flux return, which is accomplished by adding an optically thick outer region of pure scatterer to the WS cell. Recently, Pomraning and Clark[6] developed an asymptotic diffusion theory where the boundary conditions between the media (e.g. fuel and moderator) are: continuous current between the media and a specified discontinuity in the scalar flux. With this theory Pomraning[7] calculated the disadvantage factors for four of the six Thie lattices, and, since he found reasonable agreement with Clendenin's theory but not with the MC values, he suspected the validity of the latter ones for reference purposes. The values of the disadvantage factors of the Thie lattices according to the different theories are given in Table II, and some of them are plotted in Figure 1 as a function of the moderator thickness in mean free paths. The characteristics of these lattices are given in Table I. The discontinuity between the first two lattices and the other four indicates that the disadvantage factor is not solely a function of the moderator's optical thickness.

To make sure about the validity of the MC results, we calculated the disadvantage factors by

TABLE I

Lattice Characteristics [a]

Lattice No.	Pitch (cm)	W/U	Moderator cross sections (cm^{-1})	
			Σ_{am}	$\Sigma_{tm} - \Sigma_{am}$
1	1.524	4.09	0.0088	1.053
2	1.524	4.09	0.00587	0.702
3	1.143	1.87	0.0088	1.053
4	1.143	1.87	0.00587	0.702
5	1.143	1.87	0.00293	0.351
6	1.143	1.87	0.000587	0.0702

[a] Fuel radius is 0.381 cm, $\Sigma_{af} = 0.387\ cm^{-1}$, $\Sigma_{tf} = 0.780\ cm^{-1}$

[1] D. A. NEWMARCH, "Errors Due to the Cylindrical Cell Approximation in Lattice Calculations," AEEW-R34(1960).
[2] J. A. THIE, *Nucl. Sci. Eng.* **9**, 286 (1961).
[3] A. AMOUYAL *et al.*, *J. Nucl. Energy* **6**, 79 (1957).
[4] W. W. CLENDENIN, *Nucl. Sci. Eng.* **14**, 103 (1962).
[5] H. C. HONECK, *Trans. Am. Nucl. Soc.* **5**, 350 (1962).
[6] G. C. POMRANING and M. CLARK, Jr., *Nucl. Sci. Eng.* **17**, 227 (1963).
[7] G. C. POMRANING, *Nucl. Sci. Eng.* **17**, 311 (1963).
[8] N. CORNGOLD, *J. Nucl. Energy* **4**, 293 (1957).
[9] Y. FUKAI, *Nucl. Sci. Eng.* **9**, 370 (1961).

TABLE II

Disadvantage Factors By Various Methods

Lattice No.	1	2	3	4	5	6
P_1	1.051	1.039	1.036	1.030	1.023	1.018
Pomraning	1.105	1.093	1.090	1.084	-	-
P_3 (reflecting)	1.165	1.188	1.207	1.265	1.440	-
P_3 (Clendenin)	1.099	1.077	1.075	1.059	-	-
Amouyal	1.170	1.169	1.155	1.159	1.169	1.186
Monte Carlo	1.135±.031	-	-	1.137±.012	-	1.161±.010
This work (Eq. 1)	1.198	1.178	1.161	1.146	1.143	1.169
K-7 TRANSPO (refl.)	1.235	1.290	1.281	1.371	1.672	-
K-7 TRANSPO (white)	1.157	1.149	1.141	1.138	1.136	1.149

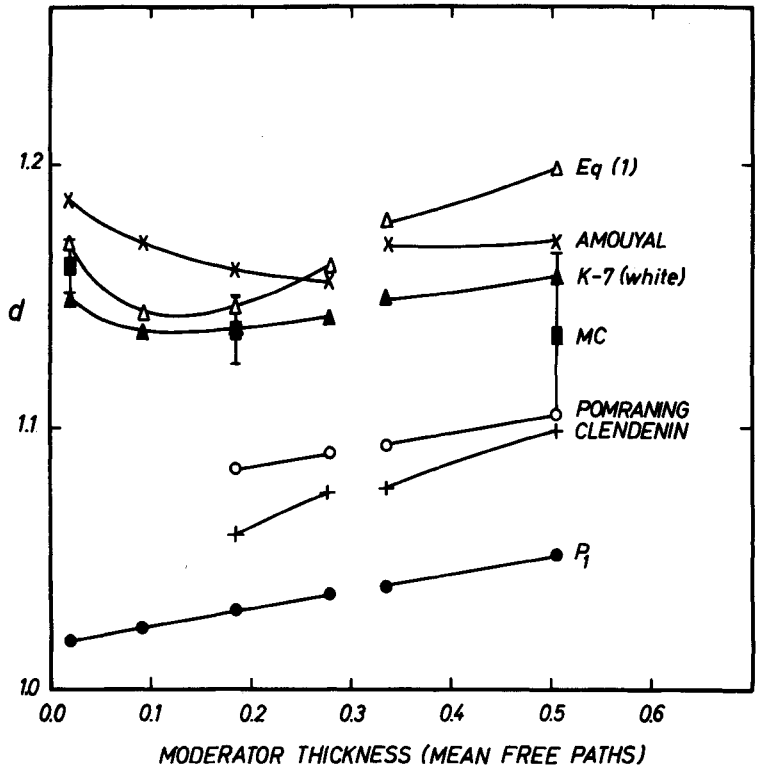

Fig. 1. Disadvantage factors by various methods.

using a collision-probability technique[1] which takes into account the squareness of the cell. The only assumption that enters, besides that of isotropic scattering, is that integrals of the type

$$\int P(\vec{r} \rightarrow \text{fuel})\,\Phi(\vec{r})\,d\vec{r}$$

may be replaced by

$$\int P(\vec{r} \rightarrow \text{fuel})\,d\vec{r} \cdot \int \Phi(\vec{r})\,d\vec{r} / \int d\vec{r}$$

where $P(\vec{r} \rightarrow \text{fuel})$ is the probability that neutrons born isotropically at r will make their first collision in the fuel, and where the integration area is either fuel or moderator. This assumption is valid for lattices where the moderator is very thin in mean free paths, because $P(\vec{r} \rightarrow \text{fuel})$ will then be close to unity for all $\vec{r}$ (keeping size and composition of the fuel rod constant). For the plane case this approximation was formulated by Corngold[8] and it was investigated by Fukai[9] who showed that, for closely packed lattices, this is a very good approximation indeed. The resulting expression for the disadvantage factor is

$$d = 1 - \frac{\Sigma_{af}}{\Sigma_{tf}} + \frac{V_f \Sigma_{af}}{V_m \Sigma_{tm}} \left(\frac{1 - P}{P} \right), \qquad (1)$$

where P is the average probability that neutrons born isotropically in the moderator will suffer

their first collision in the fuel, V means volume, Σ means macroscopic cross section, and the subscripts denote fuel, moderator, absorption and total. It will be seen that d does not depend on the ratio Σ_{am}/Σ_{tm}. The probability P was calculated following an approximate method given by Brissenden[10] which takes into account the squareness of the cell, thereby avoiding errors due to the use of cylindrical-cell approximation together with reflective-boundary conditions. The disadvantage factors obtained from (1) give good agreement with the MC values for the Thie lattices. It will be mentioned below that Brissenden's method leads to overestimates of the disadvantage factor when $V_m \Sigma_{tm} \to 0$, keeping size and composition of the fuel rod constant; this tendency can be noticed already in Figure 1.

We also calculated the disadvantage factors for the Thie lattices with K-7 TRANSPO[11], a one-velocity transport code that solves the integral transport equation in a WS cell with the aid of a THERMOS - type of transport kernel, with either a reflective or a white boundary. In case of the white-boundary condition, agreement with the MC values is good. This indicates that the WS approximation seems also to be valid for tightly packed lattices, provided one uses Honeck's[5] white-boundary condition (isotropic flux return).

Pomraning's[7] assumption, that the disadvantage factor should decrease with decreasing $V_m \Sigma_{tm}$ is not true, as the following argument will show. Write the disadvantage factor as

$$d = \frac{\bar{\Phi}_m / \Phi(r_0)}{\bar{\Phi}_f / \Phi(r_0)} = Q(1+q) \qquad (2)$$

where r_0 is the radius of the fuel rod,
Q is the self shielding effect of the fuel, i.e. $\Phi(r_0)/\bar{\Phi}_f$,
q is $\bar{\Phi}_m / \Phi(r_0) - 1$,
and a bar denotes spatial average.

In P_1 and Amouyal's theory, the inner block effect Q is independent of the properties of the moderator (our K-7 TRANSPO calculations show a very weak increase of Q with decreasing Σ_{tm}). If $\bar{\Phi}_m \to \Phi(r_0)$ in the limit of zero total cross section in the moderator, and if Q does not increase too rapidly, the disadvantage factor should indeed decrease all the way and reach the limiting value Q. This is automatically fulfilled by all differential methods that require a zero flux gradient at the cell boundary. As a matter of fact, Clendenin's and Pomraning's results do show this tendency.

However, when integral methods are used, such a behavior is no longer evident—in spite of the zero flux gradient on the cell boundary required by symmetry considerations—because of the logarithmic singularity in the transport kernel (or in its first derivative) for a number of idealized geometries. In the limit when $V_m \Sigma_{tm} \to 0$, the behavior of the disadvantage factor is determined by $(1 - P)/V_m \Sigma_{tm}$. Since $1 - P \geq 1 - P_0$, it is sufficient to investigate the behaviour of the function

$$x(\bar{\ell}\Sigma_{tm}) = (1 - P_0)/\bar{\ell}\Sigma_{tm} \qquad (3)$$

where $1 - P_0$ is the first collision probability in the moderator region assuming a black fuel rod, and is given in terms of the chord distribution function $f(\ell)$ by the following expression[12]

$$1 - P_0 = 1 - \frac{1}{\bar{\ell}\Sigma_{tm}} \int (1 - e^{-\ell \Sigma_{tm}}) f(\ell)\, d\ell \qquad (4)$$

and $\bar{\ell}$ is the average chord length, which is proportional to V_m. From (4) it follows that $x(0)$ is proportional to $\bar{\ell}^2/\bar{\ell}^2$ and that x' is for small arguments proportional to $-\bar{\ell}^3/\bar{\ell}^3$. The existence of $x(0)$ and $x'(0)$ depends on the asymptotic behavior of the chord-distribution function for large chords. In the plane case the distribution function behaves as $1/\ell^3$ so that neither $\bar{\ell}^2$ nor $\bar{\ell}^3$ are finite and x has a logarithmic singularity at zero, which implies that the corresponding disadvantage factor has the same behavior. There is little known about $f(\ell)$ for other geometrical configurations of the moderator, it can however be shown that, for square and hexagonal lattices, $f(\ell)$ behaves as $1/\ell^4$ which leads to a finite $x(0)$, but a negative logarithmically singular first derivative. This causes an uplift of d to a finite value in the limit when $\Sigma_{tm}\bar{\ell} \to 0$, which is in agreement with the MC results (see Figure 1).

In the WS approximation with reflective-boundary condition, the chord-distribution function for the moderator escape probability does not go to zero when $\ell \to \infty$ (there is a finite number of chords with infinite length, as was pointed out by Newmarch[1]). For white-boundary conditions the chord-distribution function is expected to behave as $1/\ell^4$, leading to a logarithmic singularity in x'. In K-7 TRANSPO the transport kernel for a shell behaves in the limit when $\bar{\ell}\Sigma_{tm} \to 0$ as $Ki_1(\bar{\ell}\Sigma_{tm})$ which also has a logarithmic singularity in its first derivative. Thus K-7 TRANSPO with a white boundary is expected to give results with the same behavior as the MC values for square or hexagonal lattices (see Figure 1). It is interesting to note that the use of Brissenden's[10] formula for P in (1) leads already to a logarithmical singularity in x, which is due to assumptions he made in the derivation of his formula.

[10] R. J. BRISSENDEN, "A Formula for the Escape Probability of a Rod in a Uniform Lattice," AEEW-R 282 (1963).

[11] R. J. J. STAMM'LER, to be published as a Kjeller Report.

[12] K. M. CASE *et al.*, "Introduction to the Theory of Neutron Diffusion," Los Alamos Scientific Laboratory (1963).

In conclusion we may say:

a) Thie's MC values are good, and the disadvantage factor does not decrease monotonically with decreasing moderator density.
b) Integral transport methods are to be preferred over differential methods when calculating disadvantage factors for tightly packed lattices.
c) The WS approximation with white-boundary conditions[5,11] seems to be a good approximation for use with integral methods.

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On the Variational Method Applied to the Monoenergetic Boltzmann Equation

In two papers[1] published in this journal, Pomraning and Clark have discussed the separation of the non-self-adjointness from the monoenergetic Boltzmann equation. The authors, however, have been unable to find the proper boundary terms which, added to the functional, would yield the boundary conditions corresponding to the adjoint Boltzmann equation. It is proposed to use the alternate set of boundary conditions for which the boundary terms in the functional are relatively simple to obtain.

Let us take the Boltzmann equation in the following form:

$$\mu\frac{\partial\psi}{\partial z}+\sigma\psi(z,\mu)=c\sigma\sum_{n=0}^{\infty}\frac{2n+1}{2}f_nP_n(\mu)\int_{-1}^{+1}d\mu' P_n(\mu')\psi(z,\mu'). \tag{1}$$

The notation is identical with that used in Reference 1.

[1]G. C. POMRANING and M. CLARK, Jr., "The Variational Method Applied to the Monoenergetic Boltzmann Equation." Part I and II. *Nucl. Sci. Eng.*, **16**, 147-164 (1963).

The angular distribution $\psi(z,\mu)$ can be split into the even and odd part with respect to μ:

$$\psi(z,\mu)=\psi^+(z,\mu)+\psi^-(z,\mu). \tag{2}$$

Accordingly the even and odd parts of Equation (1) are satisfied separately:

$$\mu\frac{\partial\psi^-}{\partial z}+\sigma\psi^+(z,\mu)-c\sigma\sum_{\text{even}}(2n+1)f_nP_n(\mu)\int_0^1 d\mu' P_n(\mu')\psi^+(z,\mu')=0 \tag{3}$$

$$\mu\frac{\partial\psi^+}{\partial z}+\sigma\psi^-(z,\mu)-c\sigma\sum_{\text{odd}}(2n+1)f_nP_n(\mu)\int_0^1 d\mu' P_n(\mu')\psi^-(z,\mu')=0. \tag{4}$$

Both equations are valid for μ belonging to the interval (0,1). By eliminating $\psi^-(z,\mu)$ or $\psi^+(z,\mu)$ one can get an equation for $\psi^+(z,\mu)$ or $\psi^-(z,\mu)$, respectively. For example, solving Equation (4) for $\psi^-(z,\mu)$ we get:

$$\psi^-(z,\mu)=-\frac{1}{\sigma}\mu\frac{\partial\psi^+}{\partial z}-\frac{1}{\sigma}\sum_{\text{odd}}(2n+1)\frac{cf_n}{1-cf_n}P_n(\mu)\int_0^1 d\mu' P_n(\mu')\mu'\frac{\partial\psi^+(z,\mu')}{\partial z} \tag{5}$$

and then the equation for $\psi^+(z,\mu)$ is:

$$\mu^2\frac{\partial^2\psi^+}{\partial z^2}-\sigma^2\psi^+(z,\mu)+c\sigma^2\sum_{\text{even}}(2n+1)f_nP_n(\mu)\int_0^1 d\mu' P_n(\mu')\psi^+(z,\mu')+\sum_{\text{odd}}(2n+1)\frac{cf_n}{1-cf_n}\mu P_n(\mu)\int_0^1 d\mu' P_n(\mu')\mu'\frac{\partial^2\psi^+(z,\mu)}{\partial z^2}=0. \tag{6}$$

It is the self-adjoint form of the Boltzmann equation.

To find the proper boundary conditions for Equation (6) let us consider the albedo problem for a slab. We have

$$\psi(a,\mu)=A^+(\mu)\qquad(0<\mu\le 1) \tag{7a}$$

$$\psi(b,\mu)=A^-(\mu)\qquad(-1\le\mu<0). \tag{7b}$$

Taking into account Equation (5) we can easily find boundary conditions for Equation (6).

These are