Letters to the Editor

Comment on Approximate Escape Probability Calculations

A series of recent papers[1-4] was devoted to approximate calculations of first-flight escape probabilities from convex simply connected homogeneous bodies. The increasing number of these publications illustrates how long a problem can survive its solution. To support this rather annoying statement, I would note the following: The principles and methods of calculation of escape probabilities are detailed in the early work by Case et al.[5] along with extensive tables of calculated values for the most important special geometries. There remained two possible ways of progress in the field: either give a theoretical foundation of a *reliable* approximate method for the calculation of escape probabilities for a wider class of bodies, or present simple approximate formulas for the otherwise tabulated special cases. In Ref. 1, a theoretically elaborated general method is presented, however, there is no indication of the precision of the approximation in general. The merits of the method are illustrated through application to the most common special cases of sphere, cylinder, and slab regions. Reference 2 refines to some extent the method in Ref. 1 for cylinder and slab regions. Raghav[3] proposes polynomial approximations for all the three common geometries with five (or nine) fitted parameters. The accuracy of this approximation will undoubtedly satisfy the claims of practitioners. Thus, I feel, the second method of progress came to an end and no other effort is really justifiable.

In spite of that in a recent paper Kwiat[4] proposes a new approximate method for the calculation of the same quantities. I say the same quantities since there is no hint of any kind on its applicability (and still less on its accuracy) for general geometries. Although it has the advantage over the method by Raghav[3] that it assumes one parameter to be fitted only, this advantage is rather dubious since for offhand calculations the use of the tables in Ref. 5 (with possible linear interpolation) is more comfortable than the proposed calculation, while in computer programs it hardly makes any difference whether one or nine parameters are to be pre-dated. On the other hand, Kwiat assumes the calculation of an exponential that is much more time consuming than the evaluation of a Horner scheme.

Nevertheless, a new approach to a problem (even if it is solved) may open unexpected prospectives for further investigation of more general cases. And here comes my main objection to the method in Ref. 4. The idea behind the method proposed there is the generalization of the formula

$$P_c(x) = \left[1 + x - \frac{cx}{cx+1}\right]^{-1} ,$$

by Rothenstein[6] to an explicit x-dependent $c(x)$ function as

$$c(x) = c_\infty + (c_0 - c_\infty)\exp(-x/\alpha)$$

in such a way that $c(x)$ preserves the limiting values for $x \to 0$ and $x \to \infty$ as follows from exact calculations. This condition, however, seems unnecessary since

$$\lim_{x\to 0} P_c(x) = 1 ,$$

provided $c(x)$ is such that

$$\lim_{x\to 0} xc(x) = 0 ,$$

otherwise arbitrary, while

$$\lim_{x\to\infty} P_c(x) = 0$$

for any positive $c(x)$. Furthermore, by choosing a $d(x)$ instead of $c(x)$, being bounded at small x, for the error relative to P_c we have

$$(P_c - P_d)/P_c = [c(x) - d(x)]x + O(x^2) \quad \text{for} \quad x \ll 1 ,$$

and therefore P_d may be a still better approximation than P_c in the white region as demonstrated below. For large values of x,

$$(P_c - P_d)/P_c = [1/c(x) - 1/d(x)]x^{-2} + O(x^{-3}) \quad \text{for} \quad x \gg 1 ,$$

and arbitrary nonvanishing $d(x)$ may result in an excellent approximation for the black region.

To illustrate the above assertion, I have tried the simplest linear function

$$d(x) = \alpha + \beta x$$

for cylindrical regions and a rough guess of

$$\alpha = 0.35 , \quad \beta = -\frac{1}{8}$$

resulted in the errors given in Table I. Note that this function does not necessitate the computation of exponentials. The trial function may of course still be refined [for instance by putting

$$\alpha = 0.6 , \quad \beta = 0.07 \quad \text{for} \quad x > 4$$

to yield errors <0.1% everywhere in $x \in (0.10)$] but it does not really matter for the reasons above.

A final remark is to be made concerning the usefulness of some approximations. Most of the references cited above give

[1]Y.-A. CHAO and A. S. MARTINEZ, *Nucl. Sci. Eng.*, **66**, 254 (1978).

[2]I. LUX and I. VIDOVSZKY, *Nucl. Sci. Eng.*, **69**, 442 (1979).

[3]HEM PRABHA RAGHAV, *Nucl. Sci. Eng.*, **73**, 302 (1980).

[4]D. KWIAT, *Nucl. Sci. Eng.*, **76**, 255 (1980).

[5]K. M. CASE, F. de HOFFMANN, and G. PLACZEK, "Introduction to the Theory of Neutron Diffusion," Vol. 1, Los Alamos Scientific Laboratory (1953).

[6]W. ROTHENSTEIN, *Nucl. Sci. Eng.*, **7**, 162 (1960).

TABLE I

Relative Errors in Approximate Escape Probabilities for Cylinder (%)

x	Reference 4	Present Work
0.0	0.00	0.00
0.2	0.16	0.03
0.4	0.13	0.08
0.6	−0.01	0.08
0.8	−0.19	0.05
1.0	−0.32	0.00
2.0	−0.33	−0.02
3.0	−0.04	−0.02
4.0	0.13	−0.03
5.0	0.12	−0.11
6.0	0.14	−0.12
7.0	0.07	−0.18
8.0	0.09	−0.15
9.0	0.00	−0.23
10.0	0.00	−0.22

approximate escape probabilities for spheres. The determination of these approximate values is seldom simpler essentially than the evaluation of the exact expression[5]:

$$P_{\text{sphere}(x)} = \frac{3}{8x^3}\,[2x^2 - 1 + (1 + 2x)e^{-2x}] \;;$$

where

$x = \Sigma R$

R = radius.

Iván Lux

Central Research Institute for Physics
1525 Budapest
P.O. Box 49
Hungary

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Responses to "Comment on Approximate Escape Probability Calculations"

My original motivation is not simply to play numerical games with approximations to well-known solutions, but to develop better schemes of homogenization. The point is that collision probability is very useful in formulating problems with a heterogeneous medium; however, such formulations, although very nice physics-wise, often turn out to be difficult to compute. The collision probability is, of course, introduced to represent neutron transport between regions of different compositions. A major step forward in rendering the formulations practical would be to approximate the escape probabilities such that simple schemes of homogenizing these regions could result. A well-known classical example is the so-called equivalence theorem. To this end, I would like to emphasize very much the importance of looking beyond the numerical accuracy of an approximation to ponder if the approximation has a suitable functional form for homogenization as well. To be specific and elaborate, I would like to bring the attention of my colleagues interested in this problem to Ref. 1. Some preliminary remarks relevant to this work are also given in Refs. 2 and 3.

It was of course also part of my motivation to introduce a general framework of accurately approximating the collision integral for a general geometry. I would like to mention that applications of the method[3] to Dancoff corrections and (three-region) cylindrical shells[4] have been successfully carried out. As for the Kwiat[5] approximation on which Lux[6] commented, it is misleading to say that there is only one parameter to fit, because the other two parameters, although determinable analytically through limiting behaviors, are also geometry dependent and still need to be calculated for different cases.

Finally, I would like to remark that Lux's concern about the increasing number of publications on such an old problem is perhaps a reflection on how little reactor theory is being done nowadays. However, I believe this is not because there is very little interesting reactor physics left, but the misconception that with large computation codes we no longer need physical analysis.

Yung-An Chao

Carnegie-Mellon University
Nuclear Science and Engineering Division
Pittsburgh, Pennsylvania 15213

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[1]Y.-A. CHAO and A. S. MARTINEZ, "An Accurate Background Cross-Section Method for Cell Homogenization," submitted to *Nucl. Sci. Eng.*

[2]Y.-A. CHAO, *Nucl. Sci. Eng.*, **73**, 304 (1980).

[3]Y.-A. CHAO, M. B. YARBROUGH, and A. S. MARTINEZ, *Nucl. Sci. Eng.*, **78**, 89 (1981).

[4]K. Q. RUAN and R. J. CHEN, "An Approximate Calculation of the Neutron Escape Probabilities for a Cylindrical Shell," *2nd Chinese Nuclear Society National Conf. Reactor Physics*, Suzhon, The People's Republic of China, June 1980, Private Communication.

[5]D. KWIAT, *Nucl. Sci. Eng.*, **76**, 255 (1980).

[6]I. LUX, *Nucl. Sci. Eng.*, **78**, 191 (1981).

No doubt, the use of approximations for practitioners is important. All well-known tables and approximations[1-14] only indicate that the subject is interesting as well as attractive. The problem is easy to formulate and to understand; however, as yet it has no general solution. Two major problems are faced in these calculations: (a) finding the exact expression

[1]K. M. CASE, F. de HOFFMANN, and G. PLACZEK, "Introduction to the Theory of Neutron Diffusion," Vol. 1, Los Alamos Scientific Laboratory (1953).

[2]E. P. WIGNER et al., *J. Appl. Phys.*, **26**, 260 (1955).

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[4]A. SAVER, *Nucl. Sci. Eng.*, **16**, 329 (1963).

[5]R. BONALUMI, *Energ. Nucl.*, **12**, 16 (1965).

[6]C. N. KELBER, *Nucl. Sci. Eng.*, **22**, 244 (1965).

[7]M. S. MILGRAM, *J. Math. Phys.*, **18**, 2456 (1977).

[8]Y.-A. CHAO and A. S. MARTINEZ, *Nucl. Sci. Eng.*, **66**, 254 (1978).

[9]Y.-A. CHAO, *Nucl. Sci. Eng.*, **69**, 443 (1979).

[10]M. S. MILGRAM, *J. Comp. Phys.*, **33**, 417 (1979).

[11]I. LUX and I. VIDOVSZKY, *Nucl. Sci. Eng.*, **69**, 442 (1979).

[12]H. P. RAGHAV, *Nucl. Sci. Eng.*, **73**, 302 (1980).

[13]D. KWIAT, *Nucl. Sci. Eng.*, **76**, 255 (1980).

[14]I. LUX, *Nucl. Sci. Eng.*, **78**, 191 (1981).