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 expression⁵:

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

where

 $x = \Sigma R$ R = radius.

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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 method³ to Dancoff corrections and (threeregion) cylindrical shells⁴ have been successfully carried out. As for the Kwiat⁵ approximation on which Lux⁶ 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.

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

²Y. A. CHAO, Nucl. Sci. Eng., 73, 304 (1980).

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

⁴K. 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.

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

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

No doubt, the use of approximations for practitioners is important. All well-known tables and approximations¹⁻¹⁴ 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

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

³W. ROTHENSTEIN, Nucl. Sci. Eng., 7, 162 (1960).

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

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

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

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

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

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

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

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

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

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

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

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

of the chord distribution function f(l), and (b) solving the integral

$$\frac{1}{\Sigma \overline{l}} \int f(l) \left[1 - \exp(-\Sigma l)\right] dl$$

For few simple geometries we know how to find f(l). We do not know how to solve the integral analytically. Approximations are then done using series expansions or treating the integral in different limits.^{7,10} Also numerical methods are used to give tabulated solutions for different geometries.¹

Another method of attacking the problem is to ignore the exact form of f(l) and to find closed form formulas for

$$P(x) = \frac{1}{x} \int dl f(l) [1 - \exp(-\Sigma l)]$$

where $x = \Sigma \overline{l}$. Several methods of attacking the above are known.^{2-9,11-13} Recently, Lux¹⁴ again joined the party. Showing that the conditions

$$\lim_{x \to 0} c(x) = c' \quad \text{and} \quad \lim_{x \to \infty} c(x) = c''$$

are too strong, he suggests that $c(x) = \alpha + \beta x$. This choice indeed gives for $\alpha = 0.35$ and $\beta = +\frac{1}{8}$ a very good fit for a cylinder. There is, however, no indication of how this choice is done and to its sensitivity. Indeed $\alpha = 0.6$ and $\beta = 0.007$ gives an error of more than 3.5% for x < 4. Thus, the parameter sensitivity of $c(x) = \alpha + \beta x$ seems to be high. The intention in Ref. 13 was to find an approximation that is valid in the whole spectrum and not only in parts of it. It was also indicated there that the sensitivity of the approximating function A(x) to the choice of c(x) is given by

 $\left(\frac{\partial A}{\partial C}\right)_{x,\text{constant}} = \frac{x}{[1+x+x^2c(x)]^2}$

and

$$\delta A = \frac{\partial A}{\partial C} \frac{\partial C}{\partial \alpha}; \, \delta \alpha;$$

where

$$\frac{\partial C}{\partial \alpha} \delta \alpha = \frac{\partial C}{\partial \alpha} \delta \alpha + \frac{\partial C}{\partial \beta} \delta \beta .$$

The choice $c(x) = \alpha + \beta x$ leads to

$$\frac{\partial C}{\partial \alpha}$$
; $\delta \alpha$; = $\delta \alpha \rightarrow x \, \delta \beta$

a form that is more sensitive to the proper choice of parameters.

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Comments on the Tritium Solubility in Lithium Oxide as a Solid Tritium Breeding Material

In a recent paper, Clemmer¹ estimated the tritium solubility in lithium oxide (Li₂O) from the viewpoint of blanket tritium recovery in a deuterium-tritium-fueled fusion reactor. Thermochemical calculations by Clemmer indicated that Li_2O has very high tritium solubility, to the extent that tritium inventories for Li_2O may be unacceptably high. The aim of the present Letter is to show that the model used by Clemmer is not valid for the case of Li_2O .

In our opinion, tritium oxide (T_2O) cannot be dissolved in solid Li₂O in the form of LiOT, because the crystal structure and the lattice constant (that is, lithium density) of Li₂O are quite different from those of LiOH, as shown in Table I. That is, tritium may be dissolved in Li₂O as interstitials, substitutionals, or OT, but not as LiOT. The OT species in Li₂O will be different from that of LiOT. Accordingly, we guess that a reaction

2 LiOT [in Li₂O(c)]
$$\neq$$
 Li₂O(c) + T₂O(g)

such as assumed by Clemmer, does not take place in the Li_2O lattice.

At the surface of Li_2O , the formation of LiOT(c) is conceivable. However, the equilibrium constant K for the reaction

$$2 \operatorname{LiOT}(c) \rightleftarrows \operatorname{Li}_2 O(c) + T_2 O(g)$$

should be expressed as

$$K = \frac{a(\text{Li}_{2}\text{O}) \cdot (\text{T}_{2}\text{O})}{[a(\text{LiOT})]^{2}} = P_{\text{T}_{2}\text{O}} ,$$

where a(i) is the activity of species *i* and P_{T_2O} is the equilibrium vapor pressure. The equilibrium water vapor pressure over solid LiOH has already been obtained by Gregory and Mohr.² According to their result, the equilibrium water vapor pressure at 300°C is ~1.3 Pa. From this, it is evident that LiOH on the surface of Li₂O decomposes into Li₂O and water above 300°C under the water vapor pressure of 1.3 Pa.

We are now performing experiments on the effect of water vapor pressure on the tritium release from Li_2O pellets in order to check whether Clemmer's estimation will be reasonable or not. The preliminary experiments showed that Li_2O with an initial tritium content of 2.5 wppm retained only 0.4 wppm of tritium after heat treatment at 650°C, where the Li_2O was surrounded by tritiated water vapor at 48.5 Pa. According to Clemmer's solid solution model, most of the tritium would have been held in Li_2O . Moreover, it can be concluded that

TABLE I

Crystal Structures and Lithium Densities of Li₂O and LiOH

| | Crystal Structure | Lithium Density (kg/m ³) |
|-------------------|-------------------|---|
| Li ₂ O | Antifluorite | 9.3 × 10 ² |
| LiOH | Tetragonal PbO | 4.1 × 10 ² |

¹R. G. CLEMMER, "The Development of Tritium Breeding Blankets for D-T Burning Fusion Reactors," *Proc. Fourth ANS Topl. Mtg. Technology of Controlled Nuclear Fusion*, King of Prussia, Pennsylvania, October 14-17, 1980, U.S. National Technical Information Service (1981, to be published).

²N. W. GREGORY and R. H. MOHR, J. Am. Chem. Soc., 77, 2142 (1955).