$$\mu(x)\frac{\sigma_s(x)}{\sigma_0} = \frac{2}{x^2} + \frac{10}{3\sqrt{\pi}}\frac{1}{x^3} + \frac{2}{3\sqrt{\pi}}\frac{e^{-x^2}}{x}\left(1 - \frac{5}{x^2}\right) + \\ + 2\left(\frac{1}{3} - \frac{2}{x^2}\right)\mathrm{Erf}(x) + \\ + \sqrt{\pi}\left(1 - \frac{1}{x^2}\right)\frac{e^{x^2}}{x}\mathrm{Erf}(x)\left[1 - \mathrm{Erf}(x)\right], \tag{4}$$

where $x = v/v_0$ and $v_0 = \sqrt{2kT}$.

Substituting Eq. (4) into Eq. (1) and with the appriate expression for $\langle\sigma_s(v)\rangle$ yields

$$ND(x) = \left\{3\sigma_0\left[\frac{1}{3}\frac{e^{-x^2}}{x\sqrt{\pi}} - \frac{2}{x^2} + \left(\frac{1}{3} + \frac{9}{2x^2}\right)\mathrm{Erf}(x) - \right.\right. \\ - \sqrt{\pi}\left(1 - \frac{1}{x^2}\right)\frac{e^{x^2}}{x}\mathrm{Erf}(x)\{1 - \mathrm{Erf}(x)\} - \tag{5} \\ \left.\left. - \frac{10}{3\sqrt{\pi}}\frac{1}{x^3}(1 - e^{-x^2})\right]\right\}^{-1} = \{3\sigma_0 S(x)\}^{-1}.$$

In Fig. 1 we plot the values of $\mu(x)$ and $ND(x)$ calculated from Eqs. (4) and (5), respectively, assuming $\sigma_0 = 20.7$ b.

The Maxwellian average of the diffusion coefficient, defined as

$$N\langle D\rangle = \frac{\int_0^\infty \dfrac{vM_{T_0,M}(v)}{3\sigma_s(v)[1 - \mu(v)]}dv}{\int_0^\infty vM_{T_0,M}(v)dv}, \tag{6}$$

is obtained from measurements of the diffusion properties of thermal neutrons.

From Eqs. (5) and (6) the expression for $N\langle D\rangle$ of a free proton gas is

$$N\langle D\rangle = \frac{2}{3\sigma_0}\int_0^\infty \frac{x^3 e^{-x^2}}{S(x)}dx = \frac{2}{3\sigma_0}G. \tag{7}$$

Numerical calculations yield 0.656 as the value of G.

We calculated the values of $\langle D\rangle$ from Eq. (7) for H_2O, C_6H_6 and $C_{12}H_{10}$ at $T = 300°K$. From the comparison with the values calculated by theoretical models[6,7,10], which account for the chemical binding, and with experimental results[6,8,9,10,11], we

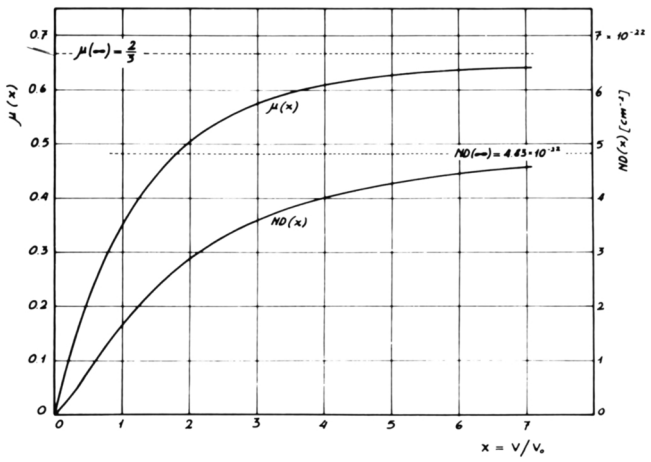

Fig. 1. Diffusion coefficient and average cosine of the scattering angle of neutrons for a free proton gas.

can conclude that using the free-proton gas model overestimates the diffusion coefficient for H_2O and hydrocarbons by a factor of 2 to 3. We neglect oxygen and carbon contributions.

B. Marsico
V. G. Molinari
R. Scozzafava

Laboratorio Gas Ionizzati
(EURATOM-CNEN),
Frascati, Roma

Received February 2, 1965
Revised March 30, 1965

ACKNOWLEDGMENTS

The authors wish to thank V. C. Boffi and D. E. Parks for useful discussions on the argument.

An Approximate Solution of the Two-Overlapping-Thermal-Group Diffusion Equations*

The use of two overlapping thermal groups to represent the spatially dependent thermal-neutron spectrum has been considered by several investigators[1-3]. The purpose of this letter is to describe

*Work performed under the auspices of the USAEC.

[1]D. S. SELENGUT, "Variational Analysis of Multi-Dimensional Systems," HW-59126, p. 89 (1950).
[2]G. P. CALAME and F. D. FEDERIGHI, *Nucl. Sci. Eng.* **10**, 190 (1961).
[3]A. J. BUSLIK, "The Description of the Thermal Neutron Spatially Dependent Spectrum by Means of Variational Principles," WAPD-BT-25, 1 (May 1962).

[6]M. S. NELKIN, *Phys. Rev.* **119**, 741 (1960).
[7]V. C. BOFFI, V. G. MOLINARI, and D. E. PARKS, B.N.L. **719**, I, 69 (1962).
[8]L. N. YUROVA, A. A. POLJAKOV, S. B. STEPANOV, and G. A. ALINOV, *Proc. Geneva Conf.* 28/P/356 (1964).
[9]T. SPRINGER, C. L. HOFMEYR, S. KORNBICHLER, and H. D. LEMMEL, *Proc. Geneva Conf.*, 28/P/763 (1964).
[10]V. C. BOFFI, F. DEMANINS, and V: G. MOLINARI, *Proc. VII Congresso Nucleare*, Roma (1962).
[11]L. PÁL, É. KISDI-KOSZÓ, L. BOD, Z. SZATAMÁRY, and I. VISI, *Proc. Geneva Conf.*, 28/P/651 (1964).

an approximate solution of one of the formulations. The approximation allows retention of the iteration strategy presently used in computer programs that solve the multidimensional few-group diffusion-theory equations.

The two-overlapping-thermal-group method assumes that the energy-dependent thermal flux can be represented as a linear combination of two predetermined trial spectra, i.e.

$$\phi(E, \boldsymbol{r}) = \psi_1(E)\chi_1(\boldsymbol{r}) + \psi_2(E)\chi_2(\boldsymbol{r}), \qquad (1)$$

where both $\psi_1(E)$ and $\psi_2(E)$ are defined over the entire thermal-neutron energy range. Substitution of Eq. (1) into the energy-dependent thermal-neutron diffusion equation, operating on the resulting equation in turn with $\int_0^{E_c} f_1(E)dE$ and $\int_0^{E_c} f_2(E)dE$ results in two equations in $\chi_1(\boldsymbol{r})$ and $\chi_2(\boldsymbol{r})$ which may be written as

$$-D_{11}\nabla^2\chi_1(\boldsymbol{r}) - D_{12}\nabla^2\chi_2(\boldsymbol{r}) + \Sigma_{11}\chi_1(\boldsymbol{r}) + \Sigma_{12}\chi_2(\boldsymbol{r}) = S_1(\boldsymbol{r}) \qquad (2a)$$

$$-D_{21}\nabla^2\chi_1(\boldsymbol{r}) - D_{22}\nabla^2\chi_2(\boldsymbol{r}) + \Sigma_{21}\chi_1(\boldsymbol{r}) + \Sigma_{22}\chi_2(\boldsymbol{r}) = S_2(\boldsymbol{r}). \qquad (2b)$$

The subscripts ij in Eqs. (2) reflect the combination of weighting functions $f_i(E)$ with trial function $\psi_j(E)$.

Equations (2) include both up- and down-coupling. Large scale two-dimensional few-group digital computer programs (like the PDQ series) take advantage of the fact that the conventional few-group equations are coupled only through down scattering and the fission source. The addition of up-coupling as exists in Eqs. (2) requires changes in iteration strategy and usually results in a large increase in the solution times.

An opportunity for further simplification of Eqs. (2) arises with the choice of trial and weight functions. The technique used by most investigators is to assume trial spectra that are both at least as soft and as hard as that expected in the reactor configuration of interest. This approach has been quite successful. Available weighting functions differ in the details but have the following general characteristics:

$f_1(E)$ is a constant (this choice assures neutron balance),

$f_2(E)$ increases with energy.

While the details do differ somewhat, little basis exists for choosing one method over the other in terms of obtaining an accurate representation of the spatially dependent spectrum.

In Buslik's formulation of the problem[3], the scattering kernel is symmetrized in order to allow the use of a variational principle for self-adjoint operators. With the Maxwellian distribution $\psi_M(E)$ chosen as one of the trial functions, the functions $f_1(E) = 1$ and $f_2(E) = \psi_H(E)/\psi_M(E)$ are obtained as weighting functions. (Here $\psi_H(E)$ is the hardened trial spectrum assumed for $\psi_2(E)$.) This choice results in the coefficients D_{22}, Σ_{22}, and S_2 in Eq. (2b) being orders of magnitude larger than the coefficients D_{21} and Σ_{21}, e.g. by a factor of 10^6 at 68°F (20°C) and by 10^2 at 535°F (279°C). This condition suggests that it may be possible to neglect the D_{21}, Σ_{21} terms in Eq. (2b) altogether. Then, if Eq. (2b) (without the D_{21} and Σ_{21} terms) is solved first, no uncoupling is required for the solution of the two-overlapping-group equations.

A comparison of Eqs. (2) with and without the D_{21} and Σ_{21} terms present yields three conditions to be satisfied for the approximation to yield an accurate solution,

$$\frac{\Sigma_{12}\Sigma_{21}}{\Sigma_{11}\Sigma_{22}} << 1, \quad \frac{\Sigma_{21}S_1}{\Sigma_{11}S_2} << 1, \quad \frac{D_{12}D_{21}}{D_{11}D_{22}} << 1. \qquad (3)$$

Several comparisons have been made between solutions of Eqs. (2) with the D_{21} and Σ_{21} terms present and not present. The M0176 (Ref. 4) computer program was used in the slab geometry for this purpose. Comparisons were made of $\chi_1(x)$, $\chi_2(x)$, and the activation rate $A = \Sigma_{11}\chi_1(x) + \Sigma_{12}\chi_2(x)$. The basic problem was a two-region cell (Table I). The slowing-in source was set proportional to the hydrogen density of the region, and the hardened trial spectrum for the basic problem was taken to be that of region 2. The maximum errors in activation rates at room temperature were less than 0.06% for all cases, except for one in which the slowing-down source was deleted from the fuel-

TABLE I

A Two-Region Cell

Region 1 (H_2O)	Region 2 (Fuel-Bearing Region)
$N_H = 0.5406\times10^{-1}$ (b cm)$^{-1}$	$N_H = 0.3004\times10^{-1}$ (b cm)$^{-1}$
$N_O = 0.2553\times10^{-1}$	$N_O = 0.24106\times10^{-1}$
Half-thickness = 10 cm	$N_{Zr} = 0.10706\times10^{-1}$
	$N_{235} = 0.92358\times10^{-3}$
	$N_{238} = 0.69517\times10^{-4}$
	Half-thickness = 10 cm

[4] R. M. CANTWELL, "M0176 - A FORTRAN Program to Solve Several P-Approximations to the Few-Group Neutron Transport Equation in Slab Geometry," WAPD-TM-320 (April 1962).

bearing region. The larger percentage error occurred at the edge of the cell, where the activation level was 10^{-4} less than at the fuel-water interface and is, consequently, insignificant.

Because of the decrease in the ratio of $\psi_H(E)/\psi_M(E)$ at high energies, the error observed when D_{21} and Σ_{21} were omitted at 535°F (279°C) was larger than at 68°F (20°C). However, in all cases, hot or cold, the error was less than 0.1%. The approximation was also applied successfully to a problem containing a heavy absorber treated with blackness theory.

The success of the approximation described above allows the conventional iteration strategy of the few-group diffusion-theory programs to be retained. As a result, the cost of using this approximation to the two overlapping groups in place of a single thermal group is essentially that of adding one conventional group to a few-group representation.

R. J. Breen
J. B. Yasinsky

Bettis Atomic Power Laboratory
Westinghouse Electric Corporation
West Mifflin, Pennsylvania 15122

Received November 2, 1964
Revised March 29, 1965