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**AN INTERPOLATION METHOD FOR
THE TRANSPORT THEORY AND ITS APPLICATION
IN FUSION-NEUTRONICS ANALYSIS**

by

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AN INTERPOLATION METHOD FOR THE TRANSPORT THEORY
AND ITS APPLICATION IN FUSION NEUTRONICS ANALYSIS

J. Jung

ABSTRACT

This report presents an interpolation method for the solution of the Boltzmann transport equation. The method is based on a flux synthesis technique using two reference-point solutions. The equation for the interpolated solution results in a Volterra integral equation which is proved to have a unique solution. As an application of the present method, tritium breeding ratio is calculated for a typical D-T fusion reactor system. The result is compared to that of a variational technique.

I. INTRODUCTION

It is quite frequent that nuclear designers face a situation where a series of similar transport calculations are required for scoping possible parameter variations of interest.¹ Over the last decades, a great deal of methodological sophistication has been developed to provide useful means for such a situation. The methods most frequently utilized are the variational and perturbation theories.²⁻²³ These methods feature: (1) evaluation of integral quantities such as eigenvalues in fission reactors and tritium production rates in fusion reactors; (2) requirement of, at least, two basic values of the forward and adjoint (or its variant) solutions of the Boltzmann transport equation;²⁴ and (3) the associated error prediction of the second order in the sense of a norm. In fact, Ref. 14 shows that several variants developed based on the variation and perturbation theories are all equivalent with respect to the accuracy as well as the required effort involved in obtaining the solution. Several authors extended their methods to high-order approximations (see e.g. Ref. 17) to improve the accuracy of the solution. It appears, however, that the effort needed to increase the accuracy by increasing the order of approximation, is not less than the effort required to solve the original Boltzmann equation.

The method presented in this report is based on a simple flux synthesis technique^{25,26} using two reference-point solutions. In this regard, the basic computational effort required for the present method is not more than that for the lowest-order variational or perturbation method. However, an attempt is made in the present method to fully utilize the information given at the two reference points in order to construct the energy- and space-dependent flux solution of the Boltzmann equation. In consequence, a variety of intergral (response rate) calculations can be done by a simple multiplication algebra.

The mathematical formulation of the present method is given in Chapt. II, along with proofs of the existence of solution and of uniqueness of the solution. Chapter III is devoted to a numerical comparison of the present method with the exact transport calculation. A comparison is also made with a variational method. Conclusions and a brief discussion of the present method are given in Chapt. IV.

II. MATHEMATICAL FORMULATION

The time-independent particle (neutron/photon) transport in a reactor system is governed by the Boltzmann transport equation,

$$L\phi = S . \quad (1)$$

along with an appropriate geometrical boundary condition. S and ϕ are the external source and the flux solution, respectively, and the linear operator L is expressed as:

$$L = \vec{\Omega} \cdot \vec{\nabla} + \Sigma_t(\vec{r}, E) - \int d\vec{\Omega}' dE' \Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) , \quad (2)$$

where Σ_t and Σ_s are the total and transfer cross sections, respectively. Given the two reference (point) solutions ϕ^1 and ϕ^2 of equations,

$$L^i \phi^i = S^i , \quad i = 1, 2 , \quad (3)$$

let's construct the solution of Eq. (1) by

$$\phi = \alpha \phi^1 + (1 - \alpha) \phi^2 . \quad (4)$$

In general, the angular flux ϕ , and hence the coefficient α , is energy E , angle $\vec{\Omega}$ and position \vec{r} dependent. Assume that in an infinitely small spatial domain, Δ , α is weakly dependent on angle, i.e.,

$$\phi \approx \alpha(E)\phi^1 + [1 - \alpha(E)]\phi^2, \quad \vec{r} \in \Delta. \quad (5)$$

Substitution of Eq. (5) into Eq. (1), using the relationship of Eq. (3), results in:

$$\begin{aligned} & \alpha(\Sigma_t - \Sigma_t^1)\phi^1 + (1 - \alpha)(\Sigma_t - \Sigma_t^2)\phi^2 \\ &= \int dE' d\vec{\Omega}' \alpha \Sigma_s \phi^1 - \alpha \int dE' d\vec{\Omega}' \Sigma_s^1 \phi^1 \\ &+ \int dE' d\vec{\Omega}' (1 - \alpha) \Sigma_s \phi^2 - (1 - \alpha) \int dE' d\vec{\Omega}' \Sigma_s^2 \phi^2. \end{aligned} \quad (6)$$

The angular flux and the transfer cross section can be expanded with the spherical harmonic functions²⁷ as follows:

$$\phi(\vec{r}, E, \vec{\Omega}) \equiv \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \phi_{\ell m}(\vec{r}, E) P_{\ell m}(\vec{\Omega}), \quad (7)$$

$$\Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \equiv \sum_{\ell=0}^{\infty} \Sigma_{s\ell}(\vec{r}, E' \rightarrow E) P_{\ell}(\mu) \quad (8)$$

assuming that the angular transfer of Σ_s is dependent solely on the cosine of scattering angle of $\mu = \vec{\Omega}' \cdot \vec{\Omega}$. The spherical harmonic functions used satisfy the following orthogonal relations:

$$\int d\vec{\Omega} P_{\ell m}(\vec{\Omega}) P_{\ell' m'}(\vec{\Omega}) = \frac{4\pi}{2\ell + 1} \delta_{\ell\ell'} \delta_{mm'} \quad (9)$$

with Kronecker deltas of $\delta_{\ell\ell'}$ and $\delta_{mm'}$.

Substitution of expansion (7) and (8) into Eq. (6), followed by integration of the resultant equation over the whole solid angle, $\vec{\Omega}$ yields a slowing-down-type equation,

$$A(E)\alpha(E) = \int_E^{E_{\max}} dE' B(E' \rightarrow E)\alpha(E') + Q(E), \quad (10)$$

where

$$A(E) = \left[\Sigma_t(E) - \Sigma_t^1(E) \right] \phi_0^1(E) - \left[\Sigma_t(E) - \Sigma_t^2(E) \right] \phi_0^2(E) + \int dE' \left[\Sigma_{s0}^1(E' \rightarrow E) \phi_0^1(E') - \Sigma_{s0}^2(E' \rightarrow E) \phi_0^2(E') \right], \quad (11)$$

$$B(E' \rightarrow E) = \Sigma_{s0}(E' \rightarrow E) \left[\phi_0^1(E') - \phi_0^2(E') \right], \quad (12)$$

$$Q(E) = \int dE' \left[\Sigma_{s0}(E' \rightarrow E) - \Sigma_{s0}^2(E' \rightarrow E) \right] \phi_0^2(E') - \left[\Sigma_t(E) - \Sigma_t^2(E) \right] \phi_0^2(E), \quad (13)$$

$$\phi_0^i(E) = \int d\vec{\Omega} \phi^i(\vec{r}, E, \vec{\Omega}) \quad i = 1, 2, \quad \vec{r} \in \Delta \quad (14)$$

and

$$\Sigma_{s0}^i(E' \rightarrow E) = \int d\vec{r} \Sigma_s^i(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}), \quad i = 1, 2 \quad \vec{r} \in \Delta. \quad (15)$$

Upon the derivation of Eq. (10) it is assumed that $S = S^1 = S^2$ for simplicity. In addition, the \vec{r} dependence of all the quantities is omitted, implicitly assuming that the equation is to be solved only within the spatial domain, Δ .

Equation (10) is solved for the parameter $\alpha(E)$ that is, in turn, used for the flux interpolation of

$$\phi_0(E) = \alpha(E)\phi_0^1(E) + [1 - \alpha(E)]\phi_0^2(E), \quad r \in \Delta \quad (16)$$

derived from Eqs. (5).

The solution technique described above can be regarded as a flux synthesis method in which the variation of the solution flux with angle and space is largely represented by the reference-point fluxes, and the transport equation is solved for the unknown α which is supposedly very weakly dependent upon angle and space. In fact, the magnitude of the term which is omitted and thereby introduces a primary error in deriving Eq. (10), i.e.,

$$R = \int d\vec{\Omega} (\phi^1 - \phi^2) \vec{\Omega} \cdot \vec{\nabla} \alpha$$

will determine the accuracy of the present method.

A. Existence of Solution

This section presents a proof of existence of the solution for Eq. (10). Assuming $A(E) \neq 0$ for an energy interval of $0 \leq E \leq E_{\max}$, Eq. (10) is rewritten as

$$\alpha(E) = \int_E^{E_{\max}} K(E, E') \alpha(E') dE' + q(E), \quad (17)$$

in which $K(E, E')$ and $q(E)$ are defined as

$$K(E, E') = B(E' \rightarrow E) / A(E) \quad (18)$$

and

$$q(E) = Q(E) / A(E). \quad (19)$$

Equation (17) is a Volterra integral equation^{28,29} of the second kind. Following the procedure of Ref. 29, the existence of solution can be verified as follows: Assume that $q(E)$ is continuous and bounded in $0 \leq E \leq E_{\max}$ and that $K(E, E')$ is continuous and bounded in $0 \leq E, E' \leq E_{\max}$. Consider an equation

$$\alpha(E) = \lambda \int_E^{E_{\max}} K(E, E') \alpha(E') dE' + q(E) \quad (20)$$

and a series expansion

$$\alpha(E) = \sum_{n=0}^{\infty} \lambda^n \alpha_n(E) . \quad (21)$$

The question is whether a bounded series of α_n 's exist. Substitution of Eq. (21) into Eq. (20) results in

$$q(E) = \alpha_0(E) + \sum_{n=1}^{\infty} \lambda^n \left\{ \alpha_n(E) - \int_E^{E_{\max}} K(E, E') \alpha_{n-1}(E') dE' \right\} . \quad (22)$$

Therefore,

$$\alpha_0(E) = q(E) \quad (23)$$

$$\alpha_n(E) = \int_E^{E_{\max}} K(E, E') \alpha_{n-1}(E') dE' , \quad n = 1, 2, \dots \quad (24)$$

Defining M and N as the maxima of $|q(E)|$ and $|K(E, E')|$, respectively, in the variable range of interest, one finds that

$$|\alpha_1(E)| \leq M \cdot N \int_E^{E_{\max}} dE' = MN(E_{\max} - E) \quad (25)$$

$$|\alpha_2(E)| \leq M \cdot N^2 \int_E^{E_{\max}} (E_{\max} - E') dE' = M \cdot N^2 \cdot \frac{(E_{\max} - E)^2}{2} . \quad (26)$$

In general,

$$|\alpha_n(E)| \leq MN^n \frac{(E_{\max} - E)^n}{n!} . \quad (27)$$

Consequently,

$$\begin{aligned}
\alpha(E) &\leq \sum_{n=0}^{\infty} \left| \lambda^n \alpha_n(E) \right| \leq M \cdot \sum_{n=0}^{\infty} \left| \lambda^n \frac{N^n (E_{\max} - E)^n}{n!} \right| \\
&\leq M \sum_{n=0}^{\infty} \frac{N^n E_{\max}^n |\lambda|^n}{n!} \\
&= M \cdot \exp \left[N |\lambda| E_{\max} \right].
\end{aligned} \tag{28}$$

Therefore, the series expansion of Eq. (21) converges uniformly in $0 \leq E \leq E_{\max}$, which completes the proof.

When $A(E) = 0$, Eq. (10) results in a Volterra equation of the first kind,^{28,29}

$$\int_E^{E_{\max}} dE' B(E' \rightarrow E) \alpha(E') = Q(E). \tag{29}$$

It is known²⁹ that the first kind Volterra equation can be transformed to its second kind equation under certain conditions. Let us assume that $\alpha(E')$ is integrable over $0 \leq E \leq E' \leq E_{\max}$, i.e.,

$$\int_E^{E_{\max}} \alpha(E') dE' = \gamma(E). \tag{30}$$

By a partial integration of Eq. (29), it follows that:

$$\int_E^{E_{\max}} dE' B(E' \rightarrow E) \alpha(E) = -B(E \rightarrow E) \gamma(E) + \int_E^{E_{\max}} dE' \frac{\partial B(E' \rightarrow E)}{\partial E'} \cdot \gamma(E') \tag{31}$$

under the condition that $B(E' \rightarrow E)$ is differentiable. Assuming another property of $B(E \rightarrow E) \neq 0$, Eq. (29) results in

$$\gamma(E) = \int_E^{E_{\max}} dE' \frac{1}{B(E \rightarrow E')} \cdot \frac{\partial B(E' \rightarrow E)}{\partial E'} \gamma(E') - \frac{Q(E)}{B(E \rightarrow E)}, \quad (32)$$

which is a Volterra equation of the second kind already studied. All the functional properties assumed for $B(E' \rightarrow E)$, such as the differentiability and $B(E \rightarrow E) \neq 0$ will hold provided that $\Sigma_{S0}(E' \rightarrow E) [\phi_0^1(E') - \phi_0^2(E)]$ is continuous and the two reference fluxes, ϕ_0^1 and ϕ_0^2 are distinct which seems to be the case in most of the practical problems of interest.

B. Uniqueness of Solution

Since the existence of solution has been proven for both cases of $A(E) \neq 0$ and $A(E) = 0$, it is sufficient to assume $A(E) \neq 0$ for the proof in this section. Suppose that $\alpha^I(E)$ and $\alpha^{II}(E)$ are two solutions of Eq. (17), then from Eq. (20),

$$\beta(E) \equiv \alpha^I(E) - \alpha^{II}(E) = \lambda \int_E^{E_{\max}} K(E', E) \beta(E') dE'. \quad (33)$$

This is a special case of $q(E) = 0$ in Eq. (17). Therefore, from Eqs. (23) and (24),

$$\beta_n(E) = \alpha_n^I(E) - \alpha_n^{II}(E) = 0, \quad n = 0, 1, 2, \dots \quad (34)$$

and then,

$$\beta(E) = \alpha^I(E) - \alpha^{II}(E) = 0, \quad (35)$$

which completes the proof that Eq. (17) has a unique solution.

C. Multigroup Formulation

This section provides a multigroup formulation of Eq. (10) in order to utilize existing cross-section libraries of multigroup format. Dividing the whole energy interval of $0 \leq E \leq E_{\max}$ into multigroups such that

$$E_{g+1} \leq E \leq E_g, \quad g = 1, 2, \dots$$

and integrating Eq. (10) over $E_{g+1} \leq E \leq E_g$, one finds that

$$A^g_{\alpha_g} \approx \sum_{g'=1}^g B^{g' \rightarrow g}_{\alpha_{g'}} + Q^g, \quad (36)$$

where

$$A^g = \left(\Sigma_t^g - \Sigma_t^{1g} \right) \phi_0^{1g} - \left(\Sigma_t^g - \Sigma_t^{2g} \right) \phi_0^{2g} + \sum_{g'=1}^g \left[\Sigma_{s0}^{1g' \rightarrow g} \phi_0^{1g'} - \Sigma_{s0}^{2g' \rightarrow g} \phi_0^{2g'} \right], \quad (37)$$

$$B^{g' \rightarrow g} = \Sigma_{s0}^{g' \rightarrow g} \left[\phi_0^{1g'} - \phi_0^{2g'} \right], \quad (38)$$

$$Q^g = \sum_{g'=1}^g \left[\Sigma_{s0}^{1g' \rightarrow g} - \Sigma_{s0}^{2g' \rightarrow g} \right] \phi_0^{2g'} - \left[\Sigma_t^g - \Sigma_t^{2g} \right] \phi_0^{2g}, \quad (39)$$

$$\phi_0^g = \int_{E_{g+1}}^{E_g} \phi_0(E) dE, \quad (40)$$

$$\alpha^g = \frac{1}{\Delta E_g} \int_{E_{g+1}}^{E_g} \alpha(E) dE \quad (41)$$

and

$$\Delta E_g = E_g - E_{g+1}. \quad (42)$$

Equation (36) can be rewritten as

$$\alpha^g = (A^g - B^{g \rightarrow g})^{-1} \left\{ \sum_{g'=1}^{g-1} B^{g' \rightarrow g} \alpha^{g'} + Q^g \right\}, \quad g = 1, 2, \dots \quad (43)$$

assuming $A^g - B^{g \rightarrow g} \neq 0$.

Once α^g is solved, the interpolated flux solution is obtained by

$$\phi_0^g = \alpha^g \phi_0^{1g} + (1 - \alpha^g) \phi_0^{2g}, \quad g = 1, 2, \dots \quad (44)$$

The formulation given here assumes that the system under consideration does not involve neutron multiplication due to fission and the neutron energy transfer is purely downward (slowing down). In the case of multiplication problems, Eq. (36) must be iteratively solved.

III. NUMERICAL EXAMPLES

As an application of the present method, a tritium production problem is considered for a D-T fusion reactor based on a one-dimensional infinite-cylindrical model. The system dimensions and material compositions used are as follows:

Zone	Radii (m)	Material Composition
1.	0-2.00	D-T source neutron (14-MeV) region; vacuum
2.	2.00-2.20	Scrape-off region; vacuum
3.	2.20-2.21	First wall, Type 316 stainless steel (SS)
4.	2.21-2.71	Blanket: 85% liquid lithium + 15% SS
5.	2.71-2.91	Shield: 45% B ₄ C + 45% SS + 10% He

The transport calculations for the reference fluxes as well as for the exact solutions which are to be compared with the present method, were performed by a one-dimensional discrete-ordinate code, ANISN³⁰ with the S8-P3 approximation. The transport cross-section library³¹ and response function library³² used are both based on ENDF/B-IV.³³ It should be noted that Ref. 34 shows that the ENDF/B-IV data for the ⁷Li(n,n α)t cross section are about 10-15% higher

than those experimentally measured. Since the liquid lithium blanket analyzed in this section has a relatively hard neutron spectrum, it is expected that the ${}^7\text{Li}$ breeding ratios (BR's) calculated here are subject to an adjustment. However, the numerical verification of the present method itself should not be affected within the consistency of the data libraries used.

Figure 1 shows the isotopic tritium BR's due to the ${}^6\text{Li}(n,\alpha)t$ (T_6) and ${}^7\text{Li}(n,n'\alpha)t$ (T_7) reactions as a function of ${}^6\text{Li}$ enrichment. In this example, the two reference-point calculations are made at ${}^6\text{Li}$ enrichments of 7.5% (natural lithium case) and 90%, and all other enrichment cases are interpolated from the reference points, based on Eqs. (43) and (44). The number of energy groups used is 46 for neutron and 21 for photon. Also shown in Fig. 1 for comparison are the BR's obtained by direct ANISN calculations. It is found that the interpolation method can predict the nonlinear T_6 variation within a maximum error of $\sim 2.5\%$ for a very wide range of ${}^6\text{Li}$ enrichment. With regard to T_7 BR, there is no appreciable difference ($\ll 1\%$) between the present method and the exact calculation by ANISN.

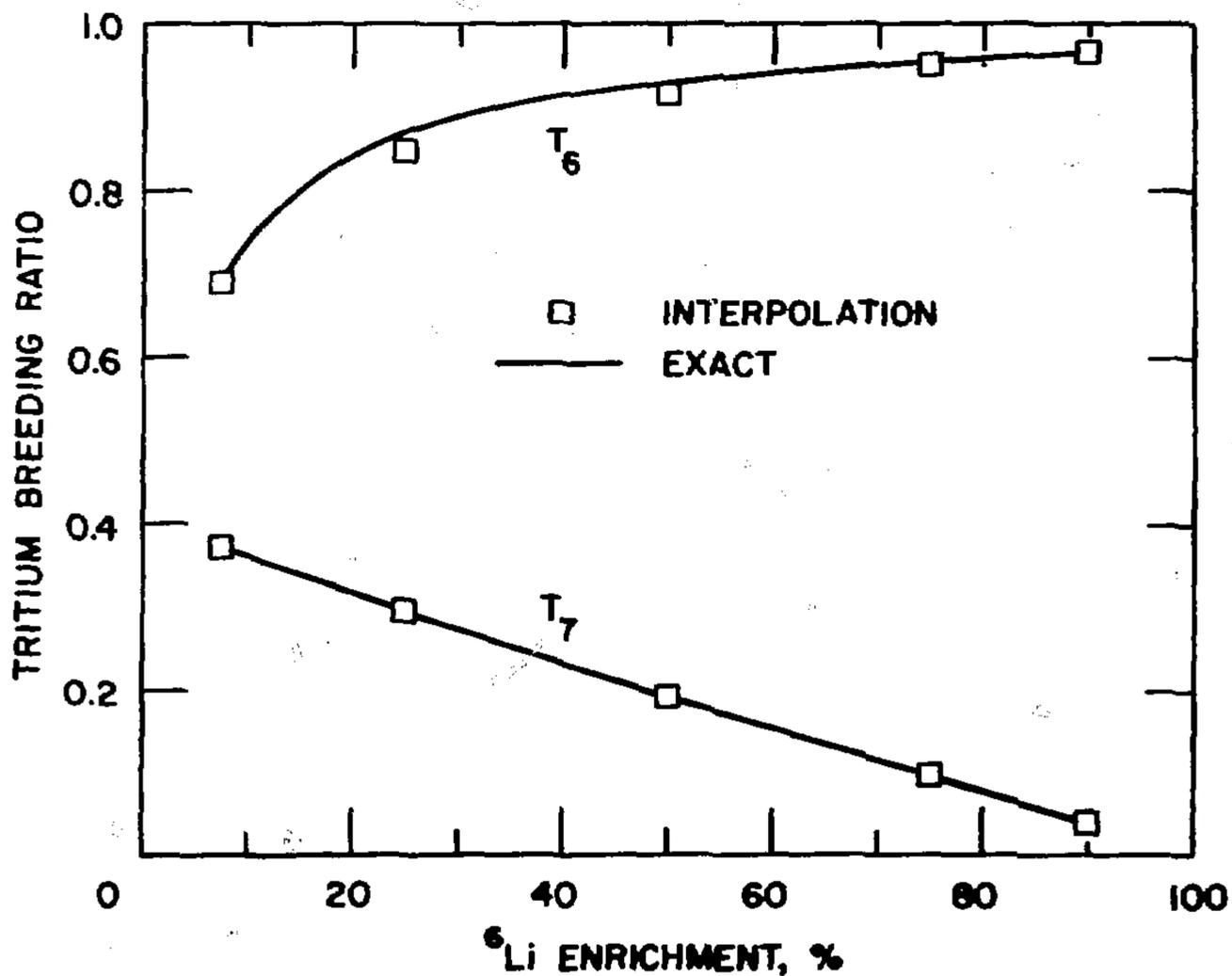


Fig. 1. Tritium breeding ratio by the interpolation method.

The interpolation method can predict not only integral quantities such as a system total BR as shown above, but also space- and energy-dependent solutions in between the two reference points. The example shown in Fig. 2 presents the spatial variation of the specific T_6 and T_7 BR's in the lithium blanket, which is interpolated for a ${}^6\text{Li}$ enrichment of 50%. The reference points are the same as those used previously. One notices an excellent agreement between the present method and direct ANISN calculations for both T_6 and T_7 . Figures 3 and 4 show, respectively, the interpolated neutron and photon spectra for the same ${}^6\text{Li}$ enrichment of 50%. The spectra are plotted at the midpoint of the lithium blanket (~ 26 cm from the first wall surface). It is seen that the difference in the neutron spectrum between the two calculations is negligible at energies above ~ 100 keV and below ~ 100 eV. The maximum error in the energy range between ~ 100 eV and ~ 100 keV is about 15%. In the case of the photon spectrum, the difference is quite trivial. Figure 5 illustrates the energy-dependent interpolation factor α used to construct the particle spectra shown in Figs. 3 and 4. As shown, the variation of α with energy is very substantial, ranging from ~ 1 to $\sim 10^{-5}$. It is inferred from this result that the effect of the transport operator change (due to the ${}^6\text{Li}$ enrichment variation in the present case) on the solution flux is mostly represented by its variation with energy, and is much less dependent upon its angular and/or spatial variation, at least for the present example.

Table I shows a comparison of the tritium BR's calculated by the present method and by E. Cheng and R. Conn's variational interpolation method.^{12,13} In Refs. 12 and 13, they have numerically proved that their method can yield much more accurate functional evaluations for a broad range of parameter variation than can conventional perturbation and variational methods. They have derived two forms of the two-point variational interpolation functional, viz., linear (Roussopoulos³) form and fractional (Schwinger⁵) form. Both of them are compared in Table I with the present interpolation method as well as the exact numerical values of ANISN. The two reference ${}^6\text{Li}$ enrichments chosen for their method are also 7.5% and 90%. Due to the unnormalized functional characteristic, the linear form solution shows nontrivial deviations from the corresponding exact calculations. The maximum error amounts to $\sim 14\%$ for the T_6 calculation, at 25% ${}^6\text{Li}$ enrichment. The result of the present method favorably compares with the Schwinger form calculation, their respective maximum deviations being only -2.5% and $+1.8\%$ relative to the ANISN calculations.

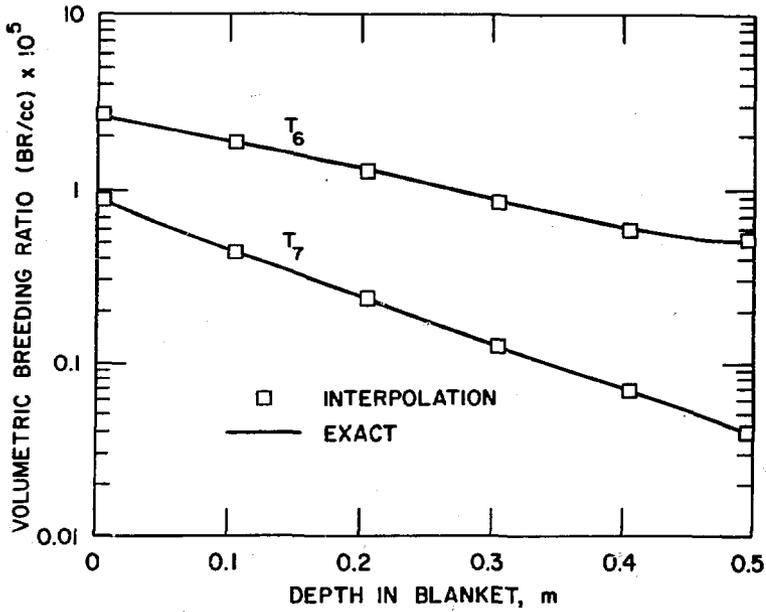


Fig. 2. Spatial dependence of tritium production.

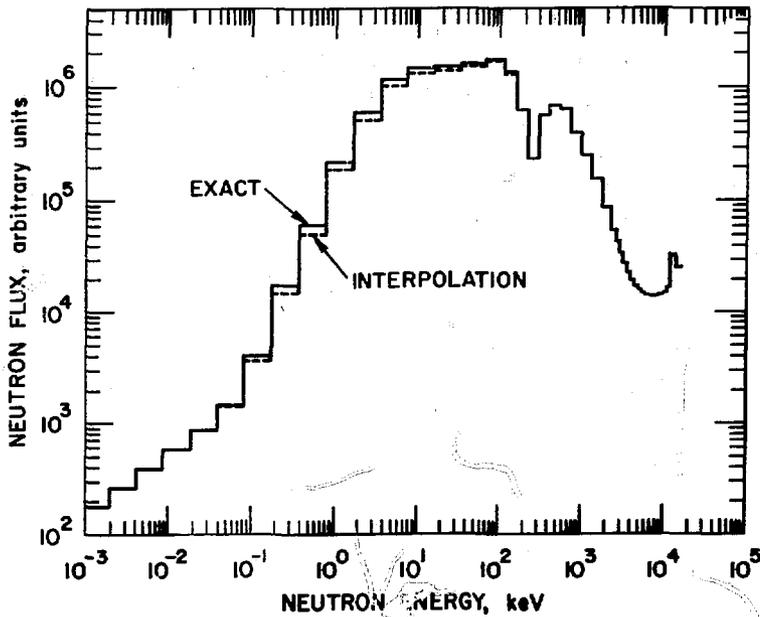


Fig. 3. Neutron spectrum by the interpolation method.

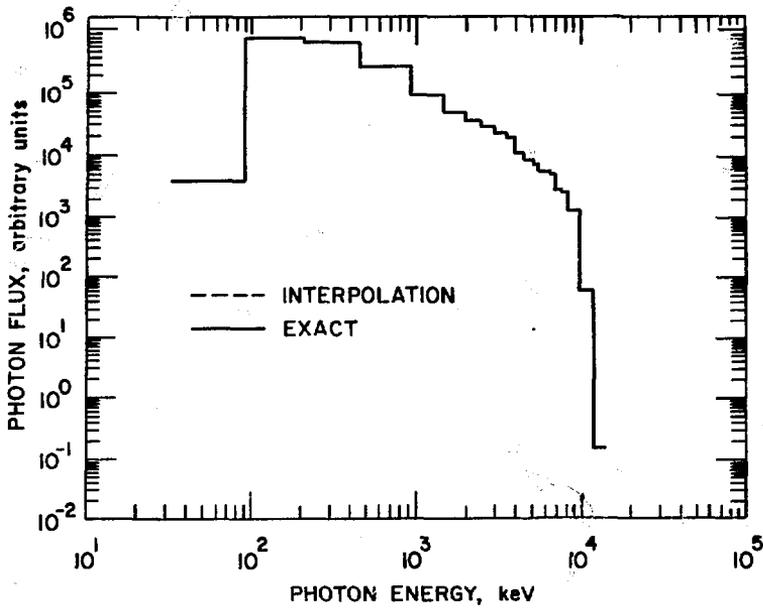


Fig. 4. Photon spectrum by the interpolation method.

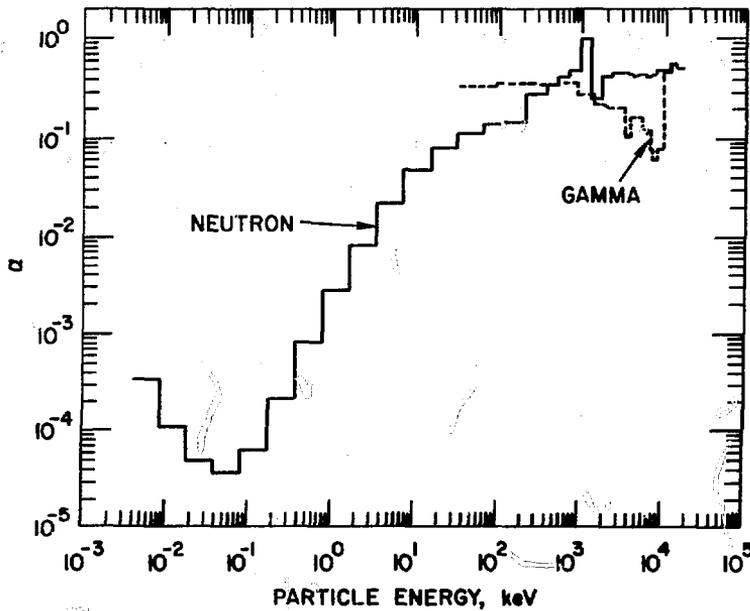


Fig. 5. The energy dependence of the interpolation factor alpha.

Table I

Comparison of Present Method with Variational Method
in Tritium Breeding Ratio Calculation

Method	⁶ Li - Enrichment					
	T ₆ - BR			T ₇ - BR		
	25%	50%	75%	25%	50%	75%
1. Variational interpolation						
i. Linear form ^a	0.749	0.832	0.916	0.297	0.197	0.0938
ii. Schwinger form ^b	0.883	0.939	0.959	0.293	0.192	0.0939
2. Present method	0.845	0.915	0.951	0.293	0.191	0.0938
3. Exact ^c	0.867	0.928	0.955	0.293	0.191	0.0938

^aRef. 13; Eq. (11).

^bRef. 13; Eq. (12).

^cS8-P3 ANISN calculation.

IV. CONCLUSIONS AND DISCUSSION

An approximate solution technique for the Boltzmann transport equation has been presented based on a flux synthesis method. The Volterra integral equation derived has been proven to have a solution which is unique. The present interpolation method can provide not only integral response rates such as BR, but also energy- and space-dependent particle fluxes. Basically, two forward transport solutions are required for the present method. The tritium BR calculated for a typical D-T fusion system shows an excellent agreement with the exact transport calculation by ANISN. The present method calculations also favorably compares with the result of Cheng and Conn's Schwinger form calculation of the two-point variational interpolation functional. It remains to be further studied whether the method presented can be applied to a broader class

of problems such as (1) variation of any blanket material compositions including structural material, coolant, etc.; and (2) different zone thicknesses (e.g., accommodation of a neutron multiplier in a fixed blanket thickness).

The choices of L^1 and L^2 given in Eq. (3) depend upon specific problems one wishes to solve. The present method allows interpolations for changes in cross sections as well as in geometries provided that a consistency among ϕ^1 , ϕ^2 , and ϕ is guaranteed with respect to the energy group structure, and the system boundary configuration. The present method has, however, no capability to provide the prediction of errors involved except for the two reference points. In this connection, the error term R shown in Sec. II, will merely afford an approximate posterior estimate on the solution precision. Prediction of errors inherent to the present interpolation also remains to be further investigated.

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