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《**Original**》

A Study of Iteration Method for 2-Dimensional 2-Group Diffusion Problems

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2차원 2군 확산 문제의 반복법에 대한 고찰

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Abstract

It is shown that the Shanks sequence E_k-transformation and the conventional extrapolation method are theoretically related. The E_1^2-transformation method is then applied for the multigroup diffusion problems. The diffusion code, CITATION, is modified for this study and the computing time is compared for each iteration tactics.

The Equipose method, in which only single inner iteration for each energy group is carried for an outer iteration, has been known as the fastest iteration method. However, in the case of 2-group problems, the proposed method, in which the number of inner iteration for the fast and thermal group is 2 and 1 respectively, gives better convergency than the Equipose method by about 12%.

The double extrapolation method results in faster computing time than the single extrapolation method without computing storage problem. It is, however, to note that this method is verified only for a two-group treatment.

요 약

본 논문에서는 Shanks의 수열 전환방법 중 E_k-전환을 연구하여 E_1-전환과 single extrapolation 방법과의 관계를 정립하고 나아가서 중성자 확산 방정식의 반복법에 E_1^2-전환을 적용하여 double extrapolation 방법을 유도하고 있으며, 이를 CITATION코드에서 적용해 보았다. 이 경우 double extrapolation은 기존의 single extrapolation 방법보다 효과적으로 외부 반복법을 가속시키고 있는데

단, double extrapolation 방법이 일어날 수 있는 조건을 만족시켜 double extrapolation이 일어나는 경우이다.

또 CITATION코드는 내부 반복법에서 'Equipose' 방법이라하여 내부 반복횟수를 1회만 하고 외부 반복법으로 넘어가는 방법이 가장 빠른 것으로 간주하고 program이 되어 있으나, 내부 반복법에서 에너지 군별로 반복횟수를 다르게 줄 경우, 예를 들면 속 중성자속과 열 중성자속을 계산하는 반복과정중 반복횟수를 각각 2번과 1번으로 줄 경우는 기존의 Equipose보다 매우 빠름을 알 수 있다. 단, 이 경우는 에너지 군이 2군일 경우 명확하게 보여주고 있다.

I. Introduction

Since the computing time for the analysis of a reactor core by the multi-group diffusion method is mainly determined by the number of iterations, the study to find the more powerful iteration method is inevitable. Many researches on the iteration have been carried out on practical problems, but for CITATION[1] code, one of the most widely used reactor analysis codes in this country, study on the code improvement has not been performed yet.

The CITATION has two special features in its iteration scheme, the extrapolation method and Equipose method, which are simply explained as follows:

1) The eigenvalue k is estimated by the following neutron balance equation.

$$k=\frac{P}{A+L}, \tag{1}$$

where P=neutron production rate,
A=neutron sink rate,
L=neutron leakage rate.

2) Only one inner iteration for each energy group is done by successive line overrelaxation (SLOR) during one outer iteration.

3) Outer iteration is accelerated by the extrapolation method,

$$\phi^{(t+1)}=\phi^{(t)}+\omega(\phi^{(t)}-\phi^{(t-1)}) \tag{2}$$

where ω is the extrapolation factor.

The above procedure is known as the Equipose method[2,3]. The procedure[3] means single extrapolation. In some of advanced codes, e.g., VENTURE[4], a double extrapolation is built in instead of this procedure[3].

In this paper the conventional extrapolation method is theoretically related with the Shanks squence E_k-transformation[5], and the double extrapolation method is then applied for multigroup diffusion problems. A modified Equipose method is tested for two group problems.

II. Theory

II. 1. E_k-Transformation of Shanks

Let $\{A_n\}$ $(n=0,1,2,\ldots)$ be a sequence of numbers of functions and

$$\Delta A_n=A_n-A_{n-1},$$
$$\Delta^2 A_n=\Delta A_n-\Delta A_{n-1}=A_n-2A_{n-1}+A_{n-2},$$
$$\vdots \qquad\qquad \vdots$$

Let k be a positive integer and define a new sequence $\{B_{k,n}\}$, "the k'th order transform of $\{A_n\}$", as follows.

$$B_{k,n}=\frac{\begin{vmatrix} A_{n-k} & \cdots & A_{n-1} & A_n \\ \Delta A_{n-k} & \cdots & \Delta A_{n-1} & \Delta A_n \\ \Delta A_{n-k+1} & \cdots & \Delta A_n & \Delta A_{n+1} \\ \vdots & & \vdots & \vdots \\ \Delta A_{n-1} & \cdots & & \Delta A_{n+k-1} \end{vmatrix}}{\begin{vmatrix} 1 & & 1 & 1 \\ \Delta A_{n-k} & \cdots & \Delta A_{n-1} & \Delta A_n \\ \Delta A_{n-k+1} & \cdots & \Delta A_n & \Delta A_{n+1} \\ \vdots & & \vdots & \vdots \\ \Delta A_{n-1} & \cdots & & \Delta A_{n+k-1} \end{vmatrix}}, \quad \text{for } n=k, k+1\cdots \tag{3}$$

Now one can introduce an operator E_k by

$$B_{k,n}=E_k(A_n), \quad \text{for } n\geq k, \tag{4}$$
$$C_{k,n}=E_k(B_{k,n})=E_k^2(A_n), \quad \text{for } n\geq 2k, \tag{5}$$
$$D_{k,n}=E_k(C_{k,n})=E_k^3(A_n), \quad \text{for } n\geq 3k. \tag{6}$$

Then $E_k(A_n)$ is called the 'E_k-transform of

$\{A_n\}$'[5].

If the sequence $\{A_n\}$ is a 'mathematical transient', i.e., if the sequence $\{A_n\}$ is function of n,

$$A_n=B+\sum_{i=1}^{k} a_i q_i, \quad \text{for } q_i<0, \tag{7}$$

where B is the 'Base' of the transient and $\lim_{n\to\infty} A_n=B$, then determining B in Eq.(7) is theoretically possible whenever exactly $2k+1$ successive values of A_n—for instance, $A_0, A_1, \ldots, A_{2k}$ is known. In practice the elimination of all the a_i's and q_i's would be too tedious, but frequently one of q_i, say q_k, predominates in Eq. (7). In such an instance one can ignore a_i, q_i for $i=1, \ldots, k-1$, so that one may obtain the following estimate for B,

$$\text{Estimate of } B=\frac{A_nA_{n-2}-A_{n-1}^2}{A_n+A_{n-2}-2A_{n-1}}$$

This is just the E_1-transform of $\{A_n\}$ ($n=n, n-1, n-2$), however it is known as the" Aitken's δ^2-process'[6] early. When the sequence A_n is a 'mathematical transient', the sequence $\{E_1(A_n)\}$ has a faster convergence than the sequence $\{A_n\}$ and the sequence $\{E_1^2(A_n)\}$ has a faster convergence than the sequence $\{E_1(A_n)\}$ and so on[5].

II. 2. E_1-Transformation

Now let's apply Shanks' sequence transformation to the neutron diffusion equation. The general iterative form of neutron diffusion difference equation can be written as follows:

$$\phi_{t+1}=(\boldsymbol{M}^{-1}\ 1/k\ \boldsymbol{F})\ \phi_t,$$
$$\text{or } \phi_{t+1}=\boldsymbol{T}_t\ \phi_t, \tag{8}$$

where the subscript t indicates the outer iteration number.

The eigenvectors of iterative matrix $\boldsymbol{T}$ are defined by

$$\boldsymbol{T}\psi_n=\mu_n\cdot\psi_n.$$

where ψ_n are the eigenvectors and μ_n are the corresponding eigenvalues, which are indexed from N in the decreasing order of μ_n as

$$\mu_N\leqslant\mu_{N-1}\leqslant\ldots\leqslant\mu_2\leqslant\mu_1.$$

The initial error vector $\boldsymbol{e}^{(0)}$ is expanded in the eigenvector series as

$$\boldsymbol{e}^{(0)}=\phi_\infty-\phi_0=\sum_{n=1}^{N} a_n\ \psi_n.$$

Then $\boldsymbol{e}^{(t)}$ is expressed by

$$\boldsymbol{e}^{(t)}=\phi_\infty-\phi_t=\sum_{n=1}^{N} (\mu_n)^t\ a_n\ \psi_n. \tag{9}$$

As the number of iterations increases, the error vector,

$$\boldsymbol{e}^{(t)}\to\mu_1^t\ a_1\ \psi_1,$$

when $\boldsymbol{T}$ is properly set up to have the spectral radius less than unity. Thus Eq. (9) can be rewritten as

$$\phi_t=\phi_\infty+\mu_1^t\ a_1\ \psi_{-1}. \tag{10}$$

Eq.(10) can be considered as a 'mathematical transient' by definition so that the E_1-transformation can be applied to Eq. (10),

$$E_1(\phi_t)=\frac{\begin{vmatrix}\phi_{t-1} & \phi_t\\ \Delta\phi_{t-1} & \Delta\phi_t\end{vmatrix}}{\begin{vmatrix}1 & 1\\ \Delta\phi_{t-1} & \Delta\phi_t\end{vmatrix}}=\frac{\phi_t\phi_{t-2}-\phi_{t-1}^2}{\phi_t+\phi_{t-2}-2\phi_{t-1}} \tag{11}$$

Eq.(11) can be rewrittent form by Eq.(10);

$$E_1(\phi_t)=\phi_t+\omega(\phi_t-\phi_{t-1}), \tag{12}$$

where

$$\omega=\frac{1}{1-\mu_1},\quad \mu_1=\frac{\phi_t-\phi_{t-1}}{\phi_{t-1}-\phi_{t-2}}.$$

Eq.(12) is the extrapolation form and ω is called the 'extrapolation factor'.

II. 3. E_1^2-Transformation

In Eq.(9), if the number of iteration is large enough and the iterative matrix is convergent, only the dominant terms $\mu_1^t\ a_1\ \psi_1$, $\mu_2^t\ a_2\ \psi_2$ remain and the other terms fade out, then Eq. (10) can be replaced by

$$\phi_t=\phi_\infty+a_1\psi_1\mu_1^t+a_2\psi_2\mu_2^t.$$

Now there are 5 unknowns, ϕ_∞, $a_1\psi_1\mu_1^t$, $a_2\psi_2\mu_2^t$, therefore the 5 consecutive values, ϕ_t, ϕ_{t-1}, ϕ_{t-2}, ϕ_{t-3}, ϕ_{t-4}, should be used to determine the unknows, especially ϕ_∞, i.e., ϕ_∞ can be obtained by E_2^1-transform of $\{\phi_t\}$ ($t=t, t-1, t-2, t-3, t-4$). This procedure can be easity illustrated by Fig. 1.

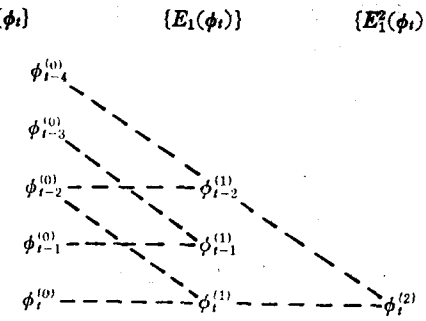

Fig. 1. The Scheme to Obtain $\phi_t^{(2)}$ with 5 Consecutive Values of ϕ_t.

In Fig. 1, one can obtain the E_1^2-transform of $\{\phi_t\}$ by using Eq. (12) as follows;

$$\phi_t^{(2)}=\phi_t^{(0)}+b(\phi_t^{(0)}-\phi_{t-1}^{(0)})+q(\phi_{t-1}^{(0)}-\phi_{t-2}^{(0)}) \quad (13)$$

where

$$q=\frac{\lambda_{t-1}(\lambda_t-\lambda_{t-1})}{\frac{\lambda_{t-2}(1-\lambda_{t-1})^2(1-\lambda_t)}{(1-\lambda_{t-2})\lambda_{t-1}}-(1-2\lambda_t+\lambda_{t-1})(1-\lambda_{t-1})}, \quad (14)$$

$$b=\frac{\lambda_t-q\left(\frac{1-\lambda_{t-1}}{\lambda_{t-1}}\right)}{1-\lambda_t}, \quad (15)$$

$$\lambda_t=\frac{\phi_t^{(0)}-\phi_{t-1}^{(0)}}{\phi_{t-1}^{(0)}-\phi_{t-2}^{(0)}}. \quad (16)$$

Eq. (13) is a form of the 'double extrapolation'.

II. 4. Double Extrapolation Adopted in VENTURE

From Eq. (13),

$$\phi_\infty-\phi_t=b_t(\phi_t-\phi_{t-1})+q_t(\phi_{t-1}-\phi_{t-2}),$$

or

$$\phi_\infty-\phi_{t-1}=b_{t-1}(\phi_{t-1}-\phi_{t-2})+q_{t-1}(\phi_{t-2}-\phi_{t-2}).$$

This recursion relationship leads to the equation:

$$\lambda_t\left(1+b_t+\frac{q_t}{\lambda_t}\right)=b_{t-1}+\frac{q_{t-1}}{\lambda_{t-1}},$$

where λ_t is defined by Eq. (16).

At some stage of calculation, it is assumed that the individual error vector contributes in such a way that the values of b_t and q_t are nearly independent of the outer iteration t, i.e., $b_t=b_{t-1}$, $q_t=q_{t-1}$. In that case,

$$q_t=\frac{\lambda_{t-1}\lambda_{t-2}(\lambda_t-\lambda_{t-1})}{\lambda_{t-2}(1-\lambda_{t-1})^2-\lambda_{t-1}(1-\lambda_t)(1-\lambda_{t-2})}, \quad (17)$$

$$b_t=\frac{\lambda_t-q_t\left(\frac{1-\lambda_{t-1}}{\lambda_{t-1}}\right)}{1-\lambda_t}. \quad (18)$$

The above double extrapolation adopted in VENTURE is different, only in the way of treatment for q_t, from that of the E_1^2-transform.

II. 5. Equipose Method

If the SLOR method is applied to 2-group diffusion equations, it leads to the equations[1]:

$$\phi_1^{(t)}=\boldsymbol{M}_1\phi_1^{(t-1)}+\boldsymbol{g}_1, \quad (19)$$

$$\phi_2^{(t)}=\boldsymbol{M}_2\phi_2^{(t-1)}+\boldsymbol{g}_2. \quad (20)$$

In a modified scheme called the 'Equipose method', essentially only one inner iteration is employed. Hence, although the number of outer iterations is increased, the total time may be minimized. The Equipose method estimates the eigenvalue k by the neutron balance equation shown in Eq. (1). This Equipose method has a validity to a large extent as shown in many literatures.[1,2,3]

The ability of arriving at a stable solution and the corresponding rate of convergence are intimately related to the properties of the iterative matrices $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$[7,8] in Eqs. (19) and (20). When $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$ have different convergence rate each other, it may be possible to employ the different number of inner iteration for each energy group, i.e., the number of inner iteration of Eq. (19) may be different from that of Eq. (20).

If one define 'flux variation' by

$$r^{t+1}=\frac{|\phi^{t+1}-\phi^t|}{|\phi_t^{t+1}|} \quad (21)$$

the different convergence rate between $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$ may be shown by comparing the fast flux variation, r_1^{t+1}, with the thermal flux variation, r_2^{t+1}.

III. Applications and Results

III. 1. Two-Dimensional Benchmark Problem

The 2-dimensional geometry of the IAEA

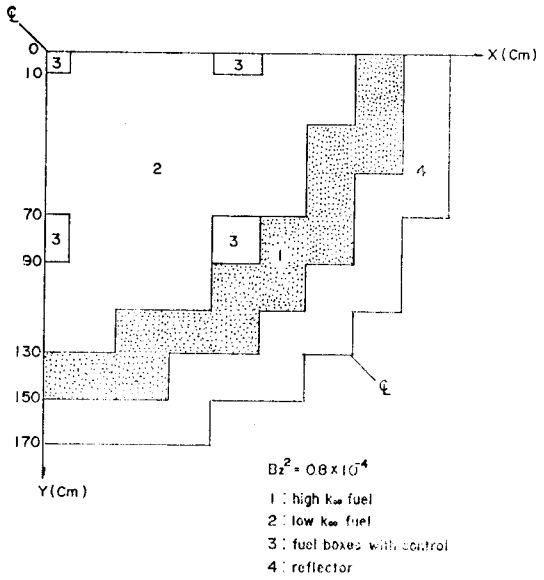

Fig. 2. 2-D Geometry of IAEA Benchmark Problem

Table 1. Assembly homogenized 2-group cross section of IAEA benchmark problem

region	group	D(cm)	Σ_r(cm^{-1})	Σ_a(cm^{-1})	Σ_f(cm^{-1})
1	1	1.5	0.02	0.01	0
	2	0.4	—	0.08	0.135
2	1	1.5	0.02	0.01	0
	2	0.4	—	0.085	0.135
3	1	1.5	0.02	0.01	0
	2	0.4	—	0.13	0.135
4	1	2.0	0.04	0	0
	2	0.3	—	0.01	0

benchmark problem[9,10] is shown in Fig. 2 and the group constants[11] are given in Table 1. To test our method, the number of meshes are fixed to 47×47.

In Table 2 is shown the change of the iteration time with the different number of inner iteration per an outer iteration, which is the same for each energy group. In Table 2, it is found that the Equipose mothod is validated for its effectiveness, i.e., when the number of inner iterations is only one for all energy groups, total iteration time is minimum. Although the number of outer iterations is the largest with single inner iteration, the total iteration time

Table 2. 2D IAEA Benchmark Problem Iteration Time
(same no. of inner iteration for groups)

group	no. of inner iteration	no. of outer iteration	total iteration time(min.)	k_{eff}
fast thermal	1 1	118	3.766	1.029383
fast thermal	2 2	103	4.447	1.029373
fast thermal	3 3	71	3.923	1.029375
fast thermal	4 4	78	5.194	1.029380
fast thermal	10 10	59	8.137	1.029377

Table 3. 2D IAEA Benchmark Problem Iteration Time
(different No. of inner iteration for groups)

group	No. of inner iteration	No. of outer iteration	total iteration time(min.)	k_{eff}
fast thermal	2 1	85	3.313	1.029382
fast thermal	3 1	74	3.344	1.029387
fast thermal	5 1	75	4.100	1.029386
fast thermal	8 1	74	5.636	1.029385

is the smallest of 3.766min.

When the number of inner iterations is different for each energy group, however, the Equipose method is not the best one as shown in Table 3. In case the number of inner iterations for the fast and for the thermal group is 2 and 1, respectivey, the total iteration time is the minimum of 3.313min. This iteration time is shorter than the 3.766min. of the Equipose method by about 12%. Also, in case the number of inner iterations for the fast and for the thermal group is 3 and 1, respectively, iteration time is shorter than that of the Equipose method by nearly 11%. Usually, the order of r_1^{t+1} in Eq. (21) is $10^{-3}\sim10^{-5}$ and that of r_2^{t+1} is $10^0\sim10^1$ during the inner iteration per outer iteration for 2-group problems.

When the condition[1] for the single extrapolation is satisfied during outer iteration in

Table 4. IAEA Benchmark Problem Comparision of Double Extrapolation to Single

extrapolation method	inner iteration		no. of outer iteration	total iteration time(min.)	total extrapolation no.	remark	SLOR
	group	number					
single	fast thermal	1 1	118	3.766	3		restrained
double	fast thermal	1 1	118	3.835	3	No double extrapolation occuring	//
single	fast thermal	3 1	74	3.344	1	1 double extrapolation occurring before convergence	//
double	fast thermal	3 1	75	3.367	1		//
single	fast thermal	3 3	71	3.923	2	2 double extrapolation occurring	//
double	fast thermal	3 3	67	3.774	2		//

CITATION, to compare the double extrapolation with the single, the double extrapolation using Eq. (17) is activated in place of the single when five consequative computations of sufficiently small error bound are carried. The comparisons in Table 4 show that the double extrapolation is very effective provided the condition for the double extraoolation is met. When the number of the inner iterations is 3 for all energy group, the double extrapolation makes the iteration scheme faster than the single extrapolation does. In this case, the total iteration time is 3.774 min., and it is faster than that of the single extrapolation by about 4%.

When the number of inner iterations is 3 for all energy groups, and the double extrapolation using Eq. (14) instead of Eq. (17) is adopted, and the condition for the double extrapolation is the same as above, the total iteration time is somewhat longer, 3.974 min., in spite of its faster convergence rate for 'mathematical transient'. The reason may be that it is not adequate to apply the condition for double extrapolatton adopted in VENTURE for the double extrapolation using Eq. (14).

In Table 4, if the double extrapolation's occurring condition is not satisfied, the double extrapolation does not occur and the total iteration time is more or less longer than that of the absence of the double extrapolation routine by negligible 1.4%. The reason is that the double extrapolation scheme needs one more outer iteration scheme, although the double extrapolation's occurring condition is not satisfied.

If the condition for the double extrapolation is satisfied, however, it is desirable to adopt the double extrapolation routine instead of the single extrapolation routine. In such a case the only disadvantage of adopting the double extrapolation routine is that one more scratch disk file is needed, which can be easily treated.

III. 2. Kori 1 Unit Reactor Core

The geometry of Kori reactor core is shown in Fig. 3 and 2-group contants obtained in the reference[12] are given in Table 5. To test our

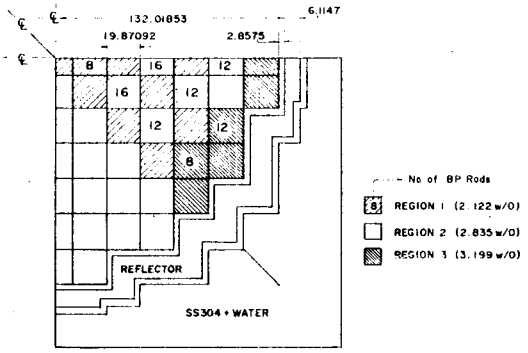

Fig. 3. 2-D Geometry of Kori Unit 1

Table 5. 2-Group Constant for Kori Unit 1

zone	group	D	Σ_f	Σ_a	Σ_{1-2}
region 1 no BP	1	1.4331	0.5432×10^{-2}	0.9190×10^{-2}	0.1700×10^{-1}
	2	0.5487	0.1819	0.1399	—
region 1 8 BP	1	1.4430	0.5432×10^{-2}	0.9580×10^{-2}	0.1632×10^{-1}
	2	0.5498	0.1844	0.1583	—
region 2 no BP	1	1.4263	0.6387×10^{-2}	0.9330×10^{-2}	0.1633×10^{-1}
	2	0.5378	0.2375	0.1665	—
region 2 12 BP	1	1.4410	0.6387×10^{-2}	1.0200×10^{-2}	0.1525×10^{-1}
	2	0.5392	0.2427	0.1962	—
region 2 16 BP	1	1.4455	0.6388×10^{-2}	1.0380×10^{-2}	0.1485×10^{-1}
	2	0.5399	0.2452	0.2068	—
region 3 no BP	1	1.4218	0.6884×10^{-2}	0.9000×10^{-2}	0.1603×10^{-1}
	2	0.5243	0.2658	0.1804	—
region 3 8 BP	1	1.4318	0.6885×10^{-2}	1.0260×10^{-2}	0.1536×10^{-1}
	2	0.5251	0.2699	0.1999	—
region 3 12 BP	1	1.4366	0.6884×10^{-2}	1.0440×10^{-2}	0.1496×10^{-1}
	2	0.5255	0.2720	0.2107	—
baffle	1	1.0703	0.	0.1200×10^{-2}	0.0140×10^{-1}
	2	0.5275	0.	0.2592	—
reflector	1	1.9552	0.	0.1150×10^{-2}	0.3904×10^{-1}
	2	0.4285	0.	0.0554	—
barrel	1	1.4732	0.	0.2530×10^{-2}	0.1731×10^{-1}
	2	0.4372	0.	0.0734	—
water+S.S.	1	0.9248	0.	0.3340×10^{-2}	0.1055×10^{-1}
	2	0.4888	0.	0.2047	—

Table 6. Kori Unit 1 Problem Iteration Time
(varying no. of inner iteration for groups)

group	no. of inner iteration	no. of outer iteration	total iteration time(min.)	SLOR
fast thermal	1 1	97	2.981	unrestrained
fast thermal	2 1	58	2.106	〃
fast thermal	3 1	57	2.370	〃
fast thermal	3 2	69	3.261	〃
fast thermal	1 1	93	2.943	restrained
fast thermal	2 2	84	3.624	〃
fast thermal	2 1	57	2.147	〃
fast thermal	3 3	53	2.905	〃

method, the number of meshes are fixed to 46×46. As done for the previous benchmark problem, the total iteration time with the different number of inner iterations is tabulated in Table 6. The table shows the cases in which the SLOR is either restrained or unrestrained[1].

In case the number of inner iteration for the fast and the thermal group is 2 and 1, respectively, the total iteration time is shorter than that of the Equipose method by 27% for the restrained SLOR and by 29% for the unrestrained SLOR.

Similiarly to the previous benchmark problem, one can also deal with the double extrapolation using Eq.(17) as shown in Table 7. In Table 7, although the double extrapolation doesn't occur, the inaccurate occurring of the single extrapolation can be repaired by adopting the double extrapolation routine as shown in case the number of the inner iteration is 3 for all energy groups.

IV. Conclusion

The results of applications of the method of varying the number of inner iteration for each energy group in 2D-problems indicates that the

Table 7. Kori Unit 1 Problem Comparision of Double Extrapolation to Single

extrapolation method	inner iteration		no. of outer iteration	total iteration time(min.)	total extrapolation no.	remark	SLOR
	group	number					
single	fast thermal	1 1	93	2.943	3		restrained
double	fast thermal	1 1	96	2.996	3	no double extrapolation occurring	〃
single	fast thermal	3 3	53	2.905	2		〃
double	fast thermal	3 3	48	2.597	1	no double extrapolation occurring	〃
single	fast thermal	1 1	97	2.981	3		unrestrained
double	fast thermal	1 1	100	3.068	3	no double extrapolation occurring	〃

method is acceptable for a two-group treatment. This method is faster than the Equipose method in the iteration convergence. Specially, in case the number of the inner iteration for the fast and thermal group is 2 and 1, respectively, the results are the best with about 12% improvement in the iteration convergence over the Equipose method. The double extrapolation is also desirable to be used in the CITATION code.

However, it is necessary to study further the condition for the double extrapolation, especially for the E_1^2-transform double extrapolation. The method of varying the number of inner iteration for each energy group in 2D-problems is verified only for a 2-group treatment. For other multi-group problems further investigations are needed.

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