JAERI 1210

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EXPANDA-5
The One-Dimensional Diffusion Equation Program for Fast Reactors Consisting of Two-Region Hexagonal Lattices

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日本原子力研究所
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EXPANDA-5

The One-Dimensional Diffusion Equation Program for Fast Reactors Consisting of Two-Region Hexagonal Lattices

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Summary

An advanced approximate treatment was developed for obtaining the effective cross sections of various nuclides in a hexagonal two-region lattice, consisting of pin-typed fuels and coolant. In this approximation, an assumption is made that the ratio ζ_1 of the flux in fuel part to the total flux ϕ in a cell does not vary significantly with energy so that the flux ϕ_i in each part of fuel and coolant can be represented by a product of ϕ and ζ_i. This ζ_1 is calculated by the transport equation describing a cell system and using ζ_1, the effective cross sections of each nuclide in the cell are estimated.

Based on the above treatment, a one-dimensional diffusion equation program EXPANDA-5 has been developed. The JAERI-fast set in 25 groups is utilized in this program.

二領域六方格子の領域を含む高速炉系の一次元拡散コード，EXPANDA-5

日本原子力研究所　東海研究所
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要　　旨

冷却材中に燃料ピンが六方格子状に配列された領域における実効断面積を求めるさい，格子内の全中性子束 ϕ に対する燃料内の中性子束の割合 ζ_1 が，エネルギーにほとんど依存しないとの仮定のもとに，格子内の燃料，冷却材の各部分における中性子束 ϕ_i を，全中性子束 ϕ と各部分での割合い ζ_i の積で表示し，格子系での輸送方程式から ζ_1 を求める式を導いた．この ζ_1 を用いて六方格子系からなる高速炉の領域における各核種の実効断面積を求め，続けて原子炉全体で，一次元拡散モデルにより臨界計算をおこなうプログラム EXPANDA-5 を作成した．炉定数ライブラリーは25群の JAERI-fast セットが用いられている．

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1. Introduction

For the criticality calculation of fast reactor systems, each spatial region of the reactor has been usually treated as a homogeneous one, that is, the effective cross sections of each nuclide in the region were calculated from the smeared densities of the elements, using the library data of a group constants set (such as YOM, HR, ABBN or JAERI) for each element, then these effective cross sections were used as the coefficients in the transport or diffusion equation.

However, it is rather a rough approximation to estimate the coefficients with homogeneous model as stated above, because, in core or blanket, fuels are arranged heterogeneously in coolant, and so, the neutron flux in each of fuel and coolant differs from that obtained by homogeneous model.

First of all, for detailed investigation of heterogeneity effects in hexagonal lattices of pin-typed fuels and coolant, two programs named ESELEM-3[1] and SDRC[2] were developed. Both these programs utilized the same nuclear data from which the JAERI-fast set[3),4)] was produced. The ESELEM-3 treats mainly the heterogeneity effects due to fission source distribution, on the other hand, the SDRC deals with the effects due to resonance absorption distribution.

Using these programs, fine and ultra-fine spectra in fuel and coolant regions in a cell were obtained, and it was confirmed that the effects are not so large for the usual fuel pins in fast reactors, and that the ratio ζ_1 of the flux in fuel region to the total flux in a cell,

$$\zeta_1=\frac{\phi_1}{\phi_1+\phi_2}$$

does not vary significantly with energy[5].

But the detailed calculations are expensive in time and cannot treat the reactor as a whole but a unit cell.

An approximate method has been developed to take the heterogeneity effects into account for estimating the effective cross sections of each nuclide in a region where pin-typed fuels are arranged hexagonally in coolant.

In this method, an assumption is made that ζ_1 does not vary much with energy, through several groups in the range of down scattering.

But this assumption is valid enough as the results of detailed calculations have shown.

And based on this method, the one-dimensional diffusion equation program EXPANDA-5 has been developed.

The applicability of the program was also examined over a wide range of lattice pitch comparing the results with those of the detailed calculations[5].

Now, let us introduce the simplified method of obtaining the effective cross sections for the heterogenous regions in 25 energy group structure of usual criticality calculation for fast reactors, using the JAERI-fast set as the library group constants data.

2. The transport equations for a cell system by the product representation of fluxes

In the stationary state, the Boltzmann equation is written as

$$\vec{\Omega}\,\mathrm{grad}\,\psi(\vec{r},\ E,\ \vec{\Omega})+\Sigma_t(E)\psi(\vec{r},\ E,\ \vec{\Omega})=q(\vec{r},\ E,\ \vec{\Omega}) \quad \cdots\cdots(1)$$

$$q(\vec{r},\ E,\ \vec{\Omega})=\iint\left[\Sigma_e(E'\to E,\ \vec{\Omega}'\to\vec{\Omega})+\frac{1}{4\pi}\Sigma_{in}(E'\to E)+\frac{1}{4\pi}\chi(E)\nu\Sigma_f(E')\right]\phi(\vec{r},\ E',\ \vec{\Omega}')dE'd\vec{\Omega}'$$

where the symbols used are usual ones. It is assumed that the spatial distribution obeys $e^{-i\vec{B}\cdot\vec{r}}$

$$\phi(\vec{r},\ E,\ \vec{\Omega})=\phi(B,\ E,\ \vec{\Omega})e^{-i\vec{B}\cdot\vec{r}}$$

Setting $\vec{\Omega}\cdot\vec{B}=\mu B$ and $\vec{\Omega}=\mu$, Eq. (1) is written as

$$(\Sigma_t-i\mu B)\phi(B,\ E,\ \mu)=q(B,\ E,\ \mu) \quad\cdots\cdots(2)$$

$$q(B,\ E,\ \mu)=\iint\left[\Sigma_e(E'\to E,\ \vec{\Omega}'\to\vec{\Omega})+\frac{1}{4\pi}\Sigma_{in}(E'\to E)+\frac{1}{4\pi}\chi(E)\nu\Sigma_f(E')\right]\phi(B,\ E',\ \mu')dE'd\vec{\Omega}'$$

With the usual spherical harmonics expansions

$$\phi(B,\ E,\ \mu)=\sum_{l=0}^{\infty}\phi^l(B,\ E)P_l(\mu)$$

$$\Sigma_e(E'\to E,\ \vec{\Omega}'\to\vec{\Omega})=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}S_l(E'\to E)P_{lm}(\vec{\Omega})P_{lm}{}^*(\vec{\Omega}'),$$

Eq. (2) becomes

$$(\Sigma_t-i\mu B)\sum_{l=0}^{\infty}\phi^l(B,\ E)P_l(\mu)$$

$$=\sum_{l=0}^{\infty}\frac{4\pi}{2l+1}P_l(\mu)\int\left[S_l(E'\to E)+\frac{1}{4\pi}\Sigma_{in}(E'\to E)\delta_{l0}+\frac{1}{4\pi}\chi(E)\nu\Sigma_f(E')\delta_{l0}\right]\phi^l(B,\ E')dE'$$

Then, operating

$$\int_{-1}^{1}d\mu P_{l'}(\mu)\left(1-\frac{i\mu B}{\Sigma_t}\right)^{-1}\cdot,$$

we obtain

$$\frac{1}{2l+1}\Sigma_t(E)\phi^l(B,\ E)$$

$$=\sum_{l'=0}^{\infty}\frac{4\pi}{2l'+1}A_{ll'}\int\left[S_{l'}(E'\to E)+\frac{1}{4\pi}\Sigma_{in}(E'\to E)\delta_{l'0}+\frac{1}{4\pi}\chi(E)\nu\Sigma_f(E')\delta_{l'0}\right]\phi^{l'}(B,\ E')dE'$$

where

$$A_{ll'}=A_{l'l}=\frac{1}{2}\int_{-1}^{1}\frac{P_l(\mu)P_{l'}(\mu)}{1-i\alpha\mu}d\mu$$

$$\alpha=B/\Sigma_t$$

When $S_l(E'\to E)=0$ for $l\geqq 2$, the resulting B_1 equation becomes[13]

$$\begin{cases}\Sigma_t\phi^0(B,\ E)=A_{00}\int[4\pi S_0(E'\to E)+\Sigma_{in}(E'\to E)+\chi(E)\nu\Sigma_f(E')]\phi^0(B,\ E')dE' \\ \qquad\qquad +\dfrac{A_{01}}{3}\int 4\pi S_1(E'\to E)\phi^1(B,\ E')dE' \quad\cdots\cdots(3) \\ \dfrac{1}{3}\Sigma_t\phi^1(B,\ E)=A_{10}\int[4\pi S_0(E'\to E)+\Sigma_{in}(E'\to E)+\chi(E)\nu\Sigma_f(E')]\phi^0(B,\ E')dE' \\ \qquad\qquad +\dfrac{A_{11}}{3}\int 4\pi S_1(E'\to E)\phi^1(B,\ E')dE' \quad\cdots\cdots(4)\end{cases}$$

where

$$A_{00}=\frac{1}{\alpha}\tan^{-1}\alpha$$

$$A_{01}=A_{10}=\frac{i}{\alpha}\left(1-\frac{1}{\alpha}\tan^{-1}\alpha\right)$$

$$A_{11}=\frac{1}{\alpha^2}\left(1-\frac{1}{\alpha}\tan^{-1}\alpha\right)$$

$$A_{00}A_{11}-A_{01}A_{10}=\frac{1}{\alpha^2}\left(1-\frac{1}{\alpha}\tan^{-1}\alpha\right),$$

and we can write

$$\psi^0(B,\ E)=\phi(B,\ E)$$
$$\psi^1(B,\ E)=3iJ(B,\ E).$$

Now we consider a hexagonal lattice of pitch t, where each hexagonal cell contains a fuel rod of radius r_1 in the center of the cell. The areas of the fuel and the remaining moderator part in the hexagon are denoted by V_1 and V_2 respectively, and

$$V=V_1+V_2$$

is the area of a hexagon. If a congruent hexagon is written on the lattice at arbitrary position and arbitrarily rotated angle, it always contains fuel and moderator regions of areas V_1 and V_2 respectively. So, we can consider the unit cell as a unit volume element for the transport equations (3) and (4) describing the lattice system. Let the total flux in a cell and the ratio be

$$\psi^0=\sum_i\psi_i{}^0=\phi$$
$$\zeta_i=\psi_i{}^0/\psi^0$$

where $i=1$ means the fuel region, and $i=2$ the moderator region. Then the flux of each region

$$\phi_i=\psi_i{}^0=\psi^0\zeta_i$$

can be represented by a product of ϕ and ζ_i.

If we neglect the $\vec{\zeta}_i{}^1$ in the spherical harmonics expansion for ζ_i

$$\zeta_i=\zeta_i{}^0+3\vec{\Omega}\cdot\vec{\zeta}_i{}^1,$$

we can write

$$\psi_i(B,\ E,\ \mu)=\psi_i{}^0+\psi_i{}^1\mu=(\psi^0+\psi^1\mu)\zeta_i{}^0=(\phi+3iJ\mu)\zeta_i{}^0.$$

As the result, we can rewrite ψ^l in the Eqs. (3) and (4),

$$\psi_i{}^l=\psi^l\zeta_i \quad (\text{for } l=0,\ 1)$$

where $\psi_i{}^l$ and ψ^l are the integrated values in the region i and the cell respectively.

Next, we introduce the collision probabilities $p_{ij}{}^*$ for a neutron uniformly generated in region i to suffer its first collision in region j including region j of all of other cells.

Another form of the transport equation is written,

$$\psi(\vec{r},\ E,\ \vec{\Omega})=\int_0^\infty ds\exp\left[-\int_0^s ds'\Sigma_t(\vec{r}-s'\vec{\Omega},\ E)\right]q(\vec{r}-s\vec{\Omega},\ E,\ \vec{\Omega})$$

Again, Fourier transformation with $e^{-i\vec{B}\cdot\vec{r}}$ is done, and integrated over a unit cell and $\vec{\Omega}$,

$$\Sigma_t\psi^0=\frac{1}{2}\int_{-1}^1 d\mu\Sigma_t\int_0^\infty ds\exp\left[-\int_0^s\Sigma_t(\vec{r}-s'\vec{\Omega},\ E)ds'+i\mu Bs\right]q(B,\ E)=A_{00}q$$

where A_{00} is the non-leakage probability of the neutrons generated in a cell out of the lattice. Then the $p_{ij}{}^*$ may be written,

$$p_{ij}{}^*=A_{00}p_{ij}$$

where p_{ij} is normalized ($\sum_j p_{ij}=1$) probabilities for the infinite cell system given in the next chapter.

From the above argument, Eqs. (3) and (4) are written for the two region cell system, with energy integration term denoted by $q_j{}^l$,

$$\Sigma_{ti}\psi^0\zeta_i=A_{00}\sum_j p_{ji}q_j{}^0+\frac{1}{3}A_{01}\sum_j p_{ji}q_j{}^1 \quad\cdots\cdots(5)$$

$$\frac{1}{3}\Sigma_{ti}\psi^1\zeta_i=A_{10}\sum_j p_{ji}q_j{}^0+\frac{1}{3}A_{11}\sum_j p_{ji}q_j{}^1 \quad\cdots\cdots(6)$$

$\sum_j p_{ji}q_j{}^l$ are solved from (5) and (6),

$$\sum_j p_{ji}q_j{}^0=\Sigma_{ti}\psi^0\zeta_i-\frac{iB}{3\Sigma_t}\Sigma_{ti}\psi^1\zeta_i=\Sigma_{ti}\phi\zeta_i+\frac{B}{\Sigma_t}\Sigma_{ti}J\zeta_i \quad\cdots\cdots(7)$$

$$\sum_j p_{ji}q_j{}^1=3\gamma^*\Sigma_{ti}\psi^1\zeta_i-\frac{3iB}{\Sigma_t}\Sigma_{ti}\psi^0\zeta_i \quad\cdots\cdots(8)$$

where $\gamma^*=\dfrac{\alpha\tan^{-1}\alpha}{3(1-(1/\alpha)\tan^{-1}\alpha)}$ and $\gamma^*\simeq 1$ for small α.

Summing (8) over subscript i,

$$q^1=3\gamma^*\Sigma_t\phi^1-3iB\phi^0$$

$$4\pi\int S_1(E'\to E)(3iJ)dE'=3\gamma^*\Sigma_t(3iJ)-3iB\phi$$

but when J is slowly varying function of lethargy u, $4\pi\int S_1(E'\to E)J(B,\ E')dE'$ is nearly equal to $3\bar{\mu}\Sigma_s J$, so that

$$9i\bar{\mu}\Sigma_s J=9i\gamma^*\Sigma_t J-3iB\phi$$

$$J=\frac{1}{3(\gamma^*\Sigma_t-\bar{\mu}\Sigma_s)}B\phi=DB\phi$$

substituting $DB\phi$ into J of Eq. (7),

$$\Sigma_{ti}\phi\zeta_i+\frac{DB^2}{\Sigma_t}\Sigma_{ti}\phi\zeta_i=\sum_j p_{ji}\int[\Sigma_{sj}(E'\to E)+\chi(E)\nu\Sigma_{f1}(E')\delta_{j1}]\phi_j(E')dE' \quad\cdots\cdots(7')$$

If the ζ_i does not vary significantly with energy, it can be put out of the integration sign on the right hand side of Eq. (7'),

$$\begin{cases}\gamma\Sigma_{t1}\phi\zeta_1=p_{11}S_1\zeta_1+p_{21}S_2\zeta_2+p_{11}\chi Q & \cdots\cdots(9)\\ \gamma\Sigma_{t2}\phi\zeta_2=p_{12}S_1\zeta_1+p_{22}S_2\zeta_2+p_{12}\chi Q & \cdots\cdots(10)\end{cases}$$

where

$$\gamma=1+\frac{DB^2}{\Sigma_t}$$

$$S_i=\int\Sigma_{si}(E'\to E)\phi(E')dE'$$

$$Q=\int\nu\Sigma_{f1}(E)\phi_1(E)dE\equiv 1$$

Using the relation $\zeta_1+\zeta_2=1$, equations (9), (10) can be rearranged about ζ_1 and ζ_2,

$$\begin{cases}(\gamma\Sigma_{t1}\phi-p_{11}S_1-p_{11}\chi Q)\zeta_1=(p_{21}S_2+p_{11}\chi Q)\zeta_2\\ (p_{12}S_1+p_{12}\chi Q)\zeta_1=(\gamma\Sigma_{t2}\phi-p_{22}S_2-p_{12}\chi Q)\zeta_2\end{cases}$$

In theses relations, the ratios of coefficients of ζ_i must be equal, so let the ratio be,

$$\theta=\frac{\gamma\Sigma_{t1}\phi-p_{11}S_1-p_{11}\chi Q}{p_{12}S_1+p_{12}\chi Q}=\frac{p_{21}S_2+p_{11}\chi Q}{\gamma\Sigma_{t2}\phi-p_{22}S_2-p_{12}\chi Q} \quad\cdots\cdots(11)$$

When the cell is homogeneous, θ is unity because

$$\Sigma_{t1}=\Sigma_{t2}=\Sigma_t$$

$$S_1=S_2=S$$

$$\theta=\frac{(\gamma\Sigma_t\phi-p_{11}S-p_{11}\chi Q)+(p_{21}S+p_{11}\chi Q)}{(p_{12}S+p_{12}\chi Q)+(\gamma\Sigma_t\phi-p_{22}S-p_{12}\chi Q)}=\frac{\gamma\Sigma_t\phi+(p_{21}-p_{11})S}{\gamma\Sigma_t\phi+(p_{12}-p_{22})S}=1$$

Considering the above result, θ may be supposed to be nearly unity for the cell with slight heterogeneity. Now, S_1 and S_2 are expressed by this θ. From the relation (11),

$$\begin{cases}(p_{11}+\theta p_{12})S_1=\gamma\Sigma_{t1}\phi-(p_{11}+\theta p_{12})\chi Q\\ (p_{21}+\theta p_{22})S_2=\theta\gamma\Sigma_{t2}\phi-(p_{11}+\theta p_{12})\chi Q\end{cases}$$

Changing the terms in parentheses like

$$p_{11}+\theta p_{12}=1-p_{12}+\theta p_{12}=1-(1-\theta)p_{12}$$

$$p_{21}+\theta p_{22}=1-p_{22}+\theta p_{22}=1-(1-\theta)p_{22},$$

S_1, S_2 become

$$\begin{cases}S_1=\dfrac{\gamma\Sigma_{t1}\phi-\{1-(1-\theta)p_{12}\}\chi Q}{1-(1-\theta)p_{12}} & \cdots\cdots(12)\\ S_2=\dfrac{\theta\gamma\Sigma_{t2}\phi-\{1-(1-\theta)p_{12}\}\chi Q}{1-(1-\theta)p_{22}} & \cdots\cdots(13)\end{cases}$$

Solving the equation (11) about ζ_1,

$$\zeta_1=\frac{\gamma\Sigma_{t2}\phi-p_{22}S_2-p_{12}\chi Q}{\gamma\Sigma_{t2}\phi+p_{12}S_1-p_{22}S_2}$$

Putting the relations (12) and (13) into S_1 and S_2 in the above equation,

$$\zeta_1=\frac{1+\dfrac{p_{22}-p_{12}}{\gamma\Sigma_{t2}\phi p_{21}}\chi Q}{1+\dfrac{p_{12}\Sigma_{t1}}{p_{21}\Sigma_{t2}}\cdot\dfrac{1-(1-\theta)p_{22}}{1-(1-\theta)p_{12}}+\dfrac{p_{22}-p_{12}}{\gamma\Sigma_{t2}\phi p_{21}}\chi Q}$$

By the relations between collision probabilities

$$p_{11}+p_{12}=p_{21}+p_{22}=1$$
$$V_1\Sigma_{t1}p_{12}=V_2\Sigma_{t2}p_{21},$$

ζ_1 finally becomes,

$$\zeta_1=\frac{1+\dfrac{p_{11}-p_{21}}{\gamma\Sigma_{t2}\phi p_{21}}\chi Q}{1+\dfrac{V_2}{V_1}\cdot\dfrac{1-(1-\theta)p_{22}}{1-(1-\theta)p_{12}}+\dfrac{p_{11}-p_{21}}{\gamma\Sigma_{t2}\phi p_{21}}\chi Q} \quad \cdots\cdots(14)$$

It can be easily proved that in homogeneous case ζ_1 becomes equal to volume ratio of the fuel region, VR_1. First, when there is no fission source (for instance, in the energy groups below the resonance region), then $\chi Q=0$ and as $\theta=1$ for homogeneous case,

$$\zeta_1=\frac{1}{1+\dfrac{V_2}{V_1}}=VR_1.$$

Secondly, when there is fission source, the terms of χQ in (9) and (10) must be replaced by $p_{11}\chi Q_1+p_{21}\chi Q_2$ and $p_{12}\chi Q_1+p_{22}\chi Q_2$ respectively, and restarting from (9) and (10) to get ζ_1 like (14),

$$\zeta_1=\frac{1+\dfrac{p_{11}-p_{21}}{\gamma\Sigma_{t2}\phi p_{21}}\chi Q_1}{1+\dfrac{V_2}{V_1}\cdot\dfrac{1-(1-\theta)p_{22}}{1-(1-\theta)p_{12}}+\left\{\chi Q_1+\dfrac{1-(1-\theta)p_{22}}{1-(1-\theta)p_{12}}\chi Q_2\right\}\dfrac{p_{11}-p_{21}}{\gamma\Sigma_{t2}\phi p_{21}}}$$

In this case θ is also unity and $Q_2=\dfrac{V_2}{V_1}Q_1$,

$$\zeta_1=\frac{1+\dfrac{p_{11}-p_{21}}{\gamma\Sigma_t\phi p_{21}}\chi Q}{\left(1+\dfrac{V_2}{V_1}\right)+\left(1+\dfrac{V_2}{V_1}\right)\dfrac{p_{11}-p_{21}}{\gamma\Sigma_t\phi p_{21}}\chi Q}=VR_1.$$

3. Collision probabilities for the two-region hexagonal lattice

Collision probabilities p_{ij} used in the previous chapter are calculated for the two-region hexagonal lattice by the BONALUMI's method[6]. And for the Dancoff correction G_m used in the method, the SAUER's approximate formula[7),8)] is adopted with the modification by BONALUMI[9]. From the fuel radius r_1 and the pin pitch t,

$$\bar{l}_2=2V_2/\pi r_1$$
$$\tau=(t-2r_1)/\bar{l}_2$$
$$\tau_1=\tau+\Sigma_{t2}\bar{l}_2/(7+2.125\,\Sigma_{t2}\bar{l}_2)$$

are defined, and giving

$$G_m=1-e^{-\tau\Sigma_{t_1}l_2}/\{1+(1-\tau_1)\Sigma_{t2}\bar{l}_2\}$$
$$G_f=2r_1\Sigma_{t1}\{1-P_c(\Sigma_{t1}r_1)\},$$

p_{ij} are calculated as follows,

$$p_{12}=\{1-P_c(\Sigma_{t1}r_1)\}G_m/\{1-(1-G_m)(1-G_f)\}$$
$$p_{11}=1-p_{12}$$
$$p_{21}=\Sigma_{t1}V_1p_{12}/\Sigma_{t2}V_2$$
$$p_{22}=1-p_{21}$$

where $P_c(x)$ is the collision probability for a single cylindrical rod of infinite length in axial direction and of optical radius x.

$P_c(x)$ is calculated by interpolation of the tabled data of CASE, *et al.*[10] making use of the function-type subprogram PC[11].

4. Calculation of the value of ζ_1

In order to calculate ζ_1 by equation (14) in the chapter 2, it is necessary to give Σ_i, B^2 and ϕ their appropriate values.

The effective macroscopic cross sections Σ_i for each region i in the cell is decided by the same way as in the EXPANDA-4[12] using the densities of the elements given in the region 1 (fuel) and region 2 (moderator). The background cross section σ_0 for interpolation of the f-tables is given as

$$\sigma_0=\sigma_{01}+\frac{VR_2}{VR_1}\sigma_{02} \quad \text{(for the elements in region 1)}$$

$$\sigma_0=\frac{VR_1}{VR_2}\sigma_{01}+\sigma_{02} \quad \text{(for the elements in region 2)}$$

This means that the interpolation is equivalent to that of the EXPANDA-4 where the homogenized densities of all the elements in the cell are used.

For the value of D and Σ_t for the cell as a whole

$$3D=(\Sigma_{tr1}VR_1+\Sigma_{tr2}VR_2)^{-1}$$
$$\Sigma_t=\Sigma_{t1}VR_1+\Sigma_{t2}VR_2,$$

then D, Σ_{t1}, Σ_{t2}, $\Sigma_{s1}{}^{l\to n}$, $\Sigma_{s2}{}^{l\to n}$ $(l\leqq n)$ are used in[14].

For the calculation of B^2 and ϕ by the relation of the material buckling and fluxes,

$$\Sigma_s{}^{l\to n}=\Sigma_{s1}{}^{l\to n}VR_1+\Sigma_{s2}{}^{l\to n}VR_2$$
$$\nu\Sigma_f{}^n=\nu\Sigma_{f1}{}^nVR_1+\nu\Sigma_{f2}{}^nVR_2$$

are also prepared, and the $B_m{}^2$ and ϕ are decided by iterative method from the relation,

$$(B_m{}^2D^n+\Sigma_t{}^n-\Sigma_s{}^{n\to n})\phi^n=\chi^n+\sum_{l<n}\Sigma_s{}^{l\to n}\phi^l$$
$$\left|\sum_n\nu\Sigma_f{}^n\phi^n-1\right|\leqq\varepsilon_1.$$

Then, D, Σ, B^2, ϕ and p_{ij} are all given for ζ_1 to be calculated in (14). But in the lowest energy groups, it sometimes occurs that the calculated value of ζ_1 becomes negative because of the strong absorption of the fuel materials which was wrongly estimated without consideration of shielding effect, like above $\Sigma_1VR_1+\Sigma_2VR_2$ (though the cross sections of the lowest groups will have no influence on the criticality calculation, the negative value of ζ_1 is not adequate in the procedure of calculating the effective cross sections described in the next chapter). To avoid this, the value of θ is calculated from both of the expressions in equation (11) as θ_1 and θ_2, and one of them which gives the larger value to

$$\xi=\frac{\dfrac{V_1}{V_2}\cdot\dfrac{1-(1-\theta)p_{22}}{1-(1-\theta)p_{12}}}{1+\dfrac{p_{11}-p_{21}}{\gamma\Sigma_{t2}\phi p_{21}}\chi Q}$$

is adoped to decide ζ_1 by

$$\zeta_1=1/(1+\xi).$$

As the macroscopic cross sections in the above process have been at first calculated with homogeneous model, it is better to recalculate ζ_1 from the cross sections modified with the ζ_i of the first step put in place of VR_i. But it is examined that the value of ζ_1 scarecely varies after the recalculation. For this reason, we use the ζ_1 of the first step in the next chapter.

5. The effective cross sections

The value of ζ_1 was obtained in the previons chapter. The value of ζ_2 is given by $1-\zeta_1$. The effective cross sections for the heterogeneous system are obtained with the ζ_i put in place of VR_i in the process deseribed before, that is, the values

$$\sigma_0=\sigma_{01}+\frac{\zeta_2}{\zeta_1}\sigma_{02}$$

$$\sigma_0=\frac{\zeta_1}{\zeta_2}\sigma_{01}+\sigma_{02}$$

for the elements in fuel and moderator region respectively are used in interpolating the table of self-shielding factors. In this procedure, all the techniques in the EXPANDA-4 are followed such as taking into account the mutual resonance interference of ^{235}U, ^{239}Pu or ^{240}Pu with the resonance of ^{238}U and as repetition of interpolating the f-table about σ_0.

After the interpolated value $\bar{f}$ is decided, the effective miroscopic cross sections are given by

$$\bar{\sigma}=\bar{f}(R,\ \sigma_0,\ T)\sigma_\infty\times\frac{\zeta_1}{VR_1}$$

$$\text{or}\quad \bar{\sigma}=\bar{f}(\sigma_0,\ T)\sigma_\infty\times\frac{\zeta_2}{VR_2}.$$

The ζ_i/VR_i is the correction factor so that $\bar{\sigma}$ should give the effective macroscopic cross sections when it is multiplied by the densities homogenized in the cell. This factor makes it possible to bring the heterogeneity effects into cross sections, even in some groups, elements or reactions, where the values of the f-table are not dependent on σ_0.

In the EXPANDA-5, each spatial region of a reactor can be treated either homogeneously or as two-region hexagonal lattice. In the latter case, the region is considered filled with the hexagonal lattice and the existence of the materials in the tube surrounding fuel assembly is ignored.

After the effective cross sections are calculated in due course of each spatial region, the one-dimensional diffusion equation is solved and the various data are printed as output, in the same way as the EXPANDA-4[12].

In order to examine the applicability of the method in the EXPANDA-5 in another scale of heterogeneity, several cases were calculated making r_1 and t of the lattice larger or smaller simultaneously. And the results were compared with those by the fine spectrum codes ESELEM-3 and SDRC. So it was confirmed that ζ_1 and k_{eff} of the EXPANDA-5 and those from the detailed calculations showed a satisfactory agreement making the pitch to 4 or 5 centimeter[5].

An example of ζ_1 in case of $t=0.76$ cm, $VR_1=0.47496$ is in the next page.

In this example, the group structure is same as that of the ABBN set. It is observed that $\zeta_1>VR_1$ in first 7 groups and $\zeta_1<VR_1$ in the remaining groups. This means the influences of the fission source distribution in the higher energy and the absorption distribution in the resonance or lower energy. The compositions of materials in the fuel and moderator region are shown in the example given in the next chapter.

gr.	ζ_1	gr.	ζ_1
1	0.47918	14	0.47005
2	0.47860	15	0.47175
3	0.47734	16	0.47070
4	0.47611	17	0.46896
5	0.47532	18	0.46501
6	0.47514	19	0.46428
7	0.47548	20	0.45965
8	0.47476	21	0.45736
9	0.47487	22	0.47049
10	0.47444	23	0.46239
11	0.47481	24	0.41562
12	0.47465	25	0.27991
13	0.47333		

6. The format of input data for EXPANDA-5

The cross section data library of JAERI-fast set of less than 30 group structure are supplied from the magnetic tape to the EXPANDA-5. This tape has been written in binary form, and each logical record in the tape corresponds to each energy group and contains the data of the group of all the 20 nuclides edited in the tape[12].

The input data by cards are nearly same as those of the EXPANDA-4[12], but a few items about the hexagonal lattice are added.

The formats and kinds of the input data in cards are described in the following.

101 (20 A 4) the title of the job

This card is necessary only once before the first problem even if the job contains more than one problems.

0 (I 1, I 6, 9 I 1, 2 I 3, 14 A 4)

- column 1——0
- the problem number

  $\begin{cases} \geqq 0 \cdots\cdots \text{the input } \Delta r \text{ is used} \\ < 0 \cdots\cdots \text{the } \Delta r \text{ resulted in the criticality adjustment in the previons case is used} \end{cases}$
- columns 8～16——the item numbers for input cards in # 1～# 9 which are necessary to be input in this problem (punched to the left side of this field without blank)

  In order to minimize the number of input cards, this code utilizes the 'blank check' method for the cards of # 1～# 9[12]. Even in the first problem, # 4, 7 or 9 can be neglected according to the nature of the problem. In the succeeding problems, only the cards of data changed are necessary.
- number of the cards in # 8
- number of the cards in # 9
- columns 23～78——the title of the problem

1 (13 I 3, 5 E 6.0)

- column 3——1
- number of spatial regions in the reactor, KMAX$\leqq$10
- boundary condition at the origin of the spatial coordinate

$$\text{ISYM}=\begin{cases} +1 \cdots\cdots \phi'(0)=0 \\ -1 \cdots\cdots \phi(0)=0 \end{cases}$$

- number of groups, IMAX≦30
- criticality adjustment

$$\text{ICRIT}=\begin{cases}+1\cdots\cdots\Delta r \text{ in a region is adjusted}\\ 0\cdots\cdots\text{no adjustment}\end{cases}$$

- selection of output data

$$\text{ISW}=\begin{cases}+2\cdots\cdots\Sigma,\ \phi,\ \psi\ (,\ B_m^2,\ BR,\ \text{condensed cross sections},\ \phi^*,\ \psi^*)\\ +1\cdots\cdots\Sigma,\ \phi\ (,\ B_m^2,\ BR,\ \text{condensed cross sections},\ \phi^*)\\ 0\cdots\cdots\phi\ (,\ B_m^2,\ BR,\ \text{condensed cross sections},\ \phi^*)\\ -1\cdots\cdots(B_m^2,\ \text{condensed cross sections},\ \phi^*)\end{cases}$$

About the items in the parentheses, the selection is given below. ϕ, ϕ^* are spectra normalized at every spatial mesh point.

- number of groups for slowing down scattering,

IDS≦IMAX-1 (IMAX=25, IDS=11 for the library tape which is now used.)

- KREG: the region number of the region where Δr is adjusted for criticality condition to be satisfied.
- geometry

$$\text{IP}=\begin{cases}0\cdots\cdots\text{slab}\\ 1\cdots\cdots\text{cylinder}\\ 2\cdots\cdots\text{sphere}\end{cases}$$

- adjoint fluxes

$$\text{NADJ}=\begin{cases}+1\cdots\cdots\text{calculated}\\ -1\cdots\cdots\text{not calculated}\end{cases}$$

- reaction rates and mass for each element

$$\text{IBR}=\begin{cases}+1\cdots\cdots\text{calculated}\\ -1\cdots\cdots\text{not calculated}\end{cases}$$

- material buckling B_m^2 for the composition of the first region

$$\text{IBSQM}=\begin{cases}+1\cdots\cdots\text{calculated}\\ 0\cdots\cdots\text{not calculated}\\ -1\cdots\cdots\text{calculated (but all the other output data are not calculated)}\end{cases}$$

- condensed cross sections

$$\text{LAPSE}=\begin{cases}N(1\leqq N\leqq 12)\cdots\cdots\text{condensed cross sections in } N \text{ group structure are calculated.}\\ 0\cdots\cdots\text{not calculated}\end{cases}$$

(When this item is preferred with IBR=+1, condensed Σ_c, Σ_a, $\bar{\sigma}_c$, $\bar{\sigma}_a$ for each element are also obtained.)

The following 5 data are in format of floating decimal point (5 E 6. 0).

- eigenvalue convergence criterion ε_1
- pointwise source convergence criterion ε_2
- $\Delta r_{\min}$, $\Delta r_{\max}$ ——the extreme values for Δr_{KREG} to be varied
- λ_2——the value of k_{eff} for which criticality adjustment is carried out

2 (I 3, 10 I 6)

- column 3——2
- number of elements in each region

(MM(K), K=1, KMAX)

1≦MM(K)≦20

3 (I 3, 10 I 6)

- columu 3——3

• mesh number of the outer boundary of each region, when the mesches are numbered 0, 1, 2, ····· from the origin, taking even number of mesh intervals in each region.

(INTER(K), K=1, KMAX)

$2 \leqq \text{INTER}(1) < \text{INTER}(2) < \cdots\cdots < \text{INTER}(\text{KMAX}) \leqq 100$

4 (I 3, 12 I 6)

• column 3——4

• last number of groups corresponding to each group of condensed structure

(IX(n), n=1, N)

$1 \leqq \text{IX}(1) < \text{IX}(2) < \cdots\cdots < \text{IX}(\text{N}) \leqq \text{IMAX}$

(The n-th coarse group corresponds to groups from IX($n-1$)+1 st to IX(n)-th in the original IMAX fine structure.)

5 (I 3, 10 E 6. 0)

• column 3——5

• mesh size for each region, Δr_k(cm)

(DR(K), K=1, KMAX)

6 (I 3, 10 E 6. 0)

• column 3——6

• absolute temperature for each region, $T_k \leqq 300$

(T(K), K=1, KMAX)

7 (I 3, 5 E 12. 5, 15 X, 2 I 1)

• column 3——7

• transverse buckling $B_\perp{}^2$ for each region

(BSQ(K), K=L+1, min{L+5, KMAX})

• column 79——1, but when there are two cards of # 7, 0 must be punched for the first card.

• column 80——NC=$\begin{cases} 1\cdots\cdots\text{for L=0} \\ 2\cdots\cdots\text{for L=5 (KMAX} \geqq 6) \end{cases}$

8 (I 3, 5(I 3, E 12. 5), 2 I 1)

• column 3——8

• code number and density (10^{24}cm^{-3}) for each element

(MCODE(M, K), AN(M, K), M=L+1, min{L+5, MM(K)})

• column 79——K (0 must be punched for the case of K=10)

• column 80——NC=$\begin{cases} 1\cdots\cdots\text{for L=0} \\ 2\cdots\cdots\text{for L=5} \\ 3\cdots\cdots\text{for L=10} \\ 4\cdots\cdots\text{for L=15} \end{cases}$

For the region K of 2-region hexagonal lattice, the elements in the first region (fuel) of the lattice must precede the elements in the second region (modetator) of the lattice in the array of

element	code number	element	code number
^{239}Pu	949	C	6
^{240}Pu	940	O	8
^{241}Pu	941	Na	11
^{234}U	924	Al	13
^{235}U	925	Cr	24
^{238}U	928	Mn	25
F. P. (^{239}Pu)	999	Fe	26
F. P. (^{235}U)	995	Ni	28
^{10}B	105	Cu	29
^{11}B	115	Mo	42

M, and the densities of these elements must be homogenized in each region in the lattice, not in each region K of reactor.

The code numbers of the elements are defined in the previous page.

9 (I3, 5(3X, E12.5), 2I1)

- column 3——9
- volume ratio for each element

  (VR(M, K), M=L+1, min{L+5, MM(K)})

  VR(M, K) is necessary only when AN(M, K) is not the effective densities, that is, AN(M, K) is not yet homogenized in the region K or in each region of lattice of the region K.
- column 79
- column 80

  ——same as in # 8

The cards in the following are treated without blank check, and must be given to each problem.

10 (10I6)

- number of elements in the first region of hexagonal lattice for each reactor region

  (MMM(K), K=1, KMAX)

  MMM(K)=0 for the reactor regions treated homogeneously.

11 (6E12.5)

- radius r_1(cm) of the first region in hexagonal lattice for each reactor region

  (R1(K), K=1, KMAX)

  (R1(K)=0. for the K of MMM(K)=0)

12 (6E12.5)

- pitch t(cm) of hexagonal lattice for each region

  (PITCH(K), K=1, KMAX)

  (PITCH(K)=0 for the K of MMM(K)=0)

When more than one problems are contained in one 'job', the cards for items from #0 to #12 are repeated in this order.

102 (I1, 79X) the last card

- column 1——1
- columns 2~80——blank

An example of input data cards is given in the next page. There, two problems are delt with in one job, and in the first problem, all the regions are treated homogeneously but in the second problem, the first, third and forth regions are hexagonal regions. So the densities of preceding MMM(K) nuclides in these regions are the quotients of those in the former problem divided by VR_1, and the densities of remaining [MM(K)-MMM(K)] nuclides are by VR_2.

The cards of # 8 in the latter problem, by this reason, can be replaced by cards of # 9 where VR(M, K)'s are $1/VR_1$ or $1/VR_2$.

7. The perturbation theory code PERTHET

From the calculations of the example in the previous chapter, the results of the effective multiplication factors for the problems were,

$k_{\text{eff}}^{\text{hom}}=1.188237$

$k_{\text{eff}}^{\text{het}}=1.188985$

$\rho=(k_{\text{eff}}^{\text{het}}-k_{\text{eff}}^{\text{hom}})/k_{\text{eff}}^{\text{het}}=0.00063.$

An auxiliary code named PERTHET has been prepared to study the detailed contribution to

```
        EXPANDA-5 DATA   JEFR 1ST LOADING     NOV.,1970  T.SUZUKI
01124011234567 8  15  0    SMEARED CELL
  1  9  1 25  0  1 11  0  1 -1  1  0  51.0E-51.0E-4 0.    0.    0.
  2    11     5    11     8     4     4    10     4     1
  3    20    22    36    52    54    58    66    72    78
  4    12    13    14    15    25
  51.01441.274 .980222.06863.023 2.824 2.875 2.66663.1677
  6 300.  300.  300.  300.  300.  300.  300.  300.  300.
  7 1.186   E-3 9.593   E-4 9.593   E-4 8.305   E-4                                          11
  8949 1.3813  E-3940 4.9332  E-4941 9.8664  E-5925 2.0833  E-3928 6.9744  E-311
  8  8 2.1841  E-2 11 8.8661  E-3 24 2.2799  E-3 26 7.4310  E-3 28 1.2760  E-312
  8 42 1.6261  E-4                                                           13
  8 11 1.9     E-2 24 2.838   E-3 26 9.25    E-3 28 1.588   E-3 42 2.024   E-421
  8949 1.3813  E-3940 4.9332  E-4941 9.8664  E-5925 2.0833  E-3928 6.9744  E-331
  8  8 2.1841  E-2 11 8.8661  E-3 24 2.2799  E-3 26 7.4310  E-3 28 1.2760  E-332
  8 42 1.6261  E-4                                                           33
  8925 3.5732  E-5928 1.4257  E-2  8 2.8586  E-2 11 5.0022  E-3 24 2.5594  E-341
  8 26 8.3420  E-3 28 1.4325  E-3 42 1.8254  E-4                           42
  8 11 4.536   E-3 24 1.468   E-2 26 4.853   E-2 28 5.853   E-3           51
  8 11 1.436   E-2 24 6.749   E-3 26 2.231   E-2 28 2.69    E-3           61
  8949 1.149   E-4940 4.103   E-5941 8.206   E-6925 1.75    E-4928 5.784   E-471
  8  8 1.817   E-3 11 1.899   E-2 24 2.323   E-3 26 7.678   E-3 28 9.259   E-472
  8 11 7.073   E-3 24 1.263   E-2 26 4.176   E-2 28 5.035   E-3            81
  8 11 2.269   E-2                                                         91
    0    0    0    0    0    0    0    0    0
 0.          0.          0.          0.          0.          0.
 0.          0.          0.
 0.          0.          0.          0.          0.          0.
 0.          0.          0.
01124028          8  0    SIMPLIFIED METHOD
  8949 2.9082  E-3940 1.0387  E-3941 2.0773  E-4925 4.3862  E-3928 1.4684  E-211
  8  8 4.5985  E-2 11 1.6887  E-2 24 4.3423  E-3 26 1.4153  E-2 28 2.4304  E-312
  8 42 3.0971  E-4                                                           13
  8949 2.9082  E-3940 1.0387  E-3941 2.0773  E-4925 4.3862  E-3928 1.4684  E-231
  8  8 4.5985  E-2 11 1.6887  E-2 24 4.3423  E-3 26 1.4153  E-2 28 2.4304  E-332
  8 42 3.0971  E-4                                                           33
  8925 5.7434  E-5928 2.2916  E-2  8 4.5947  E-2 11 1.3238  E-2 24 6.7734  E-341
  8 26 2.2077  E-2 28 3.7911  E-3 42 4.8310  E-4                           42
    6    0    6    3    0    0    0    0    0
 0.275       0.          0.275       0.68        0.          0.
 0.          0.          0.
 0.76        0.          0.76        1.642       0.          0.
 0.          0.          0.
1
```

ρ from each group, region, element and each kind of reaction by the scheme of perturbation theory. This code calculates ρ using the data supplied from two magnetic tapes. One of the tapes containes $\bar{\sigma}$, k_{eff}, ϕ and ϕ^* for the unperturbed (homogeneous) system and the another tape contains $\bar{\sigma}^p$ for perturbed (heterogeneous) system.

The calculation formula of $\rho_{x,k}{}^{ni}$, for element m, group i, reaction x and region k are derivated in the following.

The diffusion equation for the unperturbed system and its adjoint equation are,

$$-\text{div}\{D(r,E)\,\text{grad}\,\phi(r,E)\}+\Sigma_t(r,E)\phi(r,E)$$
$$=\frac{1}{k}\chi(E)\int dE'\nu\Sigma_f(r,E')\phi(r,E')+\int dE'\Sigma_s(r,E'\to E)\phi(r,E') \quad \cdots\cdots(15)$$

$$-\text{div}\{D(r,E)\,\text{grad}\,\phi^*(r,E)\}+\Sigma_t(r,E)\phi^*(r,E)$$
$$=\frac{1}{k}\nu\Sigma_f(r,E)\int dE'\chi(E')\phi^*(r,E')+\int dE'\Sigma_s(r,E\to E')\phi^*(r,E') \quad \cdots\cdots(16)$$

and, the diffusion equation for the perturbed system is,

$$-\text{div}\{D^p(r,E)\,\text{grad}\,\phi^p(r,E)\}+\Sigma_t{}^p(r,E)\phi^p(r,E)$$
$$=\frac{1}{k^p}\chi(E)\int dE'\nu\Sigma_f{}^p(r,E')\phi^p(r,E')+\int dE'\Sigma_s{}^p(r,E'\to E)\phi^p(r,E') \quad \cdots\cdots(17)$$

Multiplying $\phi^*(r,E)$ to the equation (17) and integrating over space and energy,

$$-\int dE\int dS\phi^*(r,E)D^p(r,E)\nabla_n\phi^p(r,E)+\int dE\int dV D^p(r,E)\nabla\phi^*(r,E)\nabla\phi^p(r,E)$$
$$+\int dV\int dE\phi^*(r,E)\Sigma_t{}^p(r,E)\phi^p(r,E)$$
$$=\frac{1}{k^p}\int dV\psi(r)\int dE'\nu\Sigma_f{}^p(r,E')\phi^p(r,E')+\int dV\int dE\int dE'\phi^*(r,E)\Sigma_s{}^p(r,E'\to E)\phi^p(r,E')$$
$$\cdots\cdots(18)$$

where

$$\psi(r)=\int dE\chi(E)\phi^*(r,E),$$

and the next relations were used to derivate (18) from (17),

$$\text{div}\,(D\,\text{grad}\,\phi)=D\nabla^2\phi$$
$$\int dV\phi^*D\nabla^2\phi=\int dS\phi^*D\nabla_n\phi-\int dVD\nabla\phi^*\nabla\phi$$

with $D(r,E)$ independent on r in each region.

Multiplying $\phi^p(r,E)$ to equation (16) and integrating,

$$-\int dE\int dS\phi^p(r,E)D(r,E)\nabla_n\phi^*(r,E)+\int dE\int dVD(r,E)\nabla\phi^p(r,E)\nabla\phi^*(r,E)$$
$$+\int dV\int dE\phi^p(r,E)\Sigma_t(r,E)\phi^*(r,E)$$
$$=\frac{1}{k}\int dV\psi(r)\int dE\nu\Sigma_f(r,E)\phi^p(r,E)+\int dV\int dE\int dE'\phi^p(r,E)\Sigma_s(r,E\to E')\phi^*(r,E')$$
$$\cdots\cdots(19)$$

The boundary conditions on the outer surface S are

$$\phi=\phi^*=\phi^p=0 \text{ on } S$$

or

$$\nabla_n\phi=\nabla_n\phi^*=\nabla_n\phi^p=0 \text{ on } S$$

Then subtracting (19) from (18) and using the boundary conditions, we obtain,

$$\int dV\int dE\delta D(r,E)\nabla\phi^p(r,E)\nabla\phi^*(r,E)+\int dV\int dE\delta\Sigma_t(r,E)\phi^p(r,E)\phi^*(r,E)$$
$$=-\frac{\delta k}{k^pk}\int dV\psi(r)\int dE\nu\Sigma_f{}^p(r,E)\phi^p(r,E)+\frac{1}{k}\int dV\psi(r)\int dE\delta\{\nu\Sigma_f(r,E)\}\phi^p(r,E)$$
$$+\int dV\int dE\int dE'\delta\Sigma_s(r,E\to E')\phi^p(r,E)\phi^*(r,E)$$

Now $\phi^p(r, E)$ is replaced by $\phi(r, E)$ because we consider pertubation to the first order.

$$\frac{\delta k}{k^p}\cdot\frac{1}{k}\int dV\psi(r)\int dE\nu\Sigma_f{}^p(r, E)\phi(r, E)$$

$$=-\int dV\int dE\delta D(r, E)\nabla\phi(r, E)\nabla\phi^*(r, E)-\int dV\int dE\delta\Sigma_t(r, E)\phi(r, E)\phi^*(r, E)$$

$$+\frac{1}{k}\int dV\psi(r)\int dE\delta\{\nu\Sigma_f(r, E)\}\phi(r, E)+\int dV\int dE\int dE'\delta\Sigma_s(r, E\to E')\phi(r, E)\phi^*(r, E')$$

Then the integration by energy is done in each group,

$$\rho I=-\int dV\sum_i\delta D^i(r)\nabla\phi^i(r)\nabla\phi^{*i}(r)-\int dVB_\perp{}^2(r)\sum_i\delta D^i(r)\phi^i(r)\phi^{*i}(r)$$

$$-\int dV\sum_i\delta\Sigma_a{}^i(r)\phi^i(r)\phi^{*i}(r)+\frac{1}{k}\int dV\psi(r)\sum_i\delta\{\nu\Sigma_f{}^i(r)\}\phi^i(r)$$

$$-\int dV\sum_i\phi^i(r)\{\delta\Sigma_s{}^i(r)\phi^{*i}(r)-\sum_j\delta\Sigma_s{}^{i\to j}(r)\phi^{*j}(r)\}$$

where

$$I=\frac{1}{k}\int dV\psi(r)\sum_i\nu\Sigma_f{}^{pi}(r)\phi^i(r)$$

$$\psi(r)=\sum_i\chi^i\phi^{*i}(r)$$

$$\Sigma_t{}^i=\Sigma_a{}^i(r)+\Sigma_s{}^i(r)+B_\perp{}^2(r)D^i(r).$$

Separating ρ into the parts from reactions,

$$\rho=\rho(D)+\rho(B_\perp{}^2D)+\rho(\Sigma_a)+\rho(\nu\Sigma_f)+\rho(\Sigma_e)+\rho(\Sigma_{in})$$

and using

$$\delta D=-D^2\delta\left(\frac{1}{D}\right)$$

$$\rho_{d,k}{}^{mi}=\rho_k{}^{mi}(D)=\frac{3}{I}(D_k{}^i)^2N_k{}^m\delta\sigma_{d,k}{}^{mi}\int_{V_k}dV\frac{d\phi^i(r)}{dr}\cdot\frac{d\phi^{*i}(r)}{dr}$$

$$\rho_{b,k}{}^{mi}=\rho_k{}^{mi}(B_\perp{}^2D)=\frac{3}{I}B_\perp{}^2(k)(D_k{}^i)^2N_k{}^m\delta\sigma_{d,k}{}^{mi}\int_{V_k}dV\phi^i(r)\phi^{*i}(r)$$

$$\rho_{c,k}{}^{mi}=\rho_k{}^{mi}(\Sigma_c)=-\frac{1}{I}N_k{}^m\delta\sigma_{c,k}{}^{mi}\int_{V_k}dV\phi^i(r)\phi^{*i}(r)$$

$$\rho_{a,k}{}^{mi}=\rho_k{}^{mi}(\Sigma_a)=-\frac{1}{I}N_k{}^m(\delta\sigma_{c,k}{}^{mi}+\delta\sigma_{f,k}{}^{mi})\int_{V_k}dV\phi^i(r)\phi^{*i}(r)$$

$$\rho_{f,k}{}^{mi}=\rho_k{}^{mi}(\nu\Sigma_f)=\frac{1}{kI}N_k{}^m\delta(\nu\sigma_f)_k{}^{mi}\int_{V_k}dV\phi^i(r)\psi(r)$$

$$\rho_{e,k}{}^{mi}=\rho_k{}^{mi}(\Sigma_e)=-\frac{1}{I}N_k{}^m\delta\sigma_{er,k}{}^{mi}\int_{V_k}dV\phi^i(r)\{\phi^{*i}(r)-\phi^{*i+1}(r)\}$$

$$\rho_{in,k}{}^{mi}=\rho_k{}^{mi}(\Sigma_{in})=-\frac{1}{I}N_k{}^m\left\{\delta\sigma_{in,k}{}^{mi}\int_{V_k}dV\phi^i(r)\phi^{*i}(r)\right.$$

$$\left.-\sum_j\delta\sigma_{in,k}{}^{m,i\to j}\int_{V_k}dV\phi^i(r)\phi^{*j}(r)\right\}$$

$$\rho_k{}^{mi}=\rho_{d,k}{}^{mi}+\rho_{b,k}{}^{mi}+\rho_{a,k}{}^{mi}+\rho_{f,k}{}^{mi}+\rho_{e,k}{}^{mi}+\rho_{in,k}{}^{mi}.$$

The output data of the PERTHET are:

(1) $\rho_{d,k}{}^{mi}$, $\rho_{b,k}{}^{mi}$, $\rho_{c,k}{}^{mi}$, $\rho_{a,k}{}^{mi}$, $\rho_{f,k}{}^{mi}$, $\rho_{e,k}{}^{mi}$, $\rho_{in,k}{}^{mi}$ and $\rho_k{}^{mi}$ for each i, k and m.

(2) as the sums over groups,
$\rho_{d,k}{}^m$, $\rho_{b,k}{}^m$, $\rho_{c,k}{}^m$, $\rho_{a,k}{}^m$, $\rho_{f,k}{}^m$, $\rho_{e,k}{}^m$, $\rho_{in,k}{}^m$ and $\rho_k{}^m$ for each k and m.

(3) as the sums over elements,
$\rho_{d,k}{}^i$, $\rho_{b,k}{}^i$, $\rho_{c,k}{}^i$, $\rho_{a,k}{}^i$, $\rho_{f,k}{}^i$, $\rho_{e,k}{}^i$, $\rho_{in,k}{}^i$ and $\rho_k{}^i$ for each k and i,
and

$\rho_{d,k}$, $\rho_{b,k}$, $\rho_{c,k}$, $\rho_{a,k}$, $\rho_{f,k}$, $\rho_{e,k}$, $\rho_{in,k}$ and ρ_k for each k.

(4) as the reactor totals,

$\rho_d{}^i$, $\rho_b{}^i$, $\rho_c{}^i$, $\rho_a{}^i$, $\rho_f{}^i$, $\rho_e{}^i$, $\rho_{in}{}^i$ and ρ^i for each i,

and

ρ_d, ρ_b, ρ_c, ρ_a, ρ_f, ρ_e, ρ_{in} and $\rho\left(=\dfrac{\delta k}{k^p}\right)$.

In the above, the ρ_c is of course a part of ρ_a.

(5) k (=input k_{eff})

$$\delta k=\frac{\rho}{1-\rho}k$$

$$k^p=\frac{k}{1-\rho}$$

I (the denominator)

The figure in the next page is the example of $\rho_a{}^i$ and $\rho_f{}^i$ which were calculated about the example data of the previous chapter. There $\rho_a{}^i$ and $\rho_f{}^i$ do not contain the contribution from the 4 th region.

It is observed in this example that the heterogeneity effects due to fission source distribution upper 10^{keV} is dominant while the negative effects due to resonance absorption distribution is rather small.

8. Concluding remarks

When reactivity effects like Doppler or sodium void effect are to be calculated, group structure of the ABBN set is not adequate in the energy range of the sodium resonance (the 13 th and 14 th groups in the ABBN structure). It is expected that a satisfactory result will be obtained when the original 70 group structure are used in this range, that is, each of the 13 th and 14 th groups is divided into three groups of equal lethargy width. The examination about this problem are not yet done. JAERI-fast set of 29 group structure must be first prepared for all of the 20 materials.

Another problem remained is the treatment of the tubes surrounding the fuel assembly.

Presently, the method of the EXPANDA-5 is going to be used in a two dimensional diffusion equation code.

It will be not difficult to expand this code for treating other types of lattice, for example, regular lattice, slab lattice or sphere lattice and lattice consisting of more than two regions. This method can be used in the transport equation codes such as S_n or P_n codes.

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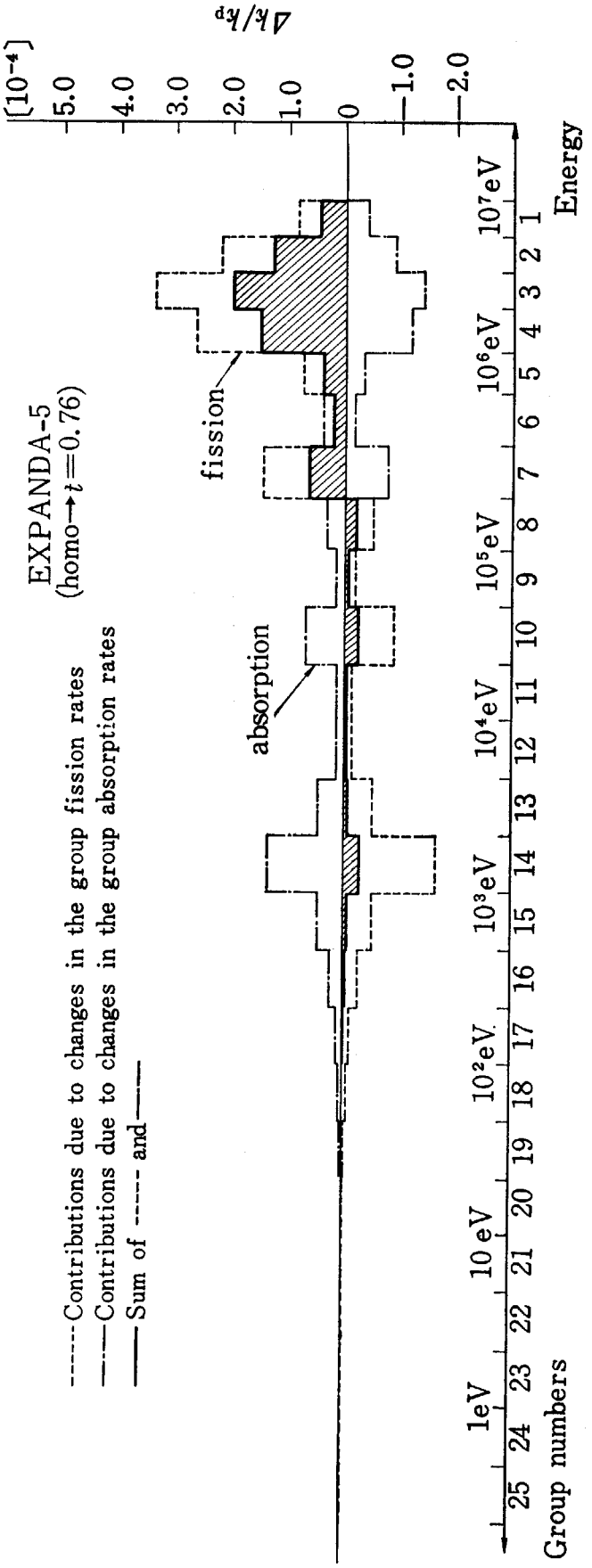
$\Delta k/k_p$
[10^{-4}]
5.0
4.0
3.0
2.0
1.0
0
1.0
2.0
EXPANDA-5
(homo→t=0.76)
fission
absorption
----Contributions due to changes in the group fission rates
—·—Contributions due to changes in the group absorption rates
——Sum of ----- and——
10^7eV
10^6eV
10^5eV
10^4eV
10^3eV
10^2eV
10 eV
1eV
Energy
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
Group numbers

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