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**DEVELOPMENT OF THE COMPUTER CODE SYSTEM
FOR THE ANALYSES OF PWR CORE**

November 1992

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Development of the Computer Code System
for the Analyses of PWR Core

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This report is one of the materials for the work titled "Development of the computer code system for the analyses of PWR core phenomena", which is performed under contracts between Shikoku Electric Power Company and JAERI.

In this report, the numerical method adopted in our computer code system are described, that is, "The basic course and the summary of the analysing method", "Numerical method for solving the Boltzmann equation", "Numerical method for solving the thermo-hydraulic equations" and "Description on the computer code system".

Keywords: Computer Code System, PWR, Steady State

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PWR炉心解析用計算コードシステムの開発

日本原子力研究所東海研究所燃料安全工学部

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本報告書は、四国電力株式会社が原研の協力のもとに行った「PWR炉心静特性解析コード・システムの開発」に関するものである。

本報告書の内容は、今回作成したコード・システムの中で採用されている「解析方法の基本的取扱い」，「ボルツマン方程式の数値解法」，「炉定数の作成方法」，「熱水力方程式の数値解法」および「計算コード・システムの概要」よりなる。

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Preface

Some PWRs have been in operation for a few years in the country. Core management of the reactors is important in utilizing the nuclear power plant. Main objects of the core management calculations are as follows:

- (1) Determination of the most economic and safe fuel exchange schedule.
- (2) Reactor startup test analyses.
- (3) Determination of the suitable operating conditions for safe operation satisfying the licences.
- (4) Evaluation of the nuclide inventories, tables of which are submitted to the government.

Many partial studies have of course been made for satisfying some of the requirements. From experiences of the present authors, however, it seems that the results from such analyses are not necessarily reliable; moreover cause for and nature of the errors are often not clear. The most important for obtaining any results is thus consistency and definiteness of the theoretical bases of data processing methods in successive calculations. Generally, the nuclear and thermo-hydraulic state of a reactor core is represented by neutron transport equation and thermo-hydraulic equations including the mass-, momentum- and energy conservation principles. However, the equations are so complicated that the analytical solution is hardly possible even for a simple system. It is thus inevitable to divide the procedure into some steps, in each of which the equation is reduced to a simple form for its numerical solution with economic computer time.

The problems included in the division above are as follows:

- (1) Consistency of the boundary conditions on each variable.
- (2) Precision of the approximate equations.

The few group reactor constants, for example, are obtained from the multi-group spectrum calculations in simpler geometries in which the boundary conditions are determined by solution of the overall equilibrium equations with natural boundary conditions. The authors have developed an analyzing scheme which has the overall consistency in the range of its applicability. In this report, the design concepts for the scheme are described in detail by reference to the results obtained by the computer code system based on the concepts.

1. The Basic Course and the Summary of the Analyzing Method

1.1 General properties of the physical quantities

In general, nuclear and thermo-hydraulic quantities to be evaluated for reactor core maintenance are determined by neutron balance equation, thermo-hydraulic equations and burnup equation. Of these equations, the neutron balance equation has a linear form if the coefficients are constant. But there may be some feedback effects of neutron flux on the coefficients through the thermo-hydraulic equations and the burnup equation; the neutron balance equation is not linear as to neutron flux in this sense, which is one of important causes of complexities in data processes for neutron balance calculations. Thermo-hydraulic equations in rigorous form which are described in terms of vector-tensor notation are very complicated from the next points of view.

- (1) Mathematical properties of the operators in the equations
- (2) Boundary conditions
- (3) Physical properties of the stress tensor

Hence there may be found no other way to treat these equations than a macroscopic treatment with unknown coefficients to be determined by empirical method. It is to be noted that super sonic transient phenomena are taken out of the description because any such phenomenon is due to an abnormal core state in a period negligibly short compared to normal operation time for which core maintenance should be performed. In other words, features are too complicated in such drastic transient states to be analyzed, that is, any analysis for such a phenomenon may be almost nonsense except when it is performed by a simple model based on many reliable experimental results.

The burnup equation is seemingly linear as to the dependent variable but the coefficients depend on it through the neutron balance equation, then some corrections may be needed.

Usually, the burn up equation is solved for the next two purposes.

- (1) Analysis of Xe-Oscillation
- (2) Calculation of fuel burnup

For the purpose (1), the feed back effects of fuel nuclide densities are negligibly small, hence the equation becomes simple. For the purpose (2), the correction for time-variations of flux distribution and effective cross sections of nuclides is important.

1.2 Summary on the basic equations

The equilibrium condition of a reactor core is determined by the next equations.

(Neutron balance⁽⁵⁾)

$$\begin{aligned} & \left[\frac{1}{V} \cdot \frac{\partial}{\partial t} + \Omega \cdot \nabla + \Sigma_t(r, E) \right] \phi(r, E, \Omega, t) \\ &= \chi_0(E) \nu_0 \psi(r, t) + \sum_{i=1}^N \chi_i(E) \nu_i \lambda_i \int_0^t \psi(r, \tau) e^{-\lambda_i(t-\tau)} d\tau \\ &+ \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(r, E' \rightarrow E, \Omega' \rightarrow \Omega) \phi(r, E', \Omega', t) \end{aligned} \quad (1.1)$$

(Mass balance)

$$\frac{\partial}{\partial t} \rho(r, t) + \text{div } \rho(r, t) V(r, t) = 0 \quad (1.2)$$

(Momentum balance⁽¹¹⁾)

$$\begin{aligned} & \frac{\partial}{\partial t} \rho(r, t) V(r, t) + [\nabla \cdot \rho(r, t) V(r, t) V(r, t)] \\ &+ \nabla p(r, t) + [\nabla \cdot \tau(r, t)] - \rho(r, t) g = 0 \end{aligned} \quad (1.3)$$

(Energy balance⁽¹¹⁾)

$$\begin{aligned} & \rho(r, t) \frac{\partial}{\partial t} e(r, t) + \rho V \text{grade} + \text{div } q \\ &+ P(r, t) \text{div } V(r, t) + [\tau(r, t) \cdot \nabla V(r, t)] = 0 \end{aligned} \quad (1.4)$$

(Burn up)

$$\frac{\partial N}{\partial t} = \Delta N \quad (1.5)$$

where

- t : time variable (sec)
- r : position vector (cm)
- E : neutron energy variable (eV)
- Ω : unit direction vector
- w : the neutron velocity corresponding to E (cm/sec)
- Σ_t : macroscopic total cross section (cm^{-1})
- Σ_s : macroscopic differential cross section ($\text{cm}^{-1} \cdot \text{eV}^{-1}$)

- Σ_f : macroscopic fission cross section (cm^{-1})
 ν : number of neutrons appearing per unit interval about the final time by a fission emerged per unit interval about an initial time (sec^{-1})
 χ : average energy spectrum of fission neutrons
 ϕ : neutron flux density per unit solid angle ($\text{cm}^{-2} \cdot \text{eV}^{-1} \cdot \text{sec}^{-1}$)
 $\psi(\mathbf{r}, t) \equiv \int_0^\infty dE \Sigma_f(E) \int_{4\pi} \phi(\mathbf{r}, E, \Omega, t) d\Omega$
 ρ : moderator density ($\text{gr} \cdot \text{cm}^{-3}$)
 \mathbf{W} : velocity vector of moderator ($\text{cm} \cdot \text{sec}^{-1}$)
 P : moderator pressure ($\text{gr} \cdot \text{cm}^{-1} \cdot \text{sec}^{-2}$)
 τ : viscosity tensor of moderator ($\text{gr} \cdot \text{cm}^{-1} \cdot \text{sec}^{-2}$)
 e : internal energy of moderator ($\text{erg} \cdot \text{cm}^{-3}$)
 \mathbf{q} : vector of heat flux density ($\text{erg} \cdot \text{cm}^{-2} \cdot \text{sec}^{-1}$)
 \mathbf{g} : the acceleration vector of gravity ($\text{cm} \cdot \text{sec}^{-2}$)
 A : coefficient matrix of burn up equation

Of course, some auxiliary equations are needed, which give nuclear cross sections^(1,2,3), the relation among the thermo-dynamic functions⁽¹¹⁾, friction and so on. However, there are some complicated relations which are not necessarily given theoretically or even if possible the forms are too complicated for utilization.

Therefore these relations should be determined by any macroscopic empirical methods for utilization as the case may be. In this report, a series of methods for solving these equations are introduced, the contents of which are partly conventional methods are partly those developed by our efforts, constituting an organic system. The solving processes are summed up as follows:

- (1) Calculation of nuclear data values at the neutron energy points required for calculating group constants.
- (2) Calculation of multi-group constants.
- (3) Calculation of few group reactor constants.
- (4) Calculation of distribution of neutron flux, power, temperature, burn up rate and so on.

The necessity of these processes is clearly shown gradually in later descriptions.

2. Numerical method for solving the Boltzmann equation

2.1 The design concept on numerical method

The neutron balance condition under a fixed thermo-hydraulic state is determined by equation (1.1).

In other words, if the distributions of temperature and pressure over a reactor core are given, the cross sections in equation (1.1) is uniquely defined by the cross section theory^(1,2), hence equation (1.1) with natural boundary conditions gives the neutron balance condition over the core.

However, it is well known to us that the dependencies of the cross sections on neutron energy are very complicated and the core of any commercial reactor has a complex geometrical structure. Therefore, no analytical solution of eq. (1.1) over the all domain of phase space can be expected. But the final purpose is to obtain the spacial distribution of reactor power and burn up rate. To obtain these quantities over a large reactor core by numerical method, it is necessary for computational economy to smooth away the neutron energy dependency of the Boltzmann equation and reduce it into a set of some few discrete group equations with the appropriate constants so called few group constants or reactor constants. These constants are given by averaging the cross sections weighted by the spectrum obtained as the solution of equation (1.1) over each unit cell such as fuel rod, etc., under simple boundary conditions. Therefore the constants depend on the weight flux, the shape of which is changed by the densities and the temperature of the absorbers and the moderator.

The fine structure of the spectrum is determined almost by the composition and the temperature of the resonance absorbers; the composition changes very slowly according to fuel burn up rate and the temperature distribution is effectively constant at a power level. The overall shape of the spectrum in a core is determined by the moderator density, the poison density in the moderator and the boundary conditions of the unit cell, where the first two of these quantities can be changed rapidly by plant control. Therefore, it is desirable to divide the reactor constant calculation procedure into two steps. The first is to calculate the fine spectrum of each unit cell and erase the resonance structure of the cross sections by averaging them using the fine spectrum as weight over each energy interval taken so appropriately that the effect of the overall shape is negligibly small. We call this step multi-

group constant calculation. The second is to calculate overall spectrum using the multi-group constants described above and reduce the multi-group constants into reactor constants. We call this step reactor constant calculation.

It is to be noted that the multi-group constant calculation has to be performed at only some points of the absorber densities and the temperature because the variation width of absorber composition and the Doppler effect is very small, while the reactor constant calculation must be performed at many points of the parameters, viz., moderator density, poison density, cell boundary conditions, and fuel enrichment because these quantities often change so far that the overall shape is distorted. In brief description it may be said that the multi-group constants are not changed by any short term transition of the reactor state but the reactor constants are not so.

Finally it may be concluded that the almost best way to solve equation (1.1) over a reactor core is to divide the solving procedure into three steps below:

- (1) Multi-group constant calculation
- (2) Reactor constant calculation
- (3) Spatial distribution calculation.

We perform the step (1) by solving the ultra-fine group integral-forms^(13,16) defined in simple one-dimensional geometries, and (2) by solving the multi-group differential-forms^(18,19) in one dimensional geometries such as rods cell or infinite slabs, while use is made of the multi-group integral form^(18,17) for more complex geometries such as assemblies to research the boundary conditions of the rod cell geometries. The step (3) is performed by the diffusion form⁽⁴⁾ consistent with the p_1 -equations; the reactor constants for the diffusion equation are determined by the p_1 -approximation at the step (2). The details of these steps are described in later sections.

2.2 Nuclear data

Almost all the reactions important for the neutron balance in a light water reactor core are picked up in table 2.1. The nuclide cross section for each of these reactions is given by ENDF⁽¹²⁾-B in the form according to the reaction. On the other hand, the neutron transport equation in seven dimensional phase space is represented using the cross sections of total, fission (multiplied by ν -value) and differential

scatter. Therefore we collect the cross sections for reactions in TABLE 2.1 into three practical quantities, namely, the cross sections of capture, fission and scatter.

The collecting manner is as follows.

(Capture cross section)

First, the cross section of reaction (a) in TABLE 2.1 is given as two parts, one is the resonance cross section given by the Breite Wigner's level formula^(1,2,12), etc., with the corresponding level parameters, while the other is the so-called smooth data giving the difference between measured value and that given by the level formula. Consequently, the cross section of the reaction (a) at any arbitrary neutron energy E is given by summing up the value given by the formula above and the smooth data:

$$\sigma_{n,\gamma}(E) = \sigma_{n,\gamma}^{\text{res}}(E) + \sigma_{n,\gamma}^{\text{sm}}(E) \quad (2.1)$$

where $\sigma_{n,\gamma}^{\text{res}}$ the resonance part is given by the level formula. Next, the cross sections of the reaction from (b) to (g) are all given as the smooth data $\sigma_{n,p}$, $\sigma_{n,\alpha}$, $\sigma_{n,t}$, σ_{n,He^3} , $\sigma_{n,\alpha}$ and $\sigma_{n,2\alpha}$ measured at finer neutron energy points.

TABLE (2.1)

(a)	(n,γ)	reaction	neutron capture	scattering	
(b)	(n,p)	"			
(c)	(n,d)	"			
(d)	(n,t)	"			
(e)	(n,He ³)	"			
(f)	(n,α)	"			
(g)	(n,2α)	"			
(h)	(n,n')	"	inelastic		
(i)	(n,n',α)	"			
(j)	(n,n',3α)	"			
(k)	(n,n',p)	"	(n,2n)		
(l)	(n,2n)	"			
(m)	(n,2n,α)	"	(n,2n)		
(n)	elastic scattering	"			
(o)	(n,f)	reaction — fission			

The capture cross section $\sigma_c(E)$ is then given as:

$$\begin{aligned}\sigma_c(E) = & \sigma_{n,\gamma}^{\text{res}}(E) + \sigma_{n,\gamma}^{\text{sm}}(E) + \sigma_{n,p}(E) + \sigma_{n,d}(E) + \sigma_{n,t}(E) \\ & + \sigma_{n,\text{He}^3}(E) + \sigma_{n,\alpha}(E) + \sigma_{n,2\alpha}(E)\end{aligned}\quad (2.2)$$

(Fission cross section)

Fission cross section is also given as the summation of resonance part $\sigma_f^{\text{res}}(E)$ and smooth part σ_f^{sm}

$$\sigma_f(E) = \sigma_f^{\text{res}}(E) + \sigma_f^{\text{sm}}\quad (2.3)$$

(ν -value and fission spectra)

It is required for the treatment of neutron kinetics equation that ν -value is given in a time dependent form^(12,21). The nuclear data library ENDF-B/4 gives this as such factors:

- $\nu_i(E)$: the number of the total neutrons emerged by decay of the i -th precursor originated from a fission by neutrons of energy E
- $\chi_i(E)$: fission spectrum of the i -th delayed neutrons
- λ_i : the decay constant of the i -th precursor ($= 0$ means "prompt", i.e., $\lambda_0 = \infty$)

These data give the time dependent fission source as

$$\chi_0(E) \nu_0 \psi(r, t) + \sum_{i=1}^N \chi_i(E) \nu_i \lambda_i \int_0^t \psi(r, \tau) e^{-\lambda_i(t-\tau)} d\tau$$

with

$$\psi(r, t) \equiv \int_0^\infty dE' \Sigma_f(E') \int_{4\pi} \phi(r, E', \Omega, t) d\Omega / 4\pi$$

(Scattering cross sections)

First, in the category of the inelastic scattering reactions described in Table 2.1, for only the (n, n') reaction excitation level data are given in ENDF-B. Namely, the data of the (n, n') reaction are given as two parts. One is composed of the k -th discrete excitation level E_k and $\sigma_{n,n'}^k(E')$ denoting the cross section value corresponding to E_k and the incident neutron energy E' , while the other is $\sigma_{n,n'}(E')$ the cross section in the unresolved excitation level energy range higher than the maximum E_k .

For another inelastic scattering reaction x , such as (n,n',α) , $(n,n',3\alpha)$ or (n,n',p) , data are given as $\sigma_x(E')$ in the unresolved excitation level energy range. Also, for each of the inelastic scattering reactions, the distribution of level energy in the unresolved region is represented by the evaporation model^(1,2,12). The total inelastic differential scattering cross section is thus given on the assumption of scattering isotropy⁽⁴⁾ in the Laboratory system.

Next, for the $(n,2n')$ reaction, data is given as $\sigma_{n,2n'}(E')$ the cross section corresponding to the incident neutron energy E' , and the evaporation model is used for the distribution of the emergent neutron energy.

Last, the elastic differential scattering cross section is practically used as a Legendre polynomial expansion with regard to the direction cosine of scattering angle. ENDF-B gives the coefficients. Finally, the total differential scattering cross section is given by the data and the models described above for incident neutron-energy larger than E_c while by thermal scattering model^(2,14,15) for the energy smaller than E_c . Note that ENDF-B gives these data at the temperature of 0°K, hence they are corrected for the Doppler effect corresponding to the actual temperature by the procedure described in APPENDIX I.

2.3 Multigroup constants

2.3.1 Consideration on multi-group constants

For the treatments of the neutron balance equations described in Sec. 2.2, it is desirable to have a set of multigroup constants satisfying the next requirements:

- (1) Closed in the sense of eigen value
- (2) Effects of resonance interference between nuclides can be taken into account
- (3) Heterogeneity effects can be taken into account
- (4) Time dependent fission source term of the Boltzmann equation can be represented without using precursor concentration variable.

Of course, there have been produced some group constants sets well known to us such as ABAGYAN⁽²³⁾, JAERI-FAST⁽²⁴⁾, GAM^(34,35) etc. But these sets may not be sufficient for the analyses of commercial light water reactor because of the next features.

- (1) ABAGYAN and JAERI-FAST sets were produced for mainly analyzing fast reactors, hence the thermal data are not sufficient for light water reactors.
- (2) GAM library is formally complete in the sense of having full data in all the necessary neutron energy range but the values are of infinite dilution and only the resonance self-shielding effect is evaluated by NR approximation on the assumption of spatially homogeneous spectrum.

However, any realistic commercial light water reactor core has strong heterogeneity, moreover the interference effect of sections must be taken into account especially in resonance energy region when plutonium isotopes override.

Moreover there are no other conventional sets than them. Therefore we have developed a computer code system for production of the multigroup constants under the design below.

- (1) ENDF-B is used as a basic nuclear data file.
- (2) The weight flux spectrum is calculated by solving the equation (1.1) in an isotropic one-dimensional form using fine energy point data of macroscopic cross sections composed of the individual microscopic cross sections given by some cross section formulae and the instruction of ENDF-B data processing methods.
Any arbitrary neutron source spectrum can be given as the fixed source term.
- (3) The group constant set of individual nuclide has one-dimensional and two-dimensional parts, the former contains the multigroup cross section vectors for capture, fission, ν -value, elastic scattering, inelastic scattering and (n,2n) reaction, while the later contains the scattering cross section matrices for elastic (p_0, p_1), inelastic (p_0) and (n,2n) reactions.
- (4) The effective values of one dimensional vectors are calculated in the realistic simple geometries of the core components such as cylindrical fuel rod cell or poison rod cell or infinite slab layer in which the one-dimensional heterogeneity is considered.
- (5) The scattering matrices are calculated by the scattering laws using a standard spectrum as the weight flux.

- (6) The table of multi-group constants of each nuclide is compiled in the form which has the infinite cross section vectors, the vector of shielding factors and the normalized scattering matrices.

2.3.2 Calculation of multi-group constants

With a suitable group structure, the values of group constants may not almost depend on the slow variation of the weight flux over an energy range wider than the group width, but they depend on the rapid variation in such a smaller energy range as a resonance width⁽²²⁾ which is extremely narrow compared to the group width. Therefore, it is sufficient for the purpose to get a fine structure and an approximate overall shape of the weight flux.

To attain this purpose, the total energy range is divided into two parts at a suitable energy point E_C , the neutrons scattered at an energy ($>E_C$) elastically or inelastically by any nuclide are all slowed down and the Boltzmann equation is then treated as a slowing down equation for a suitable fixed sources. On the other hand, in the energy range below E_C the neutrons are scattered partly up and partly down, the fractions of which are determined by the thermal scattering law, and the Boltzmann equation is then treated as a thermal equilibrium equation with the neutron source slowed down through E_C . Here, E_C is determined as:

$$E_C = 1.855 \text{ eV.}$$

For the actual problems of finding the weight flux for calculation of group constants, it is to be noted that the energy spectrum of the neutron flux in an absorber lamp has strong heterogeneity which is the reason why the equation cannot be treated in space free form. The Boltzmann equation is then treated as a static form with isotropic source in a one-dimensional geometry such as cylinder, slab or sphere.

In our calculation, the Boltzmann equation is treated fundamentally as an isotropic form because only the isotropic component of angular flux is used as weight flux. The integral transport equation is more convenient than the differential form for calculation of the isotropic component because the former is a single equation, whereas the latter is a set of more than two equations concerning some of the higher angular components.

The components of a PWR core may neutronically be classified into four categories; each of the fuel rod, control rod, burnable poison rod or the other structural components has a typical fine structure of the flux spectrum respectively. Therefore the effective values of the group constants for a nuclide is distinct by the cell in which it is contained. Hence calculation is made cell by cell to obtain the precise data for the main nuclide in the cell.

The slowing down equation is thus solved in each of the one dimensional heterogeneous geometries over the energy range from an effective upper limit to E_c under the next conditions:

- (1) The macroscopic cross sections are given at the required energy mesh points fine enough to represent the resolved resonance structure of important nuclear cross sections, and any neutron once collided in a mesh is necessarily removed from the mesh.
- (2) The scattering process of neutrons is represented by the so-called α -model.
- (3) An appropriate fixed source, e.g., a fission spectrum is given for the cell.
- (4) Boundary conditions of the cell are perfect reflective.

The calculation is performed by the RABBLE-code modified for the purpose.

The thermalization equation in the one dimensional geometry is solved under the next conditions.

- (1) The macroscopic cross sections are given at the mesh points many enough for representing the resonance cross sections and the $1/v$ cross sections in relation with the Maxwell peak of the thermal neutron flux.
- (2) The scattering process^(2,14,15) of neutrons is obedient to the Haywood model in water and to the Free Gas model in other media.
- (3) The slowing down source is given as the result of the solution of the slowing down equation.
- (4) Boundary conditions of the cell are perfect reflective.

The calculation is performed by the THERMOS code.

The multigroup meshes above E_c are taken like those of the ABAGYN-set for the reason that these mesh widths are selected by the fact that the group constants do not vary more than 2% whether the weight flux is $1/E$ or flat

shape. The multigroup meshes below E_c were determined first by considering the thermal resonances of important nuclides and thermal flux peak, and are modified afterward to decrease the neutron temperature effect on the $1/v$ cross sections to negligible size.

The fine meshes for solving the slowing down and the thermalization equations are determined by surveying the fewest necessary number of fine meshes of energy group. The multigroup structure and the fine meshes are summarized in APPENDIX A-II,

The space meshes should be determined by their optical length. Let a mesh width the Δr and the macroscopic cross section Σ_t . The size of Δr should be so determined as the next approximation

$$e^{-\Sigma_t \Delta r} \approx 1 - \Sigma_t \cdot \Delta r \quad (2.4)$$

is valid to an extent, because any discrete numerical solution is based on the assumption of mesh-wise linear dependency on space variable.

The effective group constants of a nuclide are given by the next relations,

$$\sigma_x^g = \frac{\int_{\Delta E_g} \sigma_x(E) \phi(E) dE}{\int_{\Delta E_g} \phi(E) dE} \quad (2.5)$$

$$\sigma_s^n(g \rightarrow g') = \frac{\int_{\Delta E_{g'}} dE' \int_{\Delta E_g} \sigma_s^n(E \rightarrow E') \phi(E) dE}{\int_{\Delta E_{g'}} \phi(E) dE} \quad (2.6)$$

where, $\phi(E)$ is the angle-integrated flux spectrum which is given by the fine spectrum calculation described above.

However, it is very troublesome to compile the two-dimensional data $\sigma_s^n(g, g')$ define by relation (2.6), because the scattering law becomes flux dependent and thereby it must be calculated every times. Therefore, it is desirable to make allowance of the next premises on the scattering matrix.

- (1) The total scattering cross section of every group is conserved equal to the effective value determined by relation (2.5).
- (2) The law of scattering from any group is independent of the fine spectrum in the group.

The premise (1) is indispensable to conserve scattering rate from every group. The premise (2) is an assumption meaning that the neutrons scattered in any group are transferred into other groups at the ratios

independent of energy distribution of scattering density in the group. This assumption may have little influence on the multigroup energy transfer law. Thus, $\phi(E)$ in relation (2.6) is replaced by a standard spectrum $\phi_s(E)$ representing an average spectrum of usual LWR cores as described in APPENDIX III, and the total scattering cross section in every group is normalized to unity.

Consequently, the effective scattering matrix M_e^n can be represented by the standard scattering matrix M_s^n and the effective scattering cross section matrix M_c^n as:

$$M_e^n = M_s^n \cdot M_c^n \quad (2.7)$$

where,

$$M_s^n = \begin{bmatrix} f_{1 \rightarrow 1}^n & f_{1 \rightarrow 2}^n & \dots & f_{1 \rightarrow G}^n \\ f_{2 \rightarrow 1}^n & f_{2 \rightarrow 2}^n & \dots & f_{2 \rightarrow G}^n \\ \dots & \dots & \dots & \dots \\ f_{G \rightarrow 1}^n & f_{G \rightarrow 2}^n & \dots & f_{G \rightarrow G}^n \end{bmatrix}$$

$$M_c^n = \begin{bmatrix} \sigma_1^n & \sigma_2^n & \dots & \sigma_G^n \\ \vdots & \vdots & \vdots & \vdots \\ \sigma_1^n & \sigma_2^n & \dots & \sigma_G^n \end{bmatrix}$$

$$f_{g \rightarrow g'}^n \equiv \sigma_s^n(g \rightarrow g') / \sum_{g'} \sigma_s^n(g \rightarrow g')$$

Then, it is obvious that M_e^n is obtained by calculation of only M_c^n , if once M_s^n is calculated and reserved.

2.3.3 The compilation of the multi-group constants

Concept of multi-group constant table is considered first. The effective group constants depend on the geometry, the temperature and the composition of the system. Therefore the effective value is calculated at some points of these parameters in the work. Usually, however, the group constants are calculated not by any peculiar reactor spectrum but by a standard spectrum considered as fairly suitable for almost all neutron reactors.

In these circumstances, we also compile a group constant set of the ABAGYAN type which is easily compared to other sets. The set has two new factors for LWR, i.e., the spectrum factor and the heterogeneity factor which will be described in the following sentences. In the fuel rods of the actual LWR, the fine structure of flux spectrum is determined almost by U-238, but in case of the fuel irradiated to an extent, U-236, Pu-240, Pu-242 override, and they may effect a change on the spectrum over the energy range 1.0 eV to 400 eV.

In any case, the fine spectrum is affected to an extent by the nuclides with large resonance cross section. Moreover, the effective group constants have heterogeneity for the reason described in the previous section.

Therefore we represent an effective group constant of a nuclide i as

$$\begin{aligned}\sigma_r^N(\mathbf{B}) &= \frac{\sigma_r^N(\mathbf{B})}{\bar{\sigma}^N(\mathbf{B})} \cdot \frac{\bar{\sigma}^N(\mathbf{B})}{\sigma^N(0)} \cdot \frac{\sigma^N(0)}{\sigma^0(0)} \cdot \sigma^0(0) \\ &= h_r^N(\mathbf{B}) \cdot S^N(\mathbf{B}) \cdot f(N) \cdot \sigma^0(0)\end{aligned}\quad (2.8)$$

$$\begin{aligned}\text{where } h_r^N(\mathbf{B}) &\equiv \sigma_r^N(\mathbf{B}) / \bar{\sigma}^N(\mathbf{B}) \\ S^N(\mathbf{B}) &\equiv \bar{\sigma}^N(\mathbf{B}) / \sigma^N(0) \\ f(N) &\equiv \sigma^N(0) / \sigma^0(0)\end{aligned}\quad (2.9)$$

$\sigma^0(0)$: standard spectrum weighted group average value.

$\sigma^N(0)$: real spectrum weighted group average value in case the nuclide i is contained with number density N

$\bar{\sigma}^N(\mathbf{B})$: fuel region averaged group value calculated by the weight flux determined for a cell which contains i and other resonance nuclides with number density N and respectively.

$\sigma_r^N(\mathbf{B})$: group value in region r calculated as above.

Note that $\sigma^0(0)$ is the so-called infinite value and f^N the self-shielding factor of the nuclide i and is a function of the potential scattering cross section σ_p of the other nuclides and the temperature, these quantities are all the same with those defined in usual sense. But, $S^N(\mathbf{B})$ denotes the shielding effects by other resonance nuclides contained in the cell with number density Vector \mathbf{B} , and $h_r^H(\mathbf{B})$ denotes heterogeneity effects by main resonance nuclides contained in the cell. The merit of the representation (2.8) for the compilation is that the

next relation may be permissible except few special cases,

$$\begin{aligned} s^N(B) &\approx s^0(B) \equiv s(B) \\ h_r^N(B) &\approx h_r^0(B) \equiv h_r(B) \end{aligned} \quad (2.10)$$

because, the self-shielding effects on the denominators of relations (2.9) may be comparable with those on the numerators. Thus the effective group value is given approximately by the next relation

$$\sigma_r^N(B) = h_r(B) \cdot s(B) \cdot f^N \cdot \sigma^0(0)$$

The pertinence degree of the approximation (2.10) is as exhibited in table.

As previously described, the group constants for a nuclide are compiled into one-dimensional data tables and two-dimensional data tables. The former contains the next quantities:

Infinite cross section

$$\sigma_c, \sigma_f, \sigma_e, \sigma_{in}, \sigma_{n,2n}, \sigma_t$$

ν -value and λ

$$\begin{aligned} \nu_i(E); i = 0, N \quad (i, \text{delayed neutron group}) \\ \lambda_i(E); i = 0, N \quad (= 0 \text{ means prompt}) \end{aligned}$$

Self-shielding factor

$$f_t, f_c, f_f, f_e, f_{in}$$

Spectrum factor

$$S_t, S_c, S_f, S_e$$

Heterogeneity factor

$$h_t, h_c, h_f, h_e$$

The later contains the next quantities,

Elastic scattering matrix M_{se}^n

Inelastic scattering matrix M_{in}^n

The (n,2n) reaction matrix $M_{sn,2n}^n$

Moreover, the tables must have some other data such as the parameter points at which the effective cross sections are calculated, various integers to control file utilization program and descriptions on the calculational conditions. The details of the forms of the group constant tables are shown in APPENDIX IV with the utilization rule.

2.4 Reactor constants

2.4.1 Consideration on reactor constants

The flux distribution over a reactor core is inevitably given by the few group diffusion approximation for the reason mentioned in Sec. 2.1. For practical purposes, the finest space mesh for the horizontal distribution of the neutron flux or the power over a reactor core is equal to one rod pitch. For this reason, it is sufficient to calculate and compile rod-cell-average few group constants of typical rod cells and their correction factors due to the rod cell boundary conditions. The few group constants of the typical rod cells are calculated by multigroup SN-method^(6,10,20) in cylindrical geometry, while the correction factors by multigroup FFCP-method in assembly geometry. For convenience sake, we call the former "Standard values", while the later "correction factors", and all of these values "reactor constants".

The standard values are dependent on quick parameters, namely moderator density, liquid poison density, whereas the multigroup constants are not. Hence the dependency of the standard values on these parameters can be obtained from a set of the multigroup constants substantially invariant as to these parameters. Of course, the standard values also depend on slow parameters, namely absorber nuclide densities in the fuel assembly components. This dependency would be explained in two factors; one is the number density change itself of each absorber nuclide due to burn up and the other is the variation of the multigroup constants due to the former. Consequently it is obvious that the most convenient data processing method in practice is to calculate and compile the standard values at some typical points of every quick parameter from a set of the multigroup constants corresponding to the considered ranges of the slow parameters, where the ranges of the slow parameters should be chosen so reasonably that the multigroup constants are substantially invariant over each of the ranges. By this method, the standard values are calculated and compiled step by step as the range proceeds.

The object of the correction factors are to compensate the standard

values for the discrepancy between the isotropic boundary conditions taken in the cylindrical SN calculation and the actual one. The discrepancy mainly arises from the non periodic material array of a fuel assembly, viz., PWR fuel assembly has some non fuel rods in its array. The effects of these non fuel rods on the boundary conditions of each rod cell may not largely depend on any parameter other than burnup rate of the poison rod, because other parameters are overall ones and hence have no large local effects.

It is, therefore sufficient to calculate the correction factors for each type of the assemblies only at some typical points of the poison rod burnup rate with the other parameters fixed at suitable points. For PWRs, the parameters necessary in practice are as follows:

(Quick Parameters)

- | | |
|---------------------------|-------|
| (1) fuel temperature | P_1 |
| (2) moderator density | P_2 |
| (3) liquid poison density | P_3 |

(Slow parameter)

- | | |
|-----------------------------|-------|
| (1) U-235 density | P_4 |
| (2) Pu-239 " | P_5 |
| (3) Pu-240 " | P_6 |
| (4) Pu-241 " | P_7 |
| (5) poison rod burn up rate | P_8 |

2.4.2 Calculation of reactor constants

Multi-group calculation is needed for determining reactor constants. We calculate rod-wise constants and multiplication efficiency because the over all flux spectrum is distinct cell by cell.

Usually the multi-group spectrum is calculated by the p_n , B_n , S_n or integral- p_0 method. The typical computer codes based on P_n or $^{(4)}B_n$ method, namely the moment method are MUFT and GAM.

Both of them solve only the slowing down equation derived as the Fourier transform of the one dimensional Boltzmann equation on the assumption of specially constant cross sections. In such a case the neutron thermalization equation is solved by another code such as THERMOS or the like, which means the calculation system is not closed in the sense of eigen value. It is then obvious that these systems have two disadvantageous points in practical use for commercial thermal reactors, one of which is the ambiguity or uncertainty in determination of specially constant cross

sections and the other is the difficulty in obtaining the multiplication efficiency of each rod in an assembly. Moreover there is no such practical computer code based on the moment method that can deal with a multigroup eigen value problem in a simple geometry, i.e., a cylinder, slab or sphere with one-dimensional heterogeneity.

On the contrary, some one-dimensional multi-group S_n codes have been developed for practical use, the typical two of them are well-known to us, viz., DTF(ANISN) and WDSN-II which can dispose both of the eigenvalue and the fixed source problem. The characteristic differences between them exist in the method of taking angular quadratures, the treatment of anisotropic scattering source and the treatment of void region.

We have taken WDSN-II for the purposes in favour of the merit that it can calculate the angular quadrature automatically according to a clear theory and the treatment of void region has been verified by our calculation, while DTF(ANISN) requires angular quadratures as input data and the convergence of calculation has not been certified in case of a geometry with some void regions. The anisotropic source is generally calculated by the Legendere expansion of differential cross section in regard to the direction cosine of scattering angle μ_0 under the condition of rotational invariance. WDSN-II code takes account of anisotropy of the collision source by far the first order at present, but it is easy to add the faculty of evaluating the higher order anisotropy. The method of numerical solution used in this code is described in APPENDIX V, VI and VII. One of the important factors for a rod cell calculation is the boundary condition of the cell which is determined through by the natural (or obvious) condition at the core boundary in rigorous sense, but it is impossible at present to determine the cell boundary conditions by a full core calculation. But it may be possible to obtain the approximate conditions by a multigroup calculation in the two-dimensional assembly geometry with perfect reflective boundary conditions, because the assembly boundary conditions may be nearly flat except that of assembly positioned near the core periphery, or the rod wise flux spectrum may not be influenced by the assembly boundary conditions so strongly as by rod-rod interaction even if the assembly boundary conditions are not flat. Therefore we determine the rod cell boundary conditions by the assembly calculation described above using the code COLSQ.

This code solves the Po-integral Boltzmann equation using the first flight collision probabilities. The relation between the integral transport equation and the first flight collision probability is described in detail

in APPENDIX VIII. Of course this method may be the most precise one for evaluating the details of the reaction rates and the effective cross sections in an assembly, but such a method needs so much computer time that it is hardly possible to perform many practical calculations according to various reactor states.

Therefore we execute such calculations only at some typical parameter points and the results are stored as a basic data for modification of the rod cell boundary conditions through a quantity, e.g., ALBEDO which is usable in WDSN-II code. But, the problem of finding a set of effective ALBEDO values is one of the important works for the reactor constant calculations in rod cell geometries, because the ALBEDO have strong effect on the disadvantage factors in one rod cell on which the cell average cross sections and hence the multiplication efficiency depend.

2.4.3 Formulation of the reactor constants

i) Standard value

As previously mentioned in Sec. 2.4.1 the standard values are calculated by solutions of the transport equation in the cylindrical geometries. But it is to be noted that the few group constants should be so defined that the diffusion equations, when these constants are applied as the coefficients, yield a solution consistent with that of the transport equation as precisely as possible. The definition admissible for this requirement can be derived from some troublesome manipulations. The details of the procedure⁽⁴⁾ are described in APPENDIX IX.

The diffusion approximation may be represented using a difference operator ∇_L^2 as

$$-\tilde{D}^g \nabla_L^2 \tilde{\phi}^g + \tilde{\Sigma}_{rem}^g \tilde{\phi}^g = \frac{1}{\lambda} \chi^g \sum_g \tilde{\Sigma}_f^{g' \rightarrow g} \tilde{\phi}^{g'} + \tilde{\Sigma}_{se}^{g-1 \rightarrow g} \tilde{\phi}^{g-1}$$

where

$$\tilde{\Sigma}_f^g = \sum_i \nu \Sigma_{fi}^g \tilde{\phi}_i^g V_i / \sum_i \tilde{\phi}_i^g V_i$$

$$\tilde{\Sigma}_{se}^{g \rightarrow g+1} = \tilde{R}_d^g \cdot \tilde{\Sigma}_s^{g \rightarrow g+1}$$

$$\tilde{\Sigma}_{rem}^g = \tilde{\Sigma}_a^g + \tilde{R}_r^g \cdot \tilde{\Sigma}_s^{g \rightarrow g+1} - \tilde{\Sigma}_n^g$$

$$\tilde{D}_g = \begin{pmatrix} \tilde{D}_r^g & 0 \\ 0 & \tilde{D}_a^g \end{pmatrix}$$

$$\tilde{R}_d^g = 1 + \sum_{\substack{g' \neq g \\ g' \neq g+1}} \sum_s \frac{\sum_i s_i^{g' \rightarrow g+1}}{\sum_s s^{g \rightarrow g+1}} \phi_i^{g'} V_i / \sum_i \phi_i^{g'} V_i$$

$$\tilde{R}_r^g = 1 + \sum_i \sum_{\substack{g' \neq g \\ g' = g+1}} \sum_s \frac{s_i^{g \rightarrow g'}}{\sum_s s^{g \rightarrow g+1}} \phi_i^g V_i / \sum_i \phi_i^g V_i$$

$$\sum_s^{g \rightarrow g'} = \sum_i \sum_s s_i^{g \rightarrow g'} \phi_i^g V_i / \sum_i \phi_i^g V_i$$

$$\sum_a^g = \sum_i \sum_a s_{ai}^g \phi_i^g V_i / \sum_i \phi_i^g V_i$$

$$\sum_n^g = \sum_i \sum_n s_{ni}^g \phi_i^g V_i / \sum_i \phi_i^g V_i$$

$$\tilde{D}_r^g = R / \sum_i (\Delta R_i / |D_i^g|) - \sum_\ell^g \cdot \frac{\sum_i \phi_i V_i}{\sum_i (\nabla^2 \phi^g)_i V_i}$$

$$\tilde{D}_a^g = \sum_i (|D_i^g| - \sum_{\ell i}^g / B_g^2) \phi_i^g V_i / \sum_i \phi_i^g V_i$$

$$\sum_\ell^g = \sum_i \sum_\ell s_{\ell i}^g \phi_i^g V_i / \sum_i \phi_i^g V_i$$

$$D_i^g = 1/3 \sum_{tri}^g$$

$$\sum_{\ell i}^g = \sum_{g' \neq g} \sum_{g''} \{ \sum_{fi} (\chi_i^{g'} \vee \sum_{fi}^{g''} \frac{\sum_{sli}^{g' \rightarrow g}}{\sum_{tri}^g} + \sum_{smi}^{g'' \rightarrow g' \rightarrow g} \frac{\phi_i^{g''}}{\phi_i^g} - \sum_{tmi}^{g' \rightarrow g} \cdot \frac{\phi_i^{g'}}{\phi_i^g} \}$$

$$\sum_{sli}^{g' \rightarrow g} = \int_g du \int_{g'} du' f_{li}(u' \rightarrow u) \sum_{si}(u') [\text{div} \mathbb{J}(u)]_i / [\text{div} \mathbb{J}^{g'}]_i$$

$$\sum_{tri}^g = \int_g \sum_{ti}(u) [\text{div} \mathbb{J}(u)]_i du / [\text{div} \mathbb{J}^g]_i - \sum_{sli}^{g \rightarrow g}$$

$$\sum_{smi}^{g'' \rightarrow g' \rightarrow g} = \sum_{si}^{g'' \rightarrow g'} \cdot \sum_{sli}^{g' \rightarrow g} / \sum_{tri}^g$$

$$\sum_{tmi}^{g' \rightarrow g} = \sum_{ti}^{g'} \cdot \sum_{sli}^{g' \rightarrow g} / \sum_{tri}^g$$

$$\sum_{ti}^g = \sum_{ai}^g + \sum_{si}^g + \sum_{ni}^g$$

$$\sum_{ai}^g = \int_g \sum_{ai}(u) \phi(u) du / \phi_i^g$$

$$\Sigma_{si}^g = \sum_{g'} \Sigma_{si}^{g \rightarrow g'}$$

$$\Sigma_{si}^{g \rightarrow g'} = \int_g du \int_{g'} du' f_0(u \rightarrow u') \Sigma_{si}(u) / \phi_i^g$$

$$\nu \Sigma_{fi}^g = \int_g du \nu \Sigma_{fi}(u) \phi_i(u) / \phi_i^g$$

$$\Sigma_{si}(u) = \Sigma_{ei}(u) + \Sigma_{ii}(u) + 2\Sigma_{ni}(u)$$

$$\phi_i^g = \int_g du \phi_i(u)$$

$$\phi_i(u) = \int_{V_i} \phi(u, r) dv / V_i$$

$$[\text{div} \mathbb{J}(u)]_i = \int_{V_i} \text{div} \mathbb{J}(u, r) dv / V_i$$

$$[\text{div} \mathbb{J}^g]_i = \int_g du [\text{div} \mathbb{J}(u)]_i$$

$$\phi(u, r) = \int_{4\pi} \phi(u, r, \Omega) d\Omega / 4\pi$$

$$\mathbb{J}(u, r) = \int_{4\pi} \phi(u, r, \Omega) \cdot \Omega d\Omega / 4\pi$$

$\Sigma_{ai}(u)$: macroscopic absorption cross section

$\Sigma_{ei}(u)$: macroscopic elastic scattering cross section

$\Sigma_{ii}(u)$: macroscopic inelastic scattering cross section

$\Sigma_{ni}(u)$: macroscopic (n,2n) reaction cross section

$\nu \Sigma_{fi}(u)$: macroscopic fission cross section multiplied by
v-value

R : rod cell radius

ΔR : space mesh increment

V : volume element

B^2 : axial buckling

i : mesh number

g : few energy (or lethargy) group number

ii) Correction factor

The correction factors are defined by the following consideration.
The boundary conditions of any rod cell in an assembly may be determined by the assembly array type and pison rod burn up rate as described in (i).

Thus, the correction factors, for the standard value of a quantity X in an assembly type A with a poison rod burnup rate B is defined as the next matrix:

$$M_X^A(B) \equiv \frac{1}{X_S} \begin{pmatrix} X_{11} & X_{12} & \dots & X_{1N} \\ X_{21} & X_{22} & \dots & X_{2N} \\ \dots & \dots & \dots & \dots \\ X_N & X_N & \dots & X_{NN} \end{pmatrix} \begin{matrix} A \\ \\ \\ B \end{matrix}$$

where

X_S : Standard value calculated by the cylindrical SN method under suitable values of the parameters $P_1 \sim P_7$ and $P_8 = B$.

X_{ij} : Actual value of X for (i,j) th rod in the $N \times N$ assembly array which is calculated by the FFCP method in the assembly geometry under the parameter values same as above.

Therefore, the FFCP calculation is performed for every type A or the assemblies at a burn up step B and $M_X^A(B)$ is calculated for every necessary quantity X , e.g., σ_c^g , $\sigma_s^{g \rightarrow g'}$ of the important nuclides and the macroscopic quantities Σ_c^g , $\Sigma_s^{g \rightarrow g'}$ etc.

This procedure is performed step-wise as to B with an appropriate interval ΔB in which M_X^A is nearly constant. Obviously, the rod cell-wise effective values X_e in assembly A of a quantity X corresponding to arbitrary values of parameters $P_1 \sim P_7$ are given as the next $N \times N$ matrix

$$(X_e) = X \cdot M_X^A(B)$$

through burn up interval $(B, B+\Delta B)$.

2.5 Calculation of distributions

2.5.1 Calculation of the flux distribution in a reactor core

The Boltzmann equation is so complicated that the distribution of the neutron flux over a commercial power reactor core may hardly be obtained by solving it within an appropriate computer time and capacity. Therefore, the Boltzmann equation is obtained approximately by a set of few group diffusion equations. The diffusion equations are generally solved by the so-called seven points recursion formula or a variational method such as the finite element method. In any case, the large obstacles against solving the practical problems are the following three items included in inversion⁽⁷⁾ of the spacial operators.

- (1) Difficulty in determination of the adequate boundary conditions.
- (2) Any coordinate system does not necessarily fit to the actual horizontal geometry.
- (3) Large computer capacity is required for a full core calculation.

The item (1) has the following features. For a reactor core calculation, it is desirable to know a set of external conditions defined at the surface of the core, and these conditions are homogeneous such as:

$$\left(\frac{1}{\phi} \cdot \frac{\partial \phi}{\partial n}\right)_{\text{core surface}}, \quad n: \text{normal to surface}$$

These values are however, not given previously because these are to be determined by the over-all calculation about a larger geometry including the core, at the external boundary of which naturally known conditions can be taken. But, the over-all calculation cannot be performed properly by any usual diffusion code which takes only one coordinate system for a geometry, viz., the horizontal geometry of any actual reactor is so complicated that some parts of it fit to one coordinate system, while to another do the other parts, and the item (2) means this feature.

In these circumstances, calculation is generally performed by modifying the actual geometry to fit to the computer code or by setting up the trial values of the logarithmic derivatives at some imaginary boundaries convenient for the code. The result of such a calculation is then unreliable in its distribution because these modifications often distort the overall distribution. The item (3) is the largest obstacle especially in three-dimensional calculation because the computer core capacity required for a calculation of the kind is proportional to the multiple of the numbers of meshes taken on each axis, and this capacity is very rarely admissible for usual computer in case of a large power reactor core.

Our efforts were made to remove these obstacles, and thereby a series of adequate methods has been developed. The series of methods is derived by the following consideration. The geometry of any usual commercial LWR is very complicated horizontally while simple vertically. Then for settling a part of the three items, the three-dimensional equations are first separated into horizontal ones and vertical ones. This operation is possible by the leakage iterative method⁽³³⁾. The one dimensional equations can be solved with ease but the two dimensional equations are

very difficult to be solved because of the item (1) and (2). But, for practical purposes, the item (1) and (2) can be removed by using two coordinate systems, because the horizontal geometry of any commercial LWR fits partly to the former and partly to the latter while the vertical plane geometry fits to a linear coordinate.

Two problems are included in using two coordinate systems in one geometry. The first is continuity at the interface of two horizontal plane regions, in one of which x - y - z system is used while r - θ - z systems is used in the other. The second is the inversion procedure of the spacial operator. We have settled these problems in case with the difference formula as shown in APPENDIX X, but the same problems may arise in case with a variational method.

The substance of the series of methods is as follows:

- (1) Separation of the three dimensional equations into one- and two-dimensional ones.
- (2) The geometry is divided into appropriate regions by vertical curved surfaces.
- (3) Two dimensional equations are expressed region-wise by the coordinate system taken accordingly to the shape of the region. We call this method RWM.
- (4) The spacial operator of two dimensional equation is inverted region-wise.
- (5) The rule of taking mesh line in any region is independent of those of the other regions.

The obstacles described as three items above are almost completely removed by the series of methods.

The outstanding merits of the series of methods are as follows:

- (1) It can be applied quite naturally to any horizontal plane geometry, and thereby the calculational error caused from the geometrical complexity may be extinguished.
- (2) The RWM can limit the required computer core capacity to an adequate maximum value almost independently of the total number of meshes taken in the geometry.
- (3) Nearly natural boundary condition can be taken and it is represented in the most simplified form.

2.5.2 Calculation of burnup rate

Calculation of burn-up distribution is usually accompanied with the next three problems:

- (1) Evaluation of one-group constants^(31,32) for burnup calculation^(30,36,37,38,39)
- (2) Treatment of many F.P. isotopes⁽²⁶⁾
- (3) Correction for variations of the one-group constants and flux distribution during a burnup step.

In the code system, problem (1) has been settled by calculating the effective cross sections consistent with those used for calculating the initial flux distribution, where the cross sections are assumed constant in each of "burnup regions" suitably taken independently of the flux calculation meshes.

For problem (2), the F.P. isotopes are categorized into the next four groups.

- (a) Xe^{135} , Sm^{149}
- (b) The other poisoning isotopes
- (c) Isotopes important for burn-up analyses
- (d) Isotopes important for F.P. release.

The number of the isotope kinds in group (b) is so large that the number density of the individual isotope cannot be calculated, hence they are grouped into some appropriate pseudo-F.P. nuclides. The number of isotope kinds of categories (c) and (d) is small enough that the individual calculation is possible.

The problem (3) is caused essentially from the non-linearity of the equation system. No-suitable correction for this feature can be found other than the normalization of fissile nuclide densities by integral power within the burnup step.

3. Numerical method for solving the thermo-hydraulic equations

3.1 Basic concept

Strictly speaking, the thermo-hydraulic balance condition of a PWR primary system under the required SG output power and steam quality should be described in a complete set of equations for its closed loop composed of reactor core, SG, circulating pumps and other junction parts. For statistic analysis of a reactor core however, the core boundary conditions corresponding to the required SG output power and steam quality are given as the design values, hence thermo-hydraulic equations⁽¹¹⁾ (1.2), (1.3) and (1.4) defined over a reactor core can be solved under these conditions. Of course, it is necessary for transient analysis to connect these equations to out-core balance equations considering various characteristic relation and quantities, e.g., the pump characteristics, the reactor control system characteristics, the pressure loss coefficients, etc. In this report object is restricted to only seeking the appropriate macroscopic distributions over a core under the suitable core boundary conditions.

3.2 Macroscopic treatment

The thermo-hydraulic equations are principally regarded as a set of partial differential equations about the pressure P , temperature T and velocity vector \mathbf{V} as to space variable \mathbf{r} and time variable t , where fluid density ρ , enthalpy e are the hydrodynamic quantities uniquely defined by P and T , but the distortion tensor τ is given by P , T and \mathbf{W} . These equations should be solved under the next conditions

$$V_{f=0} = 0$$

$$T(x, y, 0, t) = T_{in}(x, y, t)$$

$$P(x, y, Z_u, t) = P_{out}(x, y, t)$$

$$W(x, y, 0, t) = W_{in}(x, y, t)$$

where the next equation

$$f(x, y) = 0$$

represents the flow channel contour vertical to flow direction parallel to Z -axis. But configuration of flow area in any actual reactor core and dependency of the distortion tensor τ on T , P and \mathbf{W} are so complicated

that the analytical solution of the original equations may hardly be obtained. Hence it follows that an engineering treatment^(25,28) must be applied using macroscopic empirical data for smoothing the microscopic complexity away, and obtaining reasonable macroscopic results for practical use. The macroscopic balance equations in the form for such a treatment can be derived by integrating the equations over a sub-channel flow area and defining the appropriate average coefficients. The detailed derivation of the macroscopic equations is described in APPENDIX XI.

The balance equations about subchannel i is as follows"

(Mass balance equation)

$$A_i \frac{\partial \rho_i}{\partial t} + \frac{\partial m_i}{\partial z} = -\sum_j W_{ij} \quad (3.1)$$

(Axial momentum equation)

$$\begin{aligned} A_i \frac{\partial m_i}{\partial t} - 2A_i u_i \frac{\partial \rho_i}{\partial t} + A_i \frac{\partial P_i}{\partial z} \\ = -\left(\frac{m_i}{A_i}\right)^2 \left\{ \frac{V_i f_i \phi}{2D_i} + \frac{K_i V_i'}{2} + A_i \frac{\partial}{\partial z} \left(\frac{V_i'}{A_i} \right) \right\} A_i \\ - f_t \sum_j (u_i - u_j) W_{ij} + \sum_j (2u_j - u^*) W_{ij} - A_i \rho_i g \cos \theta \end{aligned} \quad (3.2)$$

(Radial momentum equation)

$$\frac{\partial W_{ij}}{\partial t} + \frac{\partial u^* W_{ij}}{\partial z} = \frac{d}{\ell} (P_i - P_j) - \frac{d}{\ell} C_{ij}^f W_{ij} \quad (3.3)$$

(Energy equation)

$$\begin{aligned} A_i \rho_i \frac{\partial h_i}{\partial t} + m_i \frac{\partial h_i}{\partial z} = q_i - \sum_j (T_i - T_j) C_{ij}^t \\ + \sum_j (h_i - h_j) W_{ij} + \sum_j (h_i - h^*) W_{ij} \end{aligned} \quad (3.4)$$

where the subscript i or j denotes subchannel and

t : Time variable (SEC)

z : Distance from the inlet (M)

m_i : Mass velocity (KG/SEC)

W_{ij} : Radial flow rate from channel i to j , per unit channel length (KG/SEC/M)

- W'_{ij} : Turbulent cross flow rate (KG/SEC/M)
 T_i : Temperature ($^{\circ}$ K)
 P_i : Pressure (KGW/M)
 ρ_i : Fluid density (KG/M)
 $\bar{\rho}_i$: Effective density, or energy balance refer to appendix XI
 h_i : Enthalpy (Kcal/KG)
 h^* : Enthalpy (Kcal/KG) Refer to appendix XI
 u_i : Effective momentum velocity (M/SEC)
 refer to appendix XI
 u^* : "
 V_l : Liquid specific volume
 V'_i : Effective specific volume for momentum transfer (M /KG).
 Refer to appendix XI.
 q_i : Linear heat rate (Kcal/M)
 ϕ : Two phase flow multiplier. Refer to appendix XI
 f_i : Friction factor based on all-liquid flow. Refer to
 appendix XI.
 D_i : Hydraulic diameter (M)
 K_i : Spacer loss coefficient. Refer to appendix XI
 f_t : Empirical correction factor for turbulent radial momentum
 transfer rate
 g : Gravitational constant
 e : Channel declination as to gravitational direction
 d : Rod spacing, (M). Refer to appendix XI
 l : Length of radial momentum transfer region, (M). Refer to
 appendix XI
 C^f_{ij} : Radial friction coefficient from channel i to j (SEC^{-1})
 C^t_{ij} : Heat transfer coefficient (Kcal/M/ $^{\circ}$ K)

3.3 Matrix notation and the practical form for a large core

The set of equations (3.1) ~ (3.4) can practically be solved only for a fuel bundle with some hundreds of subchannels, whereas any actual thermal reactor core without channel box has more than ten thousands of subchannels. Therefore it is inevitable to separate the calculation procedure into two steps, viz., inner iteration and outer iteration. The former means to solve equations (3.1) ~ (3.4) for each bundle under a set of guessed boundary condition obtaining subchannel-wise distributions, while the later means to solve these equation regarding each

bundle as a subchannel with equivalent coefficients obtaining new bundle boundary. In performance of these numerical calculations, it is inevitable to distinguish each assembly, subchannel, and their boundary by appropriate identification numbers. The identification numbers are defined as follows,

I : Number of assemblies in the core

J : Number of assembly boundaries in the core

K_n : Number of subchannels in assembly n

L_n : Number of subchannel boundaries in assembly n except those on assembly boundaries

M_m : Number of subchannel boundaries on the assembly boundary
No.m

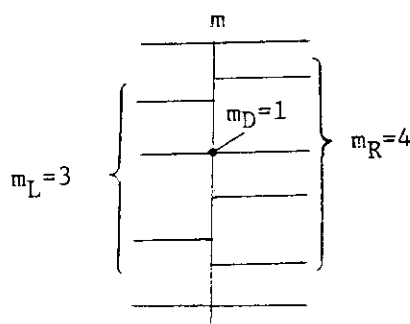
$$M_m = m_L + m_R - m_D + 1$$

where

m_L = Number of left boundaries

m_R = Number of right boundaries

m_D = Number of duplicate boundaries



i, j : Subchannel number defined as

1, 2,, K_1 in assembly No.1

$K_1+1, K_1+2, \dots, K_1+K_2$ in assembly No.2

k = Subchannel boundary number in an assembly allotted to the boundary between two subchannels i and j ($i < j$) in ascending order of j ,

m = Assembly boundary number allotted to the boundary between two assemblies n and n' ($n < n'$) in ascending order of n'

k_B = Subchannel boundary number on assembly boundary in ascending order of K_A the assembly boundary number

Under these identification, the equations for inner calculation of assembly n can be represented in vector matrix notations as

(Mass)

$$A \frac{\partial \vec{\rho}}{\partial t} + \frac{\partial \vec{m}}{\partial z} = -S\vec{W} - \vec{S}_B \vec{W}_B \quad (3.5)$$

(Axial momentum)

$$A^{-1} \frac{\partial \vec{m}}{\partial t} - 2U \frac{\partial \vec{\rho}}{\partial t} + \frac{\partial \vec{\rho}}{\partial z} = -\vec{a} + A^{-1} S \Delta U^* \vec{W} + A^{-1} S_B \Delta L_B^* \vec{W}_B \quad (3.6)$$

(Radial momentum)

$$\frac{\partial \vec{W}}{\partial t} + \frac{\partial}{\partial z} (U^* \vec{W}) + \left(\frac{dc}{\ell_c}\right) C_F \vec{W} = \left(\frac{dc}{\ell_c}\right) S + \vec{P} \quad (3.7)$$

(Energy)

$$U''^{-1} \frac{\partial \vec{h}}{\partial t} + \frac{\partial \vec{h}}{\partial z} = M^{-1} \{ \vec{q}' - S \Delta T \vec{G} + S \Delta H \vec{W}' + S \Delta H^* \vec{W} - S_B \Delta T_B \vec{C}_T^B + S_B \Delta H_B^* \vec{W}_B \} \quad (3.8)$$

(Heat source)

$$\rho_r C_r \frac{\partial T_r}{\partial t} = K_r \left(\frac{\partial^2 T_r}{\partial r^2} + \frac{1}{r} \frac{\partial T_r}{\partial r} \right) + q''' \quad (3.9)$$

$$\vec{\rho} = \begin{pmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_{kn} \end{pmatrix}$$

$$\vec{m} = \begin{pmatrix} m_1 \\ m_2 \\ \vdots \\ m_{kn} \end{pmatrix}$$

$$\vec{P} = \begin{pmatrix} P_1 \\ P_2 \\ \vdots \\ P_{kn} \end{pmatrix}$$

$$\vec{h} = \begin{pmatrix} h_1 \\ h_2 \\ \vdots \\ h_{kn} \end{pmatrix}$$

$$\vec{w} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_{Ln} \end{pmatrix}$$

$$\vec{w}' = \begin{pmatrix} w_1' \\ w_2' \\ \vdots \\ w_{Ln}' \end{pmatrix}$$

$$\vec{w}_B = \begin{pmatrix} w_{B1} \\ w_{B2} \\ \vdots \\ w_{BJ} \end{pmatrix}$$

$$\vec{w}_{Bj} = \begin{pmatrix} w_{B1} \\ w_{B2} \\ \vdots \\ w_{BMj} \end{pmatrix}$$

$$M = \begin{pmatrix} m_1 & & 0 \\ & m_2 & \\ & & \ddots \\ 0 & & & m_{kn} \end{pmatrix}$$

$$U = \begin{pmatrix} u_1 & & 0 \\ & u_2 & \\ & & \ddots \\ 0 & & & u_{kn} \end{pmatrix}$$

$$U'' = \begin{pmatrix} u_1'' & & 0 \\ & u_2'' & \\ & & \ddots \\ 0 & & & u_{kn}'' \end{pmatrix}$$

$$U^* \equiv \begin{pmatrix} u_1^* & & 0 \\ & u_2^* & \\ & & \ddots \\ & & & u_{Ln}^* \end{pmatrix}$$

$$u_k^* \equiv \begin{cases} u_i(h) & \text{for } w_k > 0 \\ u_j(h) & \text{for } w_k < 0 \end{cases}$$

$$\Delta U^* = 2U^I - U^*$$

U^I : $Ln \times Ln$ - diagonal matrix of velocity, (k, k) element of which is u_i when two subchannels i and j ($i < j$) are inter connected by k -th subchannel boundary.

U^J : $Ln \times Ln$ - diagonal matrix of velocity (k, k) element of which is u_j for the same (i, j) as above.

$$U_B^* = 2U_B^I - U_B^*$$

U_B^I, U_B^I : $J \times J$ diagonal matrices of velocity, (m, m) - th element of which is such a matrix as

$$(u_m^I) = \begin{pmatrix} u_{m,1}^i & & 0 \\ & \ddots & \\ 0 & & u_{m,Mm}^i \end{pmatrix} \quad m=1 \sim I$$

or

$$(u_m^J) = \begin{pmatrix} u_{m,1}^j & & 0 \\ & \ddots & \\ 0 & & u_{m,Mm}^j \end{pmatrix} \quad m=1 \sim J$$

respectively for subchannel pair (i, j) ($i < j$) inter-connected by assembly boundary m

$$U_B^* \equiv \begin{pmatrix} (u_1^*) & 0 \\ 0 & (u_J^*) \end{pmatrix}$$

$$(u_m^*) = \begin{pmatrix} u_{m,1}^* & 0 \\ 0 & u_{m,Mm}^* \end{pmatrix}$$

$$u_{m,n}^* = \begin{cases} u_i & \text{if } w_{Bk} > 0 \\ u_j & \text{if } w_{Bk} < 0 \end{cases} \quad n=1 \sim Mm$$

for subchannel pair (i, j) ($i < j$) inter-connected by subchannel boundary k on assembly boundary m .

$$\Delta H \equiv H^I - H^J$$

H^I, H^J : $L_n \times L_n$ - diagonal matrices of enthalpy, (k, k) - element of which is h_i or h_j respectively for the same (i, j) as those for U^I

$$\Delta H^* = H^I - H^*$$

$$H^* \equiv \begin{pmatrix} h_1^* & & 0 \\ & h_2^* & \\ & & \ddots \\ 0 & & & h_{L_n}^* \end{pmatrix}$$

$$h_k^* \equiv \begin{cases} h_i(k) & \text{for } W_k > 0 \\ h_j(k) & \text{for } W_k < 0 \end{cases}$$

$$\Delta H_B^* \equiv H_B^I - H_B^*$$

H_B^I, H_B^J : $J \times J$ - diagonal matrices of enthalpy, (m, m) - the element of which is (h_m^I) or (h_m^J) chosen by all the same manner as with that of (u_m^I) or (u_m^J)

H_B^* : $J \times J$ - diagonal matrices of enthalpy defined by all the same manner as that of U_B^*

$$\Delta T_B : T_B^I - T_B^J$$

T_B^I, T_B^J : $J \times J$ - diagonal matrices of temperature defined by all the same manner as that of U_B^I or U_B^J respectively.

$$\Delta T : T^I - T^J$$

T^I, T^J : $L_n \times L_n$ - diagonal matrices of temperature defined by all the same manner as that of U^I , or U^J respectively.

S_B^n : The n -th row vector of the next matrix S_B

$$S_B = (S_{nm}), n = 1 \sim I, m = 1 \sim J$$

$$S_{nm} = \begin{cases} M_n \times M_n - \text{zero matrix; if assembly } n \text{ has boundary } m \\ M_m \times M_m - \text{Unit matrix; if assemblies } n \text{ and } n' \text{ are inter} \\ \text{connected by boundary } m \text{ and } n < n' \\ M_n \times M_n - \text{negative unit matrix; if } n > n' \text{ in the case} \\ \text{above} \end{cases}$$

S : Summation matrix of an assembly. If any two sub-channels i and j in an assembly are interconnected

by a boundary k , the cross terms W_{ij} , W_{ij}' , C_{ij}^t , C_{ij}^f may be represented by one dimensional notation as W_k , W_k' , C_k^t , C_k^f , hence W_{ji} , W_{ji}' , C_{ji}^t , C_{ji}^f by $-W_k$, $-W_k'$, C_k^t , C_k^f .

Thus, the cross terms in the balance equations about subchannel i may be represented in the simple notations, viz., inner products of W , W' , C_T , C_F and a vector S_i , the k -th element S_{ik} of which is defined as

$$S_{ik} = \begin{cases} 0 & : \text{If subchannel } i \text{ has not boundary } k \\ +1 & : \text{If subchannel } i \text{ and } j \text{ are interconnected by the} \\ & \text{boundary } k \text{ and } i < j \\ -1 & : \text{If } i > j \text{ in the case above.} \end{cases}$$

The size of the matrix S is then determined by the assembly considered, viz., for the n -th assembly, S is determined as

$$S = (S_{ik}) \quad i = 1 \sim kn, \quad k = 1 \sim Ln$$

This matrix has the next properties

$$S^T \times S \equiv (a_{kk'}) = \begin{cases} 2 & : \text{If } k = k' \\ 0 & : \text{If no subchannel has two boundaries } k \\ & \text{and } k' \text{ at the same time.} \\ +1 & : \text{If subchannel } i \text{ is interconnected to} \\ & \text{subchannels } j \text{ and } j' \text{ by boundaries } k \text{ and} \\ & k' \text{ respectively under the next condition} \\ & j, j' > i \text{ or } j, j' < i \\ -1 & : \text{If } j > i > j' \text{ or } j < i < j' \text{ in the case above} \end{cases}$$

$$S \times S^T \equiv (b_{ii'}) = \begin{cases} I(i) & : \text{If } i = i' \text{ and subchannel } i \text{ has } I(i) \\ & \text{boundaries in the assembly} \\ -1 & : \text{If } i \neq i' \end{cases}$$

where, no two subchannels are interconnected by more than one boundary. Moreover, the matrix S is a conversion factor as

$$US = SU^I$$

$$TS = ST^I$$

$$HS = SH^I$$

$$A = \begin{pmatrix} A_1 & & 0 \\ & A_2 & \\ 0 & & A_{kn} \end{pmatrix}$$

$$(d_c/\ell_c) = \begin{pmatrix} (d_c/\ell_c)_1 & & 0 \\ & \ddots & \\ 0 & & (d_c/\ell_c)_{Ln} \end{pmatrix}$$

$$C_F = \begin{pmatrix} C_1^f & & 0 \\ & C_2^f & \\ 0 & & C_{Ln}^f \end{pmatrix}$$

$$\vec{C}_T = \begin{pmatrix} C_1^t \\ C_2^t \\ \vdots \\ C_{Ln}^t \end{pmatrix}$$

$$\vec{C}_T^B + \begin{pmatrix} C_{11}^t \\ C_{12}^t \\ \vdots \\ C_{1M1}^t \\ C_{21}^t \\ C_{22}^t \\ \vdots \\ C_{2M2}^t \\ \vdots \\ C_{J1}^t \\ \vdots \\ C_{JMJ}^t \end{pmatrix}$$

$$\vec{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_{kn} \end{pmatrix}$$

$$a_i \equiv \left(\frac{m_i}{A_i}\right)^2 \left\{ \frac{V_i f_i \phi_i}{2D_i} + \frac{K_i V_i'}{2} + A_i \frac{\partial}{\partial z} \left(\frac{V_i'}{A_i} \right) \right\} \\ + \frac{f_T}{A_i} \cdot \vec{S}_i \Delta \vec{UW}' + \rho_i g \cos \theta$$

where

- ρ_r : Density of fuel rod (gr/cc)
- C_r : Specific heat of fuel rod (kcal/°K/gr)
- T_r : Temperature of fuel rod (°K)
- K_r : Heat conductivity of fuel rod (kcal/°K/M/SEC)
- q''' : Heat source density (kcal/cc)

4. Description on the computer code system

4.1 Overall structure of the system

The code system was developed for the purposes shown in the main document. For convenience' sake, the system may be decomposed into some functional parts, eq.:

- (1) Nuclear data processing part
- (2) Multi-group constant calculation part
- (3) Reactor constant calculation part
- (4) Reactor characteristics calculation part

The following explanation concerning the code system will be given in accordance with this decomposition.

(1) Nuclear data processing part

Here, the basic data for nuclear calculation are taken mainly from ENDF-B, and the continuous data of cross sections, fission spectra and ν -values, etc. are reproduced in form of analytical functions of the neutron energy according to the cross section theories and the ENDF instruction manual. The reproduced data are then corrected for the doppler effect and changed into the ultra fine energy group data sets required by part (2).

(2) Multi-group constants calculation part

Here, two basic calculation are performed to obtain the ultra fine energy spectrum of neutron flux. One is solving the slowing equation with given fast source, and the other is solving the thermal equilibrium equation with the slowing down source given as the result of the former. These two calculations are performed in an appropriate one-dimensional geometry using the ultra fine data sets given from part (1). Averaging the ultra fine data with the ultra fine flux spectra as weight gives the multi-group constants.

(3) Reactor constant calculation part

Here, the basic work is solving the multi-group transport equation by SN or FFCP method according to the purpose described in the main document using the multi-group constants given by part (2). Averaging the multi-group constants with the multi-group spectra as weight gives the reactor constants.

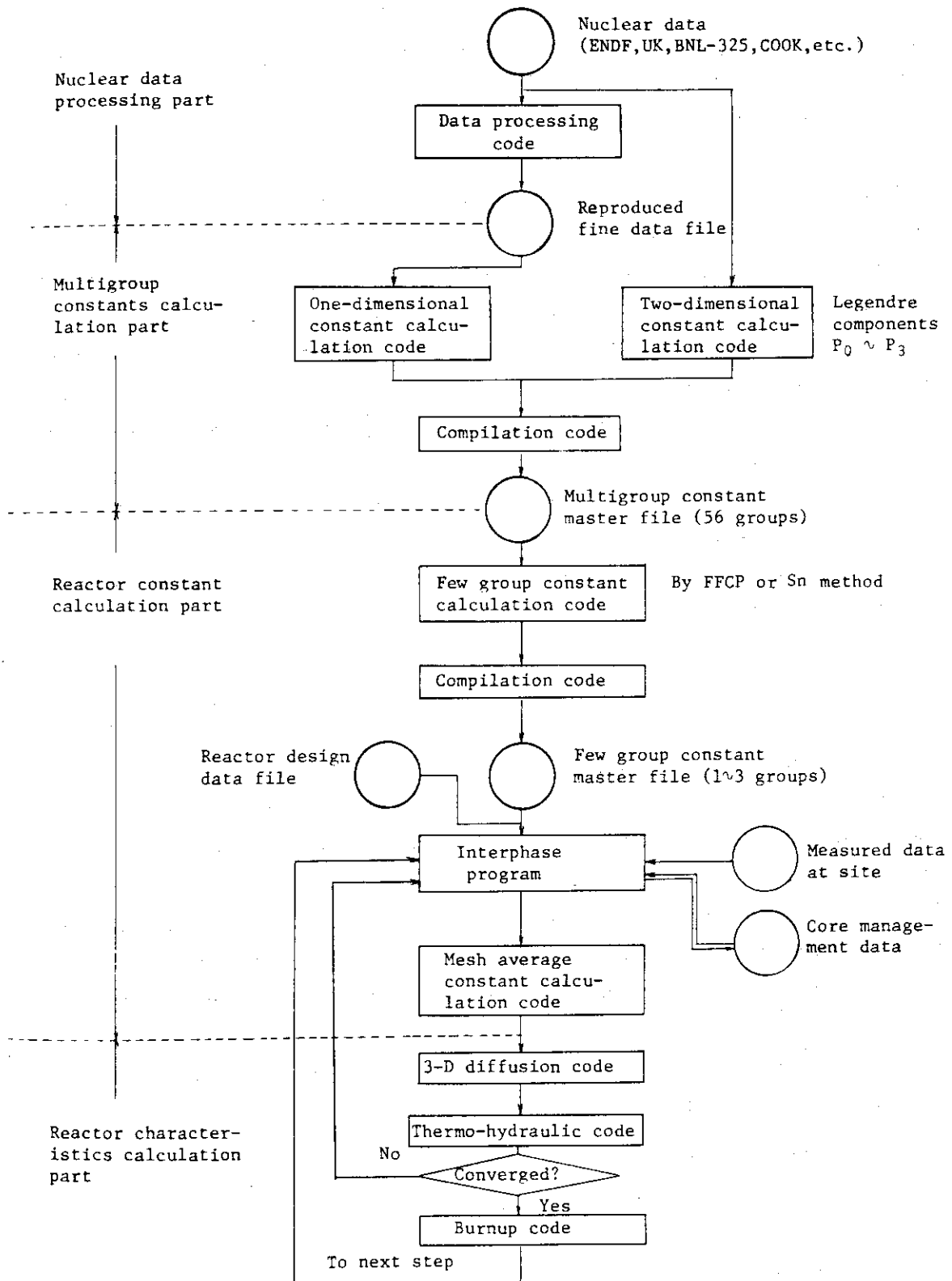
(4) Reactor characteristics calculation

The main calculations are as follows:

- (a) Neutron diffusion calculation
- (b) Thermo-hydraulic calculation
- (c) Burn up calculation

The over-all system is briefly illustrated as the next figure.

The overall system



4.2 The organic function of the code system

A series of descriptions has been made about the full steps of the numerical method for analyzing the nuclear and thermo-hydraulic behaviour of the LWR core. Every step is therefore accomplished in principle by the method described. But it is to be noted that every step of the analysis for core management is inevitably accompanied with so many input and output data that manual handling of them may scarcely be possible. Furthermore, the nuclear constants depend on the various parameters, e.g., the moderator density, poison density, fuel enrichment, etc. which are on the contrary determined by nuclear constants; the calculations are all interconnected as an iteration loop in rigorous sense.

It is then obvious that there are two important works for use of the analyzing method; one is to construct an organic computer code system, the other is to cut the loop loose from the unimportant connections and set up a practical feed back scheme for economizing computer time by avoiding much trivial tolerance. We have designed a computer code system which has partly been completed and is partly under construction. Description will be given about the system mainly from the view-point of the two works above.

4.2.1 Construction of core calculation part

As a rule, this work could be done on the FORTRAN level by undertaking the adjustment of input and output data FORMAT of every constituent code of the system. But this method requires much manpower because the code system is to be constituted by many codes. We then avoid this demerit by development of some common utility programs in the assembler languages. These utility programs may be powerful tools especially for the critical search and burnup calculations, because such calculations are multi-step ones in principle, and consequently performed by many computer codes.

All the data processed for core maintenance calculations are put into the next categories in the system.

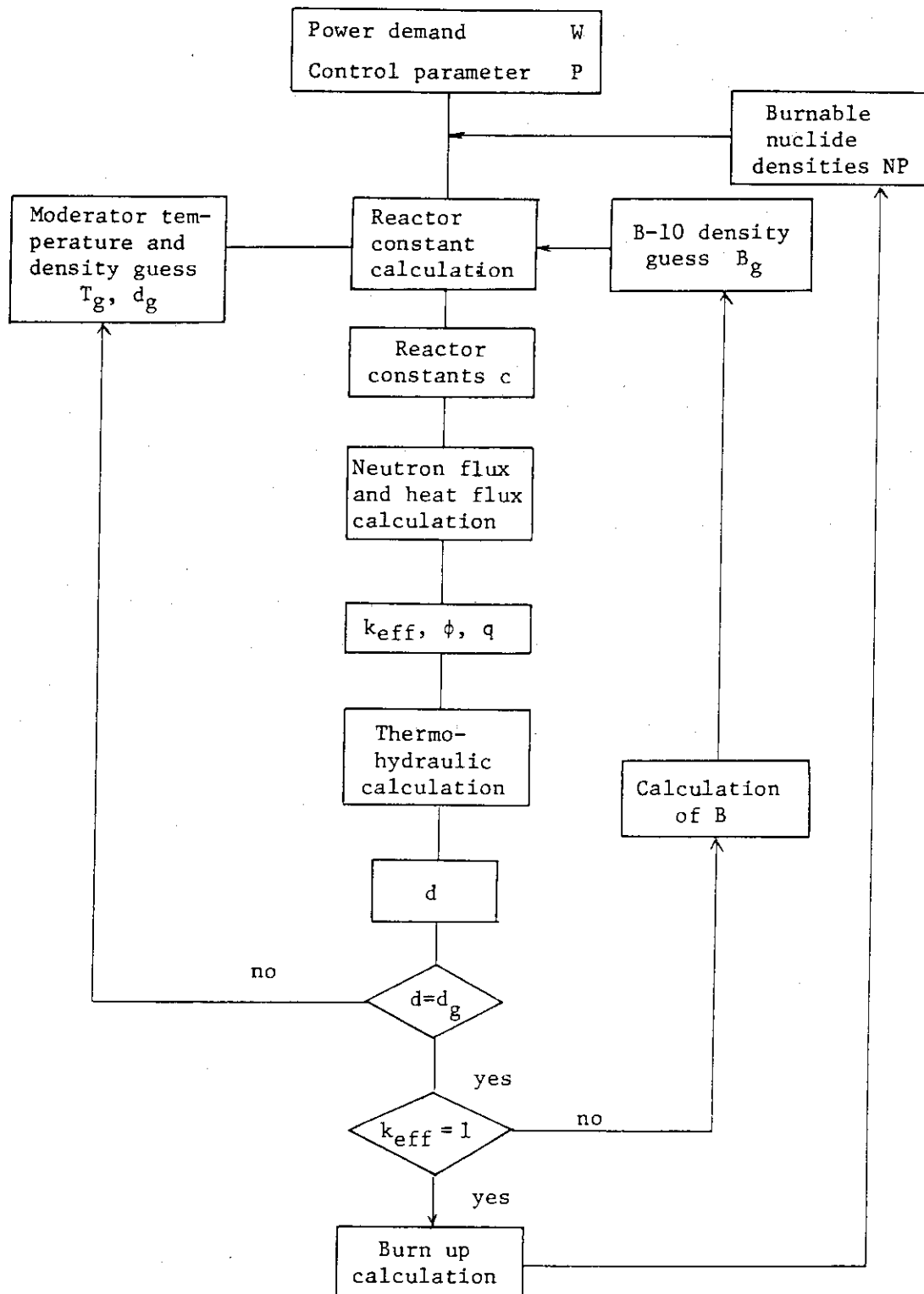
- (1) The nuclear data
- (2) Multigroup constants
- (3) Reactor constants
- (4) Fine flux spectra
- (5) Multigroup flux spectra
- (6) Spatial distributions of few group fluxes

- (7) Spacial distributions of nuclide number densities
- (8) Data of hard-wares
- (9) The control parameters of the code system

The data are usually stored in external storage units, and can be arbitrarily revised, added or eliminated if necessary.

4.2.2 Practical feed back scheme

In general, both of the multi-group constants and the reactor constants as the coefficients of the neutron balance equations depend on the flux, i.e., the solution of it, through the moderator density, poison density and burnup rate. The feedback effects on the multi-group constants are taken into account by interpolation of the resonance shielding factors which are fitted to appropriate functions of the parameters. But the treatment of the feed back effects on the multi-group constants is not so important from the view-point of the code system, because the values of the parameters having influence on the multi-group constants are fixedly given for multi-group calculations. Hence the description will be limited to the reactor core calculation using the reactor constants from now on. The summarized logic of the core calculation part of the system is simply shown in the figure below.



In this code system, the reactor constants corresponding to the parameters N , d , B are interpolated instead of being calculated from the multi-group spectrum calculation. Therefore, the multi-group calculation is cut off from the loop, thereby the substantial iteration due to the feed back effects are quickly performed in the calculation flow.

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APPENDIX I Evaluation of Doppler effect

1. Dependency of cross section on medium temperature

The nuclear cross section of a nuclide with velocity W for neutrons with velocity v is determined by the relative speed defined by

$$v_r = |v - W| \quad (1)$$

The corresponding cross section may then be denoted as $\sigma^\infty(v_r)$. If velocity distribution of the medium nuclide is subject to the Maxwell-Boltzmann's formula $P(W, T)$, the average cross section (9) $\sigma(v)$ of the medium nuclide for neutrons with velocity W is given by

$$v\sigma(v) = \iiint v_r \sigma^\infty(w) P(W, T) dW \quad (2)$$

where

$$P(W, T) = \exp(-W^2/4\theta) / (4\pi\theta)^{3/2} \quad (3)$$

$$\theta = kT/2M$$

k : Boltzmann constant (eV/°K)

M : Nuclear mass in the unit of neutron mass

T : Medium temperature (°K)

Upon substituting relation (3) into (2), the next relation is obtained,

$$v\sigma(v) = \frac{1}{(4\pi\theta)^{3/2}} \int_{-\infty}^{\infty} dV_x \int_{-\infty}^{\infty} dV_y \int_{-\infty}^{\infty} dV_z v_r \sigma^\infty(v_r) \cdot \exp(-W^2/4\theta) \quad (4)$$

Since $\sigma^\infty(v_r)$ is determined by v_r , one of the integration variables in the relation (4) must be replaced by v_r to perform the integration. Let the orientation of W be in accordance with that of V_z for calculational convenience. The speed v_r is given as

$$v_r = |v - W| = \sqrt{v_x^2 + v_y^2 + (v_z - v)^2} \quad (5)$$

which can be solved about V_z as

$$V_{z\pm} = v \pm \sqrt{v_r^2 - v_x^2 - v_y^2} \quad (6)$$

with the sign taken in the same order.

Hence, it follows that

$$dV_{z\pm} = \pm v_r \phi(v_r) dv_r \quad (7)$$

with

$$\phi(v_r) \equiv 1/\sqrt{v_r^2 - v_x^2 - v_y^2} \quad (8)$$

Substituting the relation (7) into (4) with consideration of the V_z duality as to v_r gives the integral part I of the relation (4) as

$$I = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{\sqrt{v_x^2 + v_y^2}}^{\infty} \{f(V_{z-}) + f(V_{z+})\} v_r \phi(v_r) dv_r \quad (9)$$

with

$$f(V_{z\pm}) = v_r \sigma^{\infty}(v_r) \exp(-V^2/4\theta) \quad (10)$$

Further, substitution of the next relation

$$V^2 = v_x^2 + v_y^2 + v_{z\pm}^2 = v^2 + v_r^2 \pm 2v\sqrt{v_r^2 - v_x^2 - v_y^2} \quad (11)$$

into (10) yields

$$f(V_{z\pm}) = v_r \sigma^{\infty}(v_r) \exp\left(-\frac{v^2 + v_r^2}{4\theta}\right) \cdot \exp\left(\pm \frac{v\sqrt{v_r^2 - v_x^2 - v_y^2}}{2\theta}\right) \quad (12)$$

which gives the relation:

$$v_r \{f(V_{z-}) + f(V_{z+})\} = 2v_r \sigma^{\infty}(v_r) \exp\left(-\frac{v^2 + v_r^2}{4\theta}\right) \cosh \frac{v\sqrt{v_r^2 - v_x^2 - v_y^2}}{2\theta} \quad (13)$$

Substitution of this into the definition (9) with some manipulations about the order of integration yields

$$I = 2 \exp(-v^2/4\theta) \int_0^{\infty} dz \exp(-z^2/4\theta) z^2 \sigma^{\infty}(z) K(z) \quad (14)$$

with

$$K(z) = \int \int_{x^2 + y^2 \leq z^2} dx dy \cosh \left(\frac{v\sqrt{v^2 - x^2 - y^2}}{2\theta} \right) / \sqrt{z^2 - x^2 - y^2} \quad (15)$$

Integration of $K(z)$ can be performed by the next changes of the variables:

$$\begin{aligned}
 x &= r \cos \phi \\
 y &= r \sin \phi \\
 0 &\leq r \leq z \\
 0 &\leq \phi \leq 2\pi
 \end{aligned}
 \tag{16}$$

yielding the Jacobian J as

$$J = \frac{\partial(x,y)}{\partial(r,\phi)} = r \tag{17}$$

which gives $K(z)$ as

$$\begin{aligned}
 K(z) &= 2\pi \int_0^z dr r \cosh\left(\frac{v\sqrt{z^2-r^2}}{2\theta}\right) / \sqrt{z^2-r^2} \\
 &= \frac{4\pi\theta}{v} \sinh \frac{vz}{2\theta}
 \end{aligned}
 \tag{18}$$

Substitution of the relation (18) into (14) gives $\sigma(v)$ as

$$\sigma(v) = \frac{1}{\sqrt{\pi}\theta} \frac{1}{v^2} \exp\left(-\frac{v^2}{4\theta}\right) \int_0^\infty \sigma^\infty(z) z^2 \exp\left(-\frac{z^2}{4\theta}\right) \sinh \frac{vz}{2\theta} dz \tag{19}$$

or $\sigma(E)$ as

$$\begin{aligned}
 \sigma(E) &= \frac{1}{2\sqrt{2\pi}\theta} \cdot \frac{1}{E} \int_0^\infty \sigma^\infty(z) \sqrt{z} \{ \exp\left[-\frac{1}{2\theta}(\sqrt{E} - \sqrt{z})^2\right] \\
 &\quad - \exp\left[-\frac{1}{2\theta}(\sqrt{E} + \sqrt{z})^2\right] \} dz
 \end{aligned}
 \tag{20}$$

Formula (20) is directly applied for thermal neutrons, v_{1z} , when

$$0 < E < 5kT$$

2. Calculation of Doppler function

For neutrons of kinetic energy E sufficiently large so that the relation

$$E \gg kT \tag{21}$$

holds the second exponential term of the integrand in the formula (20) can be neglected and the approximation

$$\sqrt{E} - \sqrt{z} = \frac{E-Z}{\sqrt{E} + \sqrt{z}} \approx \frac{E-Z}{2\sqrt{E}} \tag{22}$$

may be admissible.

In such a case, therefore, the formula (20) may be broken down as

$$\sigma(E) = \frac{1}{2\sqrt{2\pi}\theta} \cdot \frac{1}{E} \int_0^{\infty} \sigma^{\infty}(z) \sqrt{z} \exp\left[-\frac{(E-Z)^2}{8\theta E}\right] dz \quad (23)$$

which when Breit-Wigner's single level formula is applied for the expression of $\sigma^{\infty}(z)$ yields the so-called Doppler functions as

$$\psi(\xi, x) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{1}{1+y^2} \exp\left[-\frac{\xi^2}{4} (x-y)^2\right] dy \quad (24)$$

$$\chi(\xi, x) = \frac{\xi}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{y}{1+y^2} \exp\left[-\frac{\xi^2}{4} (x-y)^2\right] dy \quad (25)$$

Numerical values of the functions are computed as follows.

Let a complex function $W(\xi, x)$ be defined as

$$-W(\xi, x) = \frac{2}{\xi\sqrt{\pi}} \psi \frac{1}{\xi\sqrt{\pi}} \chi \quad (26)$$

This function may be represented simply as

$$-W(\xi, x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{1-iy} \exp\left[-\frac{\xi^2}{4} (x-y)^2\right] dy \quad (27)$$

Change of the integration variable by

$$\frac{\xi}{2} (y-x) = t \quad (28)$$

yields the next relation

$$\frac{1}{1-iy} = \frac{i\xi}{2} \cdot \frac{1}{z-t} \quad (29)$$

with

$$z = (\xi x + i\xi)/2 \quad (30)$$

Substitution of eq. (28) and (29) into (27) results in the next expression

$$W(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z-t} dt \quad (31)$$

For smaller $|z|$, this function can be expanded in the Taylor series as

$$W(z) = e^{-z^2} + \frac{2iz}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n n! 2^n (2z^2)^n}{(2n+1)!} \quad (32)$$

whereas it may be adequately represented by an asymptotic expansion for larger $|z|$ as

$$W(z) = \frac{i}{\pi} \sum_{n=0}^{\infty} \frac{\Gamma(n+1/2)}{z^{2n+1}} \quad (33)$$

From the expansion formula (32), it may be presumed that the integrand of (31) may properly be represented as

$$\sum_{n=0}^{\infty} A_n t^n$$

which suggests that the integration of (31) for smaller $|z|$ is better to be performed by the Gaussian integration method based on an appropriate orthogonal function set. For larger $|z|$, however, $W(z)$ may be easily calculated from the formula (33) by taking a sufficient number of terms for desired precision.

For a typical example, QUICKW-code calculates $W(z)$ by a suitable approximation for every range of $|z|$.

In range 1, $|z| < 6$,

$\psi(\xi, x)$ and $\chi(\xi, x)$ are calculated and tabulated at necessary points of the parameters ξ and x for interpolation of ψ and χ as to ξ and x .

In range 2, $6 \leq |z| < 12$,

$W(Z)$ is represented by the next Gaussian integral based on Hermite function as

$$W(Z) = \frac{1}{\pi} \lim_{n \rightarrow \infty} \sum_{k=1}^n H_k^n / (z - t_k^n)$$

which is truncated for n larger than 4 and thereby it is given as

$$\begin{aligned} W(Z) &= \frac{1}{\pi} \left\{ \frac{H_1^4}{z - t_1^4} + \frac{H_1^4}{z + t_1^4} + \frac{H_2^4}{z - t_2^4} + \frac{H_2^4}{z + t_2^4} \right\} \\ &= \frac{2}{\pi} \left\{ H_1^4 \frac{x[x^2 - y^2 - (t_1^4)^2] + 2xy^2}{4x^2y^2 + [x^2 - y^2 - (t_1^4)^2]^2} + H_2^4 \frac{x[x^2y^2 - (t_2^4)^2] + 2xy^2}{4x^2y^2 + [x^2y^2 - (t_2^4)^2]^2} \right\} \\ &\quad + \frac{2i}{\pi} \left\{ H_1^4 \frac{y[x^2 - y^2 - (t_1^4)^2] - 2x^2y}{4x^2y^2 + [x^2 - y^2 - (t_1^4)^2]^2} + H_2^4 \frac{y[x^2 - y^2 - (t_2^4)^2] - 2x^2y}{4x^2y^2 + [x^2 - y^2 - (t_2^4)^2]^2} \right\} \end{aligned}$$

Here, the zero points t_1^4 and t_2^4 of 4th-order Hermite function and the corresponding weights H_1^4 , H_2^4 are given as

$$\begin{aligned} t_1^4 &= \pm 0.5246476233 & H_1^4 &= 0.8049141 \\ t_2^4 &= \pm 1.6506801239 & H_2^4 &= 0.08131284 \end{aligned}$$

In range 3; $12 \leq |z| < 100$,

$W(Z)$ is approximated by the asymptotic expansion (33) which with aid of the Q. D. algorithm yields

$$\begin{aligned} W(Z) &= \frac{2iz}{\sqrt{\pi}} \frac{1}{2z^2-1} \\ &= \frac{1}{\sqrt{\pi}} \cdot \frac{2x^2y - y(x^2-y^2-0.5)}{(x^2-y^2-0.5)^2 - 4x^2y^2} \\ &\quad + \frac{i}{\sqrt{\pi}} \cdot \frac{x(x^2-y^2-0.5)-2xy^2}{(x^2-y^2-0.5)^2 + 4x^2y^2} \end{aligned}$$

In range 4, $|z| \geq 100$,

Only the first term of (33) is taken yielding

$$\begin{aligned} W(Z) &= \frac{i}{\sqrt{\pi}} \cdot \frac{\Gamma(1/2)}{Z} \\ &= \frac{1}{\sqrt{\pi}} \left\{ \frac{y}{x^2+y^2} + i \frac{x}{x^2+y^2} \right\} \end{aligned}$$

APPENDIX II Choice of Energy Points for Multigroup Constant Calculation

1. Thermal Energy Points

For determining the thermal neutron energy mesh points for multigroup constants calculation, it is necessary to take account of the next factors:

- (1) Thermal resonance structure of the macroscopic total cross section.
- (2) Thermal scattering property.
- (3) Energy range in which thermal neutron flux spectrum peak lies.

Of these, the factor (2) is taken into account mainly for defining the upper limit energy of thermal neutron flux; the scattering property may be an important measure for judging the energy point, e.g., such as, through which neutrons are not almost scattered up. The factor (3) is a measure of important thermal neutron energy range in which finer energy meshes may be required. But the applications of these two factors may be simple in any way. The factor (1) is the most important measure for determining the energy mesh points through which the effects of thermal resonances are efficiently evaluated in the multigroup constant calculation. Therefore the thermal energy mesh points are determined mainly by this point of view under the next two requirements.

- (a) Relative error of linear interpolation of transport kernel concerning to neutron energy is bound by an upper limit.
- (b) In the proximity of each prominent resonance energy, e is taken proportionally to $1/\Delta E$, where ΔE is the mesh width taken there.

The meaning of requirement (a) is self-evident; the transport kernel is generally represented by

$$T(x) \propto \exp(x) \quad (1)$$

with

$$x \equiv \Sigma_t(E) \cdot \ell \quad (2)$$

where $\Sigma_t(E)$ is the macroscopic total cross section and ℓ is a length. Thus if x takes two values a and ar ($r > 1$) corresponding to two distinct energy points, the value of the transport kernel at x between these two points is given as

$$\tilde{T}(x) \approx e^{-a} \left\{ 1 - \frac{1 - e^{-a(r-1)}}{a(r-1)} (x-a) \right\} \quad (3)$$

Then, the relative error $\sigma(x)$ is given by

$$\sigma(x) = e^{x-a} \left\{ 1 - \frac{1 - e^{-a(r-1)}}{a(r-1)} (x-a) \right\} - 1 \quad (4)$$

yielding the maximum value $\sigma(x_m)$ as

$$\sigma(x_m) = \frac{\exp \eta}{H \eta} - 1 \quad (5)$$

with

$$\eta \equiv \frac{S}{1 - e^{-S-1}} \quad (6)$$

$$S \equiv a(r-1) \quad (7)$$

By equating $\sigma(x_m)$ given by the formula (5) to ϵ , the next table is obtained.

ϵ	S	η
0.001	0.08947	0.0454
0.01	0.28234	0.1478
0.1	0.87796	0.5024

Requirement (b) means if the collision rate per unit neutron energy is nearly constant concerning neutron energy, the next relation may give the best harmony of precision in neutron balance calculation:

$$\Delta E_S \cdot \epsilon_S = \Delta E_C \cdot \epsilon_C$$

where

$\Delta E_C, \Delta E_S$: energy mesh width in the center or the skirt region of a resonance

ϵ_C, ϵ_S : error bound in the center or the skirt region of a resonance

Thermal resonances was taken into account of the nuclei:

U-235 (0.29, 1.14)
 Pu-239 (0.296)
 Pu-240 (1.056)

Pu-241	(0.258)
Am-241	(0.308, 0.576, 1.27)
In-115	(1.456)
Cd-113	(0.178)
Dy-163	(1.71)
Sm-149	(0.0976)

Where the numbers in the round brackets indicate resonance energy in the unit of electron Volts. Taking account of these judgements together with some other requirements, e.g., that the Bragg-cut energies of carbon nuclide had better be taken as the points, the thermal energy points were obtained as shown in the later table. Note that the multigroup boundary points were chosen so that the multigroup constants are almost independent of overall energy spectrum of the neutron flux used as weight.

2. Epithermal Energy Points

A series of survey calculations were performed to find such points through which calculated effective resonance integrals⁽²⁹⁾ are saturated. As the objective resonance nuclei, fissionable nuclei Ag-107, Ag-109 and SS-elements were taken. Thus, the best energy points were obtained as shown in the last table. It is to be noted that the ABAGYAN⁽²³⁾ Points are taken as multigroup boundaries for the same reason as the thermal part.

Thermal mesh point

No.	Energy(eV)	No.	Energy(eV)	No.	Energy(eV)	No.	Energy(eV)
1	0.0001*	31	0.1400	61	0.4500	91	1.1600
2	0.0005*	32	0.1450	62	0.4750	92	1.2000*
3	0.0015*	33	0.1500	63	0.5000*	93	1.2350
4	0.0030*	34	0.1580	64	0.5400	94	1.2700*
5	0.0050*	35	0.1600	65	0.5760*	95	1.2900
6	0.0060	36	0.1780*	66	0.6000	96	1.3100
7	0.0075	37	0.1850	67	0.6500*	97	1.3350
8	0.0090	38	0.1900	68	0.7000	98	1.3700
9	0.0100*	39	0.1950	69	0.8000	99	1.3800
10	0.0120	40	0.2020	70	0.8730*	100	1.3900
11	0.0140*	41	0.2100	71	0.9300	101	1.4000
12	0.0160	42	0.2150	72	0.9700	102	1.4100
13	0.0200*	43	0.2200	73	0.9950	103	1.4200
14	0.0250	44	0.2250	74	1.0000*	104	1.4300
15	0.0268	45	0.2300	75	1.0050	105	1.4500
16	0.0314*	46	0.2350	76	1.0100	106	1.4560*
17	0.0360	47	0.2400*	77	1.0200	107	1.4700
18	0.0420*	48	0.2450	78	1.0250	108	1.4800
19	0.0490	49	0.2580*	79	1.0450	109	1.4900
20	0.0560*	50	0.2680	80	1.0560*	110	1.5000
21	0.0642	51	0.2800*	81	1.0700	111	1.5100
22	0.0707*	52	0.2900	82	1.0750	112	1.5300
23	0.0740	53	0.2960*	83	1.0800	113	1.5700
24	0.0860	54	0.3080	84	1.0900	114	1.6300
25	0.0976*	55	0.3200	85	1.0950*	115	1.6700
26	0.1060	56	0.3300	86	1.1000	116	1.7100*
27	0.1100	57	0.3500*	87	1.1050	117	1.7500
28	0.1150	58	0.3600	88	1.1100	118	1.8550
29	0.1270*	59	0.3750	89	1.1200		
30	0.1360	60	0.3900	90	1.1400*		

(Comment) The asterisks indicate multi-group boundaries.

EPITHERMAL LETHARGY MESH

	Upper Energy	Δu_f	No. of Point	Sub total
1	10.5 MeV	0.001	480	
2	6.5	"	485	
3	4.0	"	470	
4	2.5	"	580	
5	1.4	"	560	
6	0.8	"	693	
7	0.4	"	693	
8	0.2	"	693	4654
9	100.0 Kev	0.0003	2552	
10	46.5	"	2571	
11	21.5	"	2552	
12	10.0	"	2552	10227
13	4.65	0.0001	7716	
14	2.15	"	7655	
15	1000.0 eV	"	7657	23028
16	465.0	0.0002	3857	
17	215.0	"	3828	7685
18	100.0	0.0003	2552	
19	46.5	0.0006	1286	
20	21.5	0.001	765	
21	10.0	"	766	
22	4.65	"	919	2450
	(1.855)		51882	

(*) This Table indicates the boundary lethargy points.
 These points aren't sufficient to express high energy
 resonances such as Fe's resonances.

APPENDIX III An analytic form of standard energy spectrum of neutron flux in typical light water reactor

Strictly speaking, any real neutron flux spectrum is given by the solution of the Boltzmann equation. But, we need an imaginary convenient form of flux spectrum to obtain a set of standard multigroup constants. For this reason we seek a typical spectrum which may be an averaged values over the objective reactor system. In our work, we get this by the method described below. In an infinite homogeneous system, the neutron flux $\phi(E)$ is given by the next equation.

$$\sigma_t(E)\phi(E) = \chi(E) \int_0^{\infty} \nu\sigma_f(E')\phi(E')dE' + \int_0^{\infty} \sigma_s(E' \rightarrow E)\phi(E')dE \quad (1)$$

We solve this equation through all epithermal energy region under the next assumptions:

- (1) $\sigma_t(E)$ is a constant above an energy E_h which lies in higher energy range of $1/E$ flux region.
- (2) In an energy region below E_h , $\phi(E)$ is formal given.
- (3) $\nu\sigma_f(E) = 0$ for $E \geq E_h$
- (4) $\sigma_s(E' \rightarrow E) = \sigma_s/(1-\alpha)E'$ for $\alpha E' \leq E \leq E'$
 $= 0$ for otherwise

Under these assumptions, equation (1) can be changed into the next form.

$$\sigma_t\phi(E) = a\chi(E) + \frac{\sigma_s}{1-\alpha} \int_E^{E/\alpha} \frac{\phi(E')}{E'} dE' \quad \text{for } E \geq E_h \quad (2)$$

This equation can be solved analytically by the following asymptotic method. Let

$$\phi(E) = \chi(E) \cdot \psi(E) \quad (3)$$

By substituting this into eq. (2), we get

$$\sigma_t\psi(E) = a + \frac{\sigma_s}{1-\alpha} \frac{e^{E/\theta}}{\sqrt{E}} \int_E^{E/\alpha} \frac{e^{-E'/\theta}}{\sqrt{E'}} \cdot \psi(E') dE' \quad (4)$$

Next, we define the 0-th solution of this equation by

$$\psi_0 = a/\sigma_t$$

Then we get the 1st solution $\psi_1(E)$ of eq. (4) as

$$\sigma_t \psi_1(E) = a + \frac{a}{1-\alpha} \frac{\sigma_s}{\sigma_t} \frac{e^{E/\theta}}{\sqrt{E}} \int_E^{E/\alpha} \frac{e^{-E'/\theta}}{\sqrt{E'}} dE' \quad (5)$$

This solution can be rewritten in the next form

$$\psi_1(E) = \psi_0(E) \{1 + \Delta_1(E)\} \quad (6)$$

where

$$\Delta_1(E) = 2 \frac{1}{1-\alpha} \frac{\sigma_s}{\sigma_t} \frac{\sqrt{\theta}}{\sqrt{E}} e^{E/\theta} [\text{erf}(\sqrt{E/\alpha\theta}) - \text{erf}(\sqrt{E/\theta})] \quad (7)$$

Generally speaking, the limit form of solution of equation (4) can be given as

$$\psi(E) = \psi_0 \{1 + \Delta_1(E) + \Delta_2(E) + \dots\} \quad (8)$$

where

$$\Delta_n(E) = \frac{1}{1-\alpha} \frac{\sigma_s}{\sigma_t} \frac{e^{E/\theta}}{\sqrt{E}} \int_E^{E/\alpha} \frac{e^{-E'/\theta}}{\sqrt{E'}} \Delta_{n-1}(E') dE' \quad (9)$$

By our calculation, solutions higher than $\psi_1(E)$ are not necessary in actual problem. Then we take form (6) for our needs. For energy range ($\leq E_h$) we have an empirical⁽⁴⁰⁾ form, thus we get an analytical form for full neutron energy range as follows:

$$\begin{aligned} \phi(E) = & \frac{E}{(KT_n)^2} \exp(-E/KT_n) + \gamma_1 \delta(E+2KT_n) \frac{1}{(E+2KT_n)^{1+\beta}} \\ & + \gamma_2 \psi_1(E) \chi(E) \end{aligned} \quad (10)$$

where

γ_1, γ_2 : Constants to be determined by measured data

K : Boltzmann constant

T_n : Neutron temperature AT_M

$\chi(E)$: Fission spectrum $\sqrt{E/\theta^3} \exp(-E/\theta)$

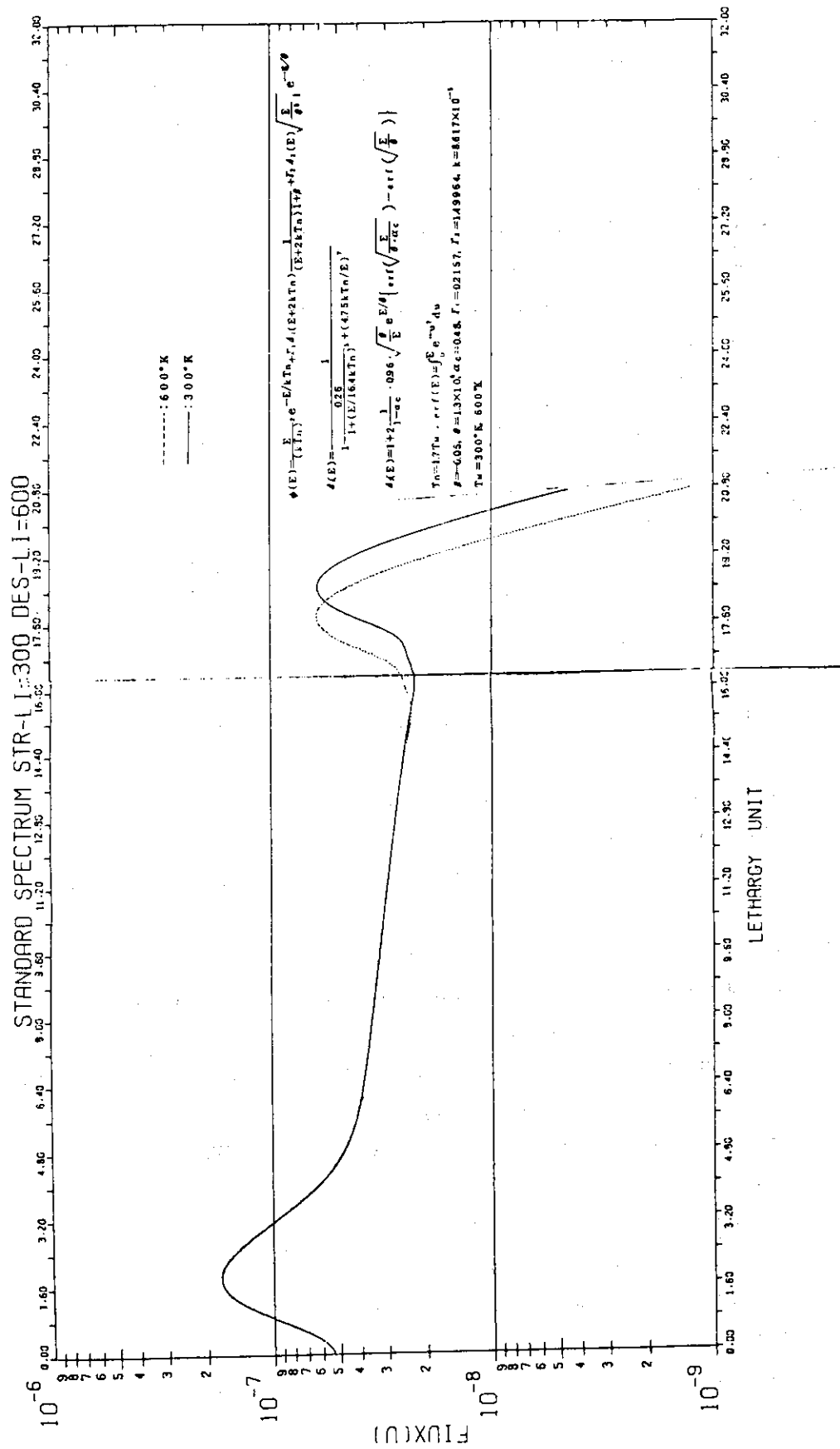
$$\delta(E) \equiv \frac{1}{1 - \frac{C}{1+(E/BKT_n)^5} + (DKT_n/E)^7} \quad (11)$$

$$\psi_1(E) \equiv 1 + \frac{2}{1-\alpha_c} \frac{\sigma_s}{\sigma_t} \frac{\sqrt{\theta}}{\sqrt{E}} e^{E/\theta} \{\text{erf}(\sqrt{E/\theta\alpha_c}) - \text{erf}(\sqrt{E/\theta})\} \quad (12)$$

$$\text{erf}(E) \equiv \int_0^E e^{-u^2} du$$

We obtained the values of constants γ_1 , γ_2 , A, B, C, D, α_c , σ_s/σ_t , β , θ , from JPDR's data, etc., as shown in Fig. 14.1.

Fig. 14. 1



APPENDIX IV Form of the group constant table

This group constant table was named SEPCO-set and has the next form⁽⁴¹⁾.

RECORD 1

- Set number NST
- Number of nuclides contained NUC
- Number of neutron energy groups NGR
- Nuclide identification numbers NID (I), I=1, NUC
- Group energy mesh points E(I), I=1, NGR
- Description

From RECORD 2 to RECORD 11 are given to every nuclide.

RECORD 2

- Nuclide identification number NID (I)
- Number of regions in body where the cross section of this nuclide is calculated NRE
- Maximum Legendre order of elastic scattering matrix+1 NEIG
- Maximum Legendre order of inelastic scattering matrix+1 NILG
- The length of elastic scattering cross section vector and self-scatter position of every group NEL (I,J) I=1,2, J=1,NGR
- The length of inelastic scattering cross section vector of every group NIN (I), I=1, NGR
- The length of (n,2n) reaction cross section vector of every group N2N (I), I=1, NGR
- Upper and lower limit of energy group numbers for f \neq 1, 0 NFL, NFU
- The same as above for S \neq 1, 0 NSL, NSU
- The same as above for hr \neq 1, 0 NHL, NHU
- Number of σ_p - points taken for f, S, hr-calculation NSP
- The same as above for T- points NTP
- Dimension of B NC

- Nuclide identification numbers which construct B NID (I), I=1, NC
 - Number of points of every component of B NP (I), I=1, NC
- RECORD 3
- Capture cross section CSIG (I), I=1, NGR
- RECORD 4
- Fission cross section FSIG (I), I=1, NGR
 - $\gamma\sigma_f$ FNSIG (I), I=1, NGR
 - Fission spectrum FSP (I), I=1, NGR
- RECORD 5
- Elastic scattering matrix SCATE (I,J,K), I=1,
NEL (1,J); J=1, NGR;
K=1, NELG
- RECORD 6
- Inelastic scattering matrix SCATI (I,J,K) I=1, NIN (J);
J=1, NGR; K=1, NILG
- RECORD 7
- (n,2n) scattering matrix SCATN (I,J), I=1, N2N(J),
J=1, NGR
- RECORD 8
- Total cross section TSIG (I), I=1, NGR
- RECORD 9
- σ_p - value SIG (I), I=1, NSP
 - T - value T (I), I=1, NTP
 - B - value XN (I,J), I=1, NP(J) J=1, NC
- RECORD 10
- Self-shielding factor FT (I,J,K), FC (I,J,K)
 $f_t(\sigma_p, t)$, $f_c(\sigma_p, t)$ FF (I,J,K), FE (I,J,K)
 $f_t(\sigma_p, T)$, $f_e(\sigma_p, T)$ FI (I,J,K) I=NFL, NFU;
 $f_{in}(\sigma_p, T)$ J=1, NSP, K=1, NTP

RECORD 11

Spectrum factor

ST I, N(I);.....N(NC)

I=NSL, NSU; N(1)=1, NP(1);..

...N(NC)=1, NP(NC)

RECORD 12

Heterogeneity factor

HT I,J,N(1).....N(NC)

I=NIL, NHU; J=1, NRE;

N(1)=1, NP(1); ;

N(NC)=1, NP(NC)

The utilization procedure of this table is divided into the next four steps per group.

(1) Calculation of $\sigma^N(0)$

The total σ_{exo} of infinite inelastic scattering and (n,2n) reaction cross sections is given as

$$\sigma_{\text{exo}} = \sigma_{\text{to}} - (\sigma_{\text{eo}} + \sigma_{\text{co}} + \sigma_{\text{fo}})$$

where σ_{to} , σ_{eo} , σ_{co} or σ_{fo} is infinite total, elastic scattering, capture or fission cross section respectively. Then, the factors f_t , f_e , f_c , f_{in} are determined by iterative method as to σ_p -value so as the next relation is satisfied:

$$f_t \sigma_{\text{to}} = f_e \sigma_{\text{eo}} + f_c \sigma_{\text{co}} + f_f \sigma_{\text{fo}} + f_{\text{in}} \sigma_{\text{exo}}$$

Each of the terms is written as $\sigma_t^N(0)$, $\sigma_e^N(0)$, $\sigma_c^N(0)$, $\sigma_f^N(0)$ and $\sigma_{\text{ex}}^N(0)$ from the left hand side of this relation.

(2) Calculation of $\overline{\sigma^N(B)}$

The mutual shielding effect is evaluated by multiplying the S-factor corresponding to input B-value

$$\sigma_t^N(B) = S(B) \cdot \sigma_t^N(0)$$

$$\sigma_e^N(B) = S(B) \cdot \sigma_e^N(0)$$

$$\sigma_c^N(B) = S(B) \cdot \sigma_c^N(0)$$

$$\sigma_f^N(B) = S(B) \cdot \sigma_f^N(0)$$

(3) Calculation of $\sigma_r^N(B)$

Heterogeneity factor is evaluated by multiplying $h_r(B)$ factor corresponding to the region γ and input B

$$\sigma_{tr}^N(B) = h_r(B) \cdot \sigma_t^N(B)$$

$$\sigma_{er}^N(B) = h_r(B) \cdot \sigma_e^N(B)$$

$$\sigma_{cr}^N(B) = h_r(B) \cdot \sigma_c^N(B)$$

$$\sigma_{fr}^N(B) = h_r(B) \cdot \sigma_{fr}^N(B)$$

(4) Calculation of effective scattering matrix

The effective scattering matrix M_e^M is given by multiplying M_s^M the standard scattering low by M_c^M constructed by effective scattering cross sections given by the processes (1) ~ (3).

APPENDIX V Basic theories used in WDSN (2)-code

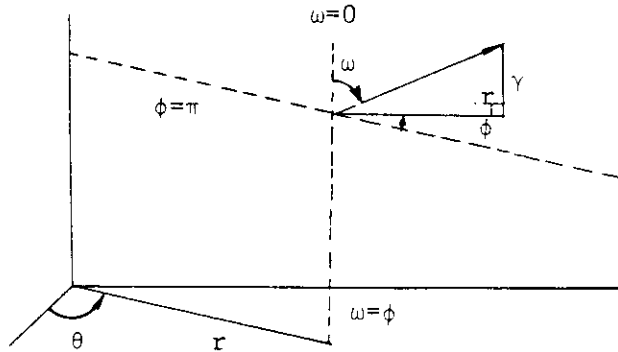
1. Derivation of the discrete form

One-dimensional neutron transport equation is represented on the coordinate system in the figure below.

$$\left[\eta \cos \frac{\partial}{\partial r} - \eta \frac{\sin \phi}{r} \frac{\partial}{\partial \phi} + \Sigma_t \right] N(r, w, \phi, E) = S(r, w, \phi, E) \quad (1)$$

with

$$\begin{aligned} S(r, w, \phi, E) \equiv & Q(r, w, \phi, E) + \chi(E) \int_{\pi/2}^{\pi} dw' \int_{\pi/2}^{\pi} d\phi' \int_0^{\infty} dE' \\ & \times v \Sigma_f(V, E') N(r, w', \phi', E') + \int_{\pi/2}^{\pi} dw' \int_{\pi/2}^{\pi} d\phi' \int_0^{\infty} dE' \\ & \times \Sigma_s(r, w' \rightarrow w, \phi' \rightarrow \phi, E' \rightarrow E) \cdot N(r, w', \phi', E') \end{aligned} \quad (2)$$



In this code, the angular variables are represented by discrete notations⁽¹⁸⁾ n_j ($j=1 \sim n$) and ϕ_{ji} ($k=0 \sim j$), where j denotes the division points of the azimuthal angle ω , and i the division points of the polar angle ϕ , with the division rule described in the next section.

Integration of equation (1) over the polar increment $\Delta\phi_{ji}$ under the assumptions

$$\int_{\Delta\phi_{ji}} N d\phi = \bar{N}_{ji} \cdot \Delta\phi_{ji} \quad (3)$$

$$\int_{\Delta\phi_{ji}} N \cos \phi d\phi = \bar{N}_{ji} \cdot \bar{\mu}_{ji} \cdot \Delta\phi_{ji} \quad (4)$$

$$\sin \phi_{ji} + \sin \phi_{j,i-1} \approx -b_{ji} \Delta\phi_{ji} \quad (5)$$

$$\bar{N}_{jir} \equiv (N_{jir} + N_{ji-1r})/2 \quad (6)$$

$$\mu_{ji} \cdot \Delta\phi_{ji-2} \sin\phi_{ji} \equiv b_{ji} \cdot \Delta\phi_{ji} \quad (7)$$

yields the equation

$$\eta_j \bar{\mu}_{ji} \frac{\partial \bar{N}_{ji}}{\partial r} + \frac{\eta_j b_{ji}}{r} \bar{N}_{ji} - \frac{\eta_j b_{ji}}{r} N_{ji-1} + N_{ji} = S \quad (8)$$

with b_{ji} given by eqs. (5) and (7) as

$$b_{ji} = \bar{\mu}_{ji} - \frac{2}{\phi_{ji}} \sum_{k=1}^i \bar{\mu}_{jk}$$

where $\bar{\mu}_{ji}$ is defined in the next section. Further integration of equation (8) over the space mesh increment ΔR gives the final discrete form as

$$\begin{aligned} & (\eta_j \bar{\mu}_{ji} + \frac{1}{2} \eta_j b_{ji} Pr + h_r) \bar{N}_{jir} \\ & + (-\eta_j \mu_{ji} + \frac{1}{2} \eta_j b_{ji} Pr + h_r) \bar{N}_{jir-1} \\ & - \eta_j b_{ji} Pr \bar{N}_{ji-1r} = \Delta S \end{aligned} \quad (10)$$

where

$$\begin{aligned} Pr & \equiv \Delta R / \bar{R} \\ hr & \equiv \Sigma_t \cdot \Delta R \\ \bar{R} & \equiv (R_r + R_{r-1})/2 \\ N_{jir} & \equiv (N_{jir} + N_{jir-1})/2 \end{aligned} \quad (11)$$

Note that \bar{N}_{jir} is the i -th direction cell average value defined at the outer edge of the r -th space cell, while \bar{N}_{jir} is the r -th space mesh average value defined at the outer edge of the i -th direction cell. These values are connected by other relations. i.e. the diamond difference relations

$$2\tilde{N}_{jir} = \tilde{N}_{jir} + \tilde{N}_{ji-1r} = \bar{N}_{jir} + \bar{N}_{jir} \quad (12)$$

Here, \tilde{N}_{jir} is the average value for the r -th space cell the for the guess values of \bar{N}_{jir} and \bar{N}_{jir-1} . Therefore, by substituting the guess

values of \bar{N}_{jir} and N_{jir-1} . Therefore, by substituting the guess value \bar{N}_{jir} and the corresponding solution \bar{N}_{jir-1} into the relation (12), \tilde{N}_{jir} is obtained which gives \tilde{N}_{jir} by use of the guess \tilde{N}_{ji-1r} . The code does not edit the space cell edge value \bar{N}_{jir} , but edits the phase-space averaged value \tilde{N}_{jir} as an angular flux density in space mesh, additionally editing the boundary cell edge value \bar{N}_{jir} .

2. Choice of angular quadrature ordinates and weights⁽¹⁹⁾

Let the angular components of unit direction vector Ω be ϕ and ω , as shown in the figure of section 1.

Then, in one-dimensional geometry, it is sufficient for the flux calculation to consider only the next range of ω and ϕ

$$\pi/2 \leq \omega \leq \pi \text{ and } \pi/2 \leq \phi \leq \pi$$

The angular mesh points of order n are then defined as

$$\gamma_j \equiv \cos \omega_j \frac{4j(j+1)}{n(n+2)} - 1$$

$$(j=1, 2, \dots, n/2) \quad (13)$$

$$\phi_{ji} \equiv \pi(1 - i/2j) \quad (i=0, 1, \dots, j) \quad (14)$$

The mesh increment is given as

$$d\gamma_j \equiv \gamma_j - \gamma_{j-1} = \frac{8j}{n(n+2)} \quad (15)$$

$$d\phi_{ji} \equiv \phi_{ji-1} - \phi_{ji} = \pi/2j \quad (16)$$

They give a constant increment of solid angle as

$$d\gamma_j d\phi_{ji} = 4\pi/n(n+2) \quad (17)$$

The representative direction of each direction cell is defined by either of the following two methods.

(1) Carlson's method

Let the representatives be $\bar{\gamma}_j$ and $\bar{\mu}_{ji}$. They are defined by the

relations:

$$\bar{\gamma}_j \equiv \frac{1}{2} (\gamma_j + \gamma_{j+1}) (1 + \Sigma) = \left[\frac{4j^2}{n(n+2)} - 1 \right] (1 + \Sigma) \quad (18)$$

$$\bar{\mu}_{ji} \equiv \cos \frac{1}{2} (\phi_{ji} + \phi_{ji-1}) = \cos \pi \left(1 + \frac{1}{4j} - \frac{1}{2j} \right) \quad (19)$$

Here, Σ is a modification factor determined by the diffusion approximation condition which requires that the integral

$$\int_{\pi/2}^{\pi} \sin^3 \omega d\omega \int_{\pi/2}^{\pi} \cos^2 \phi d\phi$$

be given rigorously by the discrete ordinates and weights as $\pi/6$.

This requirement determines Σ as

$$\Sigma = \sqrt{\frac{n+2n}{n^2+2n+2} - 1} \quad (20)$$

(2) Brissenden's method

The representatives are determined by the next two requirements

(a) The first and the second moment conditions are satisfied as

$$\Sigma \bar{\eta}_j \bar{\mu}_{ji} = n(n+2)/16 \quad (21)$$

$$\Sigma \bar{\eta}_j^2 \bar{\mu}_{ji}^2 = 1/24 n(n+2) \quad (22)$$

(b) The flux peak near a reflective boundary is best given by having

$$\Sigma_j \bar{\eta}_j = \frac{1}{32} (n+2) \quad (23)$$

$$\Sigma_j \bar{\eta}_j^2 = \frac{1}{12} n(n+2) \quad (24)$$

$$\Sigma \bar{\mu}_{ji}^2 = \frac{1}{16} n(n+2) \quad (25)$$

These conditions determine $\bar{\eta}_j$ and $\bar{\mu}_{ji}$ as

$$\bar{\eta}_j = a \eta_j' + b \quad (26)$$

$$\bar{\mu}_{ji} = C_{ji} \mu'_{ji} + d_j \quad (27)$$

Here, η'_j is defined by

$$\eta_j'^2 = \frac{1}{\Delta_j} \int_{\Delta_j} \eta^2 dr = 1 - \frac{\gamma_j^2 + \gamma_j \gamma_{j-1} + \gamma_{j+1}^2}{3} \quad (28)$$

and μ'_{ji} is equal to that of Carlson's and

$$a = \sqrt{\frac{1 - \frac{3}{32} \pi^2}{1 - \frac{3}{32} \pi^2 \sigma^2}} \quad (29)$$

$$b = \frac{\pi}{4} (1 - a\sigma) \quad (30)$$

$$\sigma = \frac{m/2}{\sum_{j=1}^m j \eta'_j} \frac{\pi n(n+2)}{32} \quad (31)$$

$$C_j = \sqrt{\frac{j/2 - \frac{1}{j} \left(\sum_{i=1}^j \mu_{ji}'^2 \right) \lambda^2}{\sum_{i=1}^j \mu_{ji}'^2 - \frac{1}{j} \left(\sum_{i=1}^j \mu_{ji}' \right)^2}} \quad (32)$$

$$d_j = \frac{\lambda - C_j}{j} \sum_{i=1}^j \mu_{ji}' \quad (33)$$

3. Boundary conditions

The left-boundary condition is always fixed as perfect reflective one, whereas free, perfect reflective or isotropic one is admissible at the right boundary. These three conditions are as follows.

The free boundary condition is defined by setting the angular fluxes in the direction $\phi (\leq \pi/2)$ as zero at the outer boundary. By the notation of the angular quadrature used in the code, this condition is represented as

$$N_{ji} = 0 \quad \text{for} \quad j = 1 \sim n/2, \quad i = 0 \sim j \quad (34)$$

Here, j denotes the azimuthal angle mesh point and i the polar angle mesh

point. The perfect reflective or isotropic condition is represented by the boundary matrix B_j defined for azimuthal angular slab j . The perfect reflective condition is defined as

$$N_j^- = N_j^+ \quad (34)$$

The vector N_j^- or N_j^+ denotes an inward or outward angular flux vector at the outer boundary, the components of which correspond to ϕ_{ji} described above. The isotropic condition is represented as

$$N_j^- = N_j^- \cdot U_j \quad (36)$$

Here, U_j is a vector the components of which are all unity, and N_j^- is a scalar determined by the next non-leaking condition

$$\int_{\Omega} (N_j^- U - N_j^+) r_o \cdot d\Omega = 0 \quad (37)$$

Here, r_o denotes a unit vector directed toward the space coordinate. The relation is rewritten by discrete notation as

$$U_j \cdot (N^+ - N_j^+ U_j) = 0 \quad (38)$$

Then, N_j^- is given as

$$N_j^- = \frac{\sum_{i \neq 0}^j \mu_i N_i^+}{\sum_{i \neq 0}^j \mu_i} \quad (39)$$

The isotropic non-leaking condition is represented by (36) and (39) as

$$N_j^- = W_j \cdot N_j^+ \quad (40)$$

The matrix W_j is defined as

$$W_j \equiv \begin{pmatrix} 0 & \mu_1 & \dots & \mu_j \\ \vdots & & & \vdots \\ 0 & \mu_1 & \dots & \mu_j \end{pmatrix} \quad (41)$$

The actual non leaking condition is neither perfect reflective nor

isotropic, but it is an intermediate one which may be represented as

$$N_j^- = B_j N_j^+ \quad (42)$$

The intermediate boundary matrix B_j is defined as

$$B_j = \lambda I + (1-\lambda)W_j \quad (43)$$

It is evident that the relation (42) satisfies the non-leaking condition:

$$\mu_j \cdot (N_j^+ \cdot N_j^-) = 0 \quad (44)$$

Note that $\lambda=0$ implies the isotropic condition while $\lambda=1$ the perfect one. The expressions above are used in the original WDSN(2) code as the boundary conditions. In actuality, however, it is not satisfactory for the cell calculations to use only the free or non-leaking condition. That is, to seek the precise spectrum, it is necessary to have the possibility of using the semi-reflective or semi-leaking condition. Such a condition may be attained as follows.

Consider that the fraction λ of the outward vector N_j^+ is perfectly reflected while the fraction of the residue $(1-\lambda)N_j^+$ is reflected isotropically and the residue $(1-\omega)(1-\lambda)N_j^+$ leaks out. Then, the boundary matrix B_j may be modified as

$$B_j = \lambda I + \omega(1-\lambda)W_j \quad (45)$$

implying

$$\text{leak out if} \quad 0 \leq \omega \leq 1$$

$$\text{not leak if} \quad \omega = 1$$

$$\text{leak in if} \quad \omega > 1$$

The relation (42) with B_j defined by (45) is equivalent to the relation.

$$\mu_j (\alpha \cdot N_j^+ - N_j^-) = 0 \quad (46)$$

Here, the scalar α is given as

$$\alpha = \lambda + \omega(1-\lambda) \quad (47)$$

which is the so-called ALBEDO; it is determined by calculation in a larger geometry such as an assembly.

Much effort is required in performing the series of works to find a set of the ALBEDO, because the calculation is made only by the integral transport method which needs much computer time and core capacity especially for multi-group calculation.

APPENDIX VI Representation of collision source term in the Boltzmann equation in terms of multigroup constants.

The collision source terms S in the Boltzmann equation is generally written as

$$S = \int_0^{\infty} dE' \int \frac{d\Omega'}{4\pi} \Sigma(E' \rightarrow E, \Omega' \rightarrow \Omega) \phi(E', \Omega') \quad (1)$$

where $\Sigma(E' \rightarrow E, \Omega' \rightarrow \Omega)$ is the macroscopic differential scattering cross section. Under the rotation invariance condition, it can be represented as

$$\Sigma(E' \rightarrow E, \Omega' \rightarrow \Omega) = \Sigma(E' \rightarrow E, \mu) / 2\pi \quad (2)$$

with

$$\mu \equiv \Omega' \cdot \Omega$$

$$\Sigma(E' \rightarrow E, \mu) = \sum_i \Sigma_i(E' \rightarrow E, \mu) \quad (3)$$

where i denotes an individual constituent nuclide of the medium. The emergent energy E of neutrons scattered at incident energy E' , however, is not independent of but uniquely determined by E' , viz.,

$$E = E_0 \equiv f(\mu)$$

or

$$\mu = \mu_0 \equiv g(E) \quad (4)$$

It is therefore quite natural that the differential scattering cross section is measured as E -dependent $\sigma^i(E', E)$ or μ -dependent $\sigma^i(E', \mu)$. Consequently, it follows that the microscopic cross section must be derived from $\sigma^i(E', E)$ or $\sigma^i(E', \mu)$ for source calculation. This can be done as follows. It is easily found that the next relation holds for an independent variable μ :

$$\sigma^i(E' \rightarrow E, \mu) = \sigma^i(E', \mu) \delta(\mu - \mu_0) \cdot \frac{\partial \mu_0}{\partial E} \quad (5)$$

from which $\Sigma(E' \rightarrow E, \Omega' \rightarrow \Omega)$ is derived by use of the measurable data $\sigma^i(E', \mu)$; δ is the Dirac's delta function.

For practical convenience, S is generally represented by a series of

Legendre moments about angular variables by the following procedure. Cross section $\Sigma(E' \rightarrow E, \Omega' \rightarrow \Omega)$ and angular flux $\phi(E', \Omega')$ are expanded by Legendre function of angular variables as

$$\begin{aligned}\Sigma(E' \rightarrow E, \Omega' \rightarrow \Omega) &\equiv \Sigma(E' \rightarrow E, \mu)/2\pi \\ &= \sum_{n=0}^{\ell} \frac{2n+1}{4} P_n(\mu) \Sigma_n(E' \rightarrow E)\end{aligned}\quad (6)$$

$$\phi(E', \Omega') = \sum_{\ell=0}^{\infty} \sum_{k=-\ell}^{\ell} \phi_{\ell}^k(E') Y_{\ell}^k(\Omega') \quad (7)$$

where

$$P_n(\mu) = \sum_{m=-n}^n \frac{(n-m)!}{(n+m)!} P_n^m(\lambda) P_n^m(\lambda') e^{im(\psi-\psi')} \quad (8)$$

$$Y_{\ell}^k(\Omega') = H_{\ell}^k P_{\ell}^k(\lambda') e^{ik\psi'} \quad (9)$$

$$H_{\ell}^k = \left[\frac{(2\ell+1)(\ell-k)!}{4\pi(\ell+k)!} \right]^{1/2} \quad |k| \leq \ell \quad (10)$$

$$P_n^m(\lambda) = \sin^m \theta \frac{d^m}{d\mu^m} P_n(\lambda) \quad (11)$$

$$P_n^{-m}(\lambda) = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m(\lambda) \quad m = 0 \sim n$$

$$\lambda \equiv \cos \theta \quad (12)$$

$$\lambda' \equiv \cos \theta'$$

The integrand of relation (1) is then represented as

$$\Sigma(E' \rightarrow E, \Omega' \rightarrow \Omega)(E', \Omega') = \sum_{n=0}^{\infty} \sum_{\ell=0}^{\infty} S(n, \ell) \quad (13)$$

where

$$\begin{aligned}S(n, \ell) &= \sum_{k=-\ell}^{\ell} \sum_{m=-n}^n \frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!} H_{\ell}^k P_n^m(\lambda) P_n^m(\lambda') \\ &\quad \times P_{\ell}^k(\lambda') e^{im\psi + i(k-m)\psi'} \cdot \Sigma_n(E' \rightarrow E) \phi_{\ell}^k(E')\end{aligned}\quad (14)$$

Integration of $S(n, \ell)$ over Ω' with aid of the next relation

$$\int_{4\pi} \tilde{Y}_{\ell}^k(\Omega) Y_n^m(\Omega) d\Omega = \delta_m^k \cdot \delta_n^{\ell} \quad (15)$$

yields

$$\begin{aligned} \int_{4\pi} d\Omega' S(n, \ell) &= \frac{2n+1}{4\pi} \delta_n^{\ell} \sum_{k=-\ell}^{\ell} \sum_{m=-n}^n \delta_m^k \frac{(n-m)!}{(n+m)!} \\ &\times P_n^m(\lambda) e^{im\psi} \Sigma_n(E' \rightarrow E) \phi^k(E') \end{aligned} \quad (16)$$

Therefore it is evident that only the term $S(n, n)$, ($n=0, 1, \dots$) contributes to the scattering source, and the integral of $S(n, n)$ is rewritten simply as

$$\begin{aligned} \int_{4\pi} d\Omega' S(n, n) &= \frac{2n+1}{4\pi} \sum_{m=-n}^n \frac{(n-m)!}{(n+m)!} \cdot \frac{1}{H_n^m} P_n^m(\lambda) e^{im\psi} \\ &\times \Sigma_n(E' \rightarrow E) \phi_n^m(E') \end{aligned} \quad (17)$$

Here, $\phi_n^m(E')$ is given by relation (7) as

$$\phi_n^m(E') = H_n^m \int_{-1}^1 d\lambda' \int_0^{2\pi} d\psi' \phi(E', \Omega') P_n^m(\lambda') e^{-im\psi'} \quad (18)$$

Finally the scattering source in expanded form is represented as

$$\begin{aligned} S &= \frac{1}{4\pi} \sum_{m=0}^{\infty} \sum_{n=-\infty}^{\infty} \frac{2n+1}{H_n^m} \cdot \frac{(n-m)!}{(n+m)!} P_n^m(\lambda) e^{im\psi} \\ &\times \int_0^{\infty} dE' \Sigma_n(E' \rightarrow E) \phi_n^m(E') \end{aligned} \quad (19)$$

If we take only the first and the second terms neglecting all other higher terms, P_1 -approximation of the collision source is obtained from relation (19) as

$$\begin{aligned} S &= \frac{1}{2\sqrt{\pi}} \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \phi_0^0(E') \\ &+ \frac{3}{2\sqrt{\pi}} \int_0^{\infty} dE' \{ \lambda \phi_1^0(E') + \sqrt{\frac{1-\lambda^2}{2}} [e^{i\psi} \phi_1^1(E') - e^{-i\psi} \phi_1^{-1}(E')] \} \\ &\times \Sigma_1(E' \rightarrow E) \end{aligned} \quad (20)$$

Here, the moments $\phi_0^0(E')$, $\phi_1^0(E')$, $\phi_1^1(E')$ and $\phi_1^{-1}(E')$ are given from the relation (18) by some manipulations as

$$\phi_0^0(E') = \frac{1}{2\sqrt{\pi}} \int_{4\pi} d\Omega' \phi(E', \Omega') \quad (21)$$

$$\begin{aligned} \lambda \phi_1^0(E') &= \frac{1-\lambda^2}{2} [e^{i\psi} \phi_1^0(E') - e^{-i\psi} \phi_1^{-1}(E')] \\ &= \frac{1}{2} \frac{3}{\pi} \int_{\pi} d\Omega' \phi(E', \Omega') \cdot (\Omega \cdot \Omega') \end{aligned} \quad (22)$$

Finally, substituting relations (21) and (22) into (20) yields the next expression

$$\begin{aligned} S &= \int_0^\infty dE' \Sigma_0(E' \rightarrow E) \bar{\phi}(E') \\ &\quad + 3 \int_0^\infty dE' \Sigma_0(E' \rightarrow E) \Omega \cdot \mathbb{J}(E') \end{aligned} \quad (23)$$

with the definitions

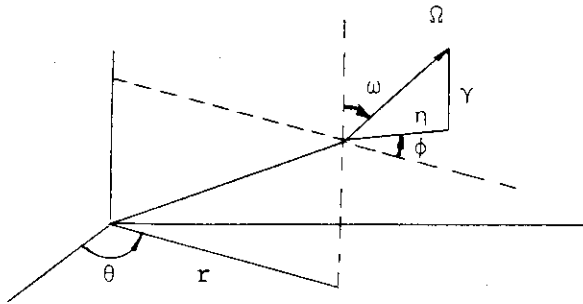
$$\bar{\phi}(E') \equiv \int_{4\pi} d\Omega' \phi(E', \Omega') / 4\pi \quad (24)$$

$$\mathbb{J}(E') \equiv \int_{4\pi} d\Omega' \Omega \phi(E', \Omega') / 4\pi \quad (25)$$

APPENDIX VII Transverse buckling correction and time absorption
in one-dimensional cylindrical transport equation.

The Boltzmann equation in the cylindrical coordinate system shown in the figure below is represented as

$$\left[\frac{1}{v} \frac{\partial}{\partial t} + \frac{\mu}{r} \frac{\partial}{\partial r} r + \frac{\eta \sin \phi}{r} \frac{\partial}{\partial \theta} + \gamma \frac{\partial}{\partial z} - \frac{1}{r} \frac{\partial}{\partial \phi} \eta \sin \phi + \sigma_t \right] N = S \quad (1)$$



$$\begin{aligned} \gamma &\equiv \cos \omega \\ \eta &\equiv \sin \omega \\ \mu &= \sin \omega \cos \phi \end{aligned}$$

If the angular flux N is independent of θ , the equation (1) is reduced into the next form.

$$\left[\frac{1}{v} \frac{\partial}{\partial t} + \frac{\mu}{r} \frac{\partial}{\partial r} r + \gamma \frac{\partial}{\partial z} - \frac{1}{r} \frac{\partial}{\partial \phi} \eta \sin \phi + \sigma_t \right] N = S \quad (2)$$

Let the flux N be approximated by the first and the second moments of solid angle as

$$N = \bar{N} + 3\Omega \cdot \mathbf{J} \quad (3)$$

with

$$\bar{N} = \int_{4\pi} N d\Omega / 4\pi, \quad \mathbf{J} = \int_{4\pi} N \Omega d\Omega / 4\pi \quad (4)$$

and substitute relation (3) into equation (2), one obtains the next form;

$$\begin{aligned} & \left(\frac{1}{v} \frac{\partial}{\partial t} + \mu \frac{\partial}{\partial r} + \gamma \frac{\partial}{\partial z} + \sigma_t \right) \bar{N} \\ & + 3 \left(\frac{\mu}{v} + \mu^2 \frac{\partial}{\partial r} + \mu \gamma \frac{\partial}{\partial z} + \mu \sigma_t \right) J_r \\ & + 3 \left(\frac{\gamma}{v} \frac{\partial}{\partial t} + \mu \gamma \frac{\partial}{\partial r} + \gamma^2 \frac{\partial}{\partial z} + \gamma \sigma_t \right) J_z = S \end{aligned} \quad (5)$$

where, J_r or J_z is r or z -component respectively.

Upon integrating both hand side of equation (5) over Ω and dividing through by 4π , the next equation is obtained.

$$\left(\frac{1}{v} \frac{\partial}{\partial t} + \sigma_t\right) \bar{N} + \frac{\partial J_r}{\partial r} + \frac{\partial J_z}{\partial z} = S_0 \quad (6)$$

with

$$S_0 = \int \frac{S d\Omega}{4\pi}$$

Two other equations are obtained by Ω -integration of equation (2) multiplied by μ or γ :

$$\frac{1}{3} \frac{\partial \bar{N}}{\partial r} + \frac{1}{v} \frac{\partial J_r}{\partial t} + \sigma_t J_r = S_\mu \quad (7)$$

$$\frac{1}{3} \frac{\partial \bar{N}}{\partial r} + \frac{1}{v} \frac{\partial J_z}{\partial t} + \sigma_t J_z = S_\gamma \quad (8)$$

where

$$S_\mu = \int \frac{S \mu d\Omega}{4\pi}$$

$$S_\gamma = \int \frac{S \gamma d\Omega}{4\pi}$$

Hence if the source is isotropic ($S_\mu = S_\gamma = 0$), J_r and J_z may be given by (7) and (8) as

$$J_r = -\frac{1}{3D_t} \cdot \frac{\partial \bar{N}}{\partial r} \quad (9)$$

$$J_z = -\frac{1}{3D_t} \cdot \frac{\partial \bar{N}}{\partial r} \quad (10)$$

Substitution of these relations into equation (6) yields the next equation

$$\left(D_t - \frac{1}{3D_t} \frac{\partial^2}{\partial z^2}\right) \bar{N} - \frac{1}{3D_t} \frac{\partial^2 \bar{N}}{\partial r^2} = S_0 \quad (11)$$

Thus, by substitution of the next assumptions

$$\bar{N} = \bar{N}(r) \exp(\alpha t) \cos(\pi z/2\ell) \quad (12)$$

$$S_0 = S_0(r) \exp(\alpha t) \cos(\pi z/2\ell) \quad (13)$$

- $\ell \leq z \leq \ell$ -

into equation (11), one obtains the next equation

$$[D_t + \frac{1}{3D} (\frac{\pi}{2\ell})^2] \bar{N}(r) - \frac{1}{3D_t} \cdot \frac{d^2 \bar{N}(r)}{dr^2} = S_0(r) \quad (14)$$

with

$$D_t \equiv \sigma_t + \alpha/v \quad (15)$$

This result means that the transverse buckling effects and time-dependency in γ -dependent cylindrical problem can be disposed at a time by replacing the total cross section σ_t by σ_t' given by

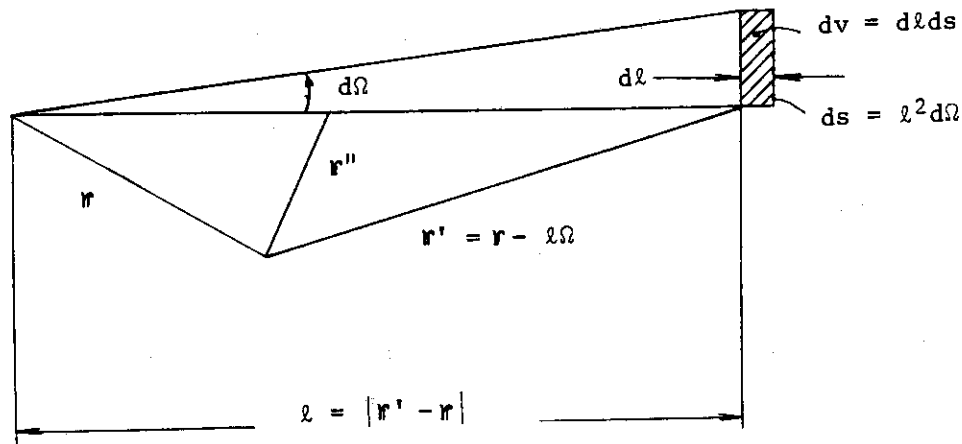
$$\sigma_t' = \sigma_t [1 + \frac{\alpha}{v\sigma_t} + \frac{1}{3} \frac{1}{1 + \alpha/v\sigma_t} (\frac{\pi}{2\ell\sigma_t})^2] \quad (16)$$

where

- α : Time constant of flux change
- ℓ : Effective buckling height of the cylinder
- v : Neutron velocity

APPENDIX VIII Derivation of integral transport equation and first flight collision probability

Consider the Boltzmann equation at a phase space point $P(\mathbf{r}-\Omega\ell, t-\ell/v)$ for ℓ taken as the distance between two spacial points indicated by position vector \mathbf{r} and \mathbf{r}' as shown in the next figure.



The expression⁽⁸⁾ is then given by replacing the coordinates \mathbf{r} by $\mathbf{r}-\Omega\ell$ and t by $t-\ell/v$:

$$\begin{aligned} & \left(\frac{1}{v} \frac{\partial}{\partial t} + \Omega \cdot \nabla + \Sigma_t(\mathbf{r}-\Omega\ell, E) \right) f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v) \\ &= S(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v) \\ &+ \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma(\mathbf{r}-\Omega'\ell, E' \rightarrow E, \Omega' \rightarrow \Omega) f(\mathbf{r}-\Omega\ell, E', \Omega', t-\ell/v) \quad (1) \end{aligned}$$

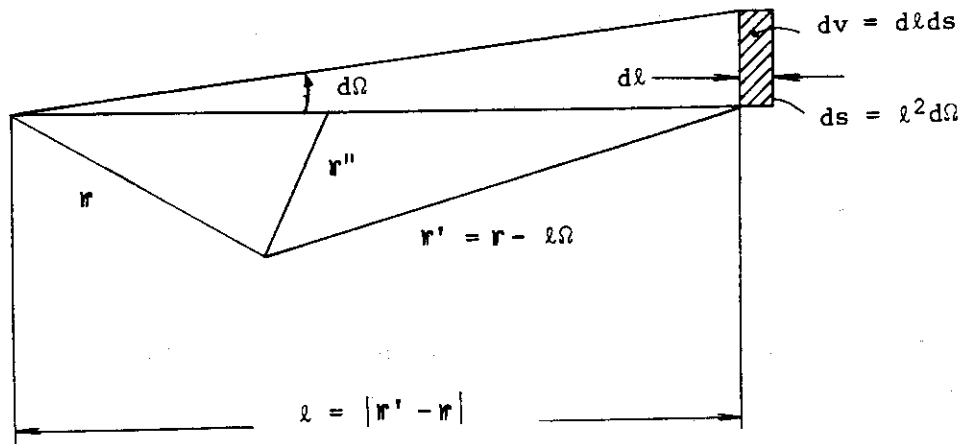
The two derivatives on the left-hand side of eq. (1) are rewritten as,

$$\begin{aligned} & \frac{1}{v} \frac{\partial}{\partial t} f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v) \\ &= \lim_{\Delta\ell \rightarrow 0} \frac{f(\mathbf{r}-\Omega\ell, E, \Omega, t-(\ell+\Delta\ell)/v) - f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v)}{\Delta\ell} \\ & \Omega \cdot \nabla f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v) \\ &= \lim_{\Delta\ell \rightarrow 0} \frac{f(\mathbf{r}-\Omega(\ell+\Delta\ell), E, \Omega, t-\ell/v) - f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v)}{\Delta\ell} \end{aligned}$$

It is evident, therefore, that the sum of these two derivatives is equal

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The expression⁽⁸⁾ is then given by replacing the coordinates \mathbf{r} by $\mathbf{r}-\Omega\ell$ and t by $t-\ell/v$:

$$\begin{aligned} & \left(\frac{1}{v} \frac{\partial}{\partial t} + \Omega \cdot \nabla + \Sigma_t(\mathbf{r}-\Omega\ell, E) \right) f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v) \\ &= S(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v) \\ &+ \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma(\mathbf{r}-\Omega'\ell, E' \rightarrow E, \Omega' \rightarrow \Omega) f(\mathbf{r}-\Omega\ell, E', \Omega', t-\ell/v) \quad (1) \end{aligned}$$

The two derivatives on the left-hand side of eq. (1) are rewritten as,

$$\begin{aligned} & \frac{1}{v} \frac{\partial}{\partial t} f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v) \\ &= \lim_{\Delta\ell \rightarrow 0} \frac{f(\mathbf{r}-\Omega\ell, E, \Omega, t-(\ell+\Delta\ell)/v) - f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v)}{\Delta\ell} \\ & \Omega \cdot \nabla f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v) \\ &= \lim_{\Delta\ell \rightarrow 0} \frac{f(\mathbf{r}-\Omega(\ell+\Delta\ell), E, \Omega, t-\ell/v) - f(\mathbf{r}-\Omega\ell, E, \Omega, t-\ell/v)}{\Delta\ell} \end{aligned}$$

It is evident, therefore, that the sum of these two derivatives is equal

to the total derivative of $f(\mathbf{r}-\mathbf{R}\ell, E, \Omega, t-\ell/v)$ as to ℓ , viz.;

$$\begin{aligned} & \left(\frac{1}{v} \frac{\partial}{\partial t} + \mathbf{R} \cdot \nabla \right) f(\mathbf{r}-\mathbf{R}\ell, E, \Omega, t-\ell/v) \\ & \equiv - \frac{d}{d\ell} f(\mathbf{r}-\mathbf{R}\ell, E, \Omega, t-\ell/v) \end{aligned} \quad (2)$$

Equation (1) is thus rewritten as follows by some manipulations:

$$\begin{aligned} & - \frac{d}{d\ell} \left\{ e^{-\int_0^\ell \Sigma_t(\mathbf{r}-\mathbf{R}\ell', E) d\ell'} \cdot f(\mathbf{r}-\mathbf{R}\ell, E, \Omega, t-\ell/v) \right\} \\ & = e^{-\int_0^\ell \Sigma_t(\mathbf{r}-\mathbf{R}\ell', E) d\ell'} \cdot q(\mathbf{r}-\mathbf{R}\ell, E, \Omega, t-\ell/v) \end{aligned} \quad (3)$$

with q representing the total source. Integration of eq. (3) on both sides over ℓ from zero to infinity under the natural condition

$$e^{-\int_0^\infty \Sigma_t(\mathbf{r}-\mathbf{R}\ell', E) d\ell'} \cdot f(-\infty, E, \Omega, -\infty) = 0$$

yields the formal integral:

$$f(\mathbf{r}, E, \Omega, t) = \int_0^\infty e^{-\int_0^\ell \Sigma_t(\mathbf{r}-\mathbf{R}\ell', E) d\ell'} q(\mathbf{r}-\mathbf{R}\ell, E, \Omega, t-\ell/v) d\ell \quad (4)$$

where

$$\begin{aligned} q(\mathbf{r}-\mathbf{R}\ell, E, \Omega, t-\ell/v) & \equiv S(\mathbf{r}-\mathbf{R}\ell, E, \Omega, t-\ell/v) \\ & + \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma(\mathbf{r}-\mathbf{R}\ell, E' \rightarrow E, \Omega' \rightarrow \Omega) \phi(\mathbf{r}-\mathbf{R}\ell, E', \Omega', t-\ell/v) \end{aligned} \quad (5)$$

Integration on both sides of eq. (4) over Ω with aid of the relation

$$d\ell d\Omega = dV(\mathbf{r}') / |\mathbf{r}' - \mathbf{r}|^2 \quad (6)$$

gives

$$\begin{aligned} \phi(\mathbf{r}, E, t) & = \frac{1}{4\pi} \int_V dV(\mathbf{r}') \frac{1}{|\mathbf{r}' - \mathbf{r}|} \text{Exp} \left[- \int_{\mathbf{r}}^{\mathbf{r}'} \Sigma_t(\mathbf{r}'', E) dV'' \right] \\ & \times [S(\mathbf{r}', E, \Omega, t-|\mathbf{r}-\mathbf{r}'|/v) + \int_{4\pi} d\Omega' \int_0^\infty dE' f(\mathbf{r}', E', \Omega', t-|\mathbf{r}-\mathbf{r}'|/v) \\ & \times \Sigma(\mathbf{r}', E' \rightarrow E, \Omega' \rightarrow \Omega)] \end{aligned} \quad (7)$$

Here,

$$\phi(r, E, t) \equiv \int_{\pi} d\Omega f(r, E, \Omega, t) / 4\pi \quad (8)$$

$$\Omega \equiv (r - r') / |r - r'| \quad (9)$$

For practical purposes, description will be limited to only quasistatic form thereafter.

The static form of eq. (7) becomes as

$$\begin{aligned} \phi(r, E) &= \frac{1}{4\pi} \int_V dV(r') \frac{1}{|r' - r|^2} \text{Exp} \left[- \int_r^{r'} \Sigma_t(r'', E) dr'' \right] \\ &\times [S(r', E, \Omega) + \int_{4\pi} d\Omega' \int_0^\infty dE' f(r', E', \Omega') \Sigma(r', E' \rightarrow E, \Omega' \rightarrow \Omega)] \end{aligned} \quad (10)$$

If a synthetic kernel such as

$$\Sigma(r', E' \rightarrow E, \Omega) \equiv \frac{\int_{4\pi} f(r', E', \Omega') \Sigma(r', E' \rightarrow E, \Omega' \rightarrow \Omega) d\Omega'}{\int_{4\pi} d\Omega' f(r', E', \Omega')} \quad (11)$$

is given, eq. (10) is rewritten as

$$\begin{aligned} \phi(r, E) &= \int_V dV(r') \frac{1}{|r' - r|} \text{Exp} \left[- \int_r^{r'} \Sigma_t(r'', E) dr'' \right] \\ &\times \left[\frac{1}{4} S(r', E, \Omega) + \int_0^\infty dE' \phi(r', E') \Sigma(r', E' \rightarrow E, \Omega) \right] \end{aligned} \quad (12)$$

by which $\phi(r, E)$ is determined.

Equation (12) is generally solved using a kernel, such as transmission probability or first flight collision probability. The code COLSQ, for example, uses the first flight collision probability P_{ij} which is defined as below. The definition of a probability $P(E, r' \rightarrow r)$ such as

$$P(E, r' \rightarrow r) \equiv \frac{\Sigma_t(r, E)}{|r' - r|^2} \text{Exp} \left[- \int_r^{r'} \Sigma_t(r'', E) dr'' \right] \quad (13)$$

and substitution of this into eq. (12) yields the next equation.

$$\begin{aligned} \Sigma_t(r, E) \phi(r, E) &= \int_V dV(r') P(E, r' \rightarrow r) \\ &\times \left[\frac{1}{4} S(r', E, \Omega) + \int_0^\infty dE' \phi(r', E') \Sigma(r', E' \rightarrow E, \Omega) \right] \end{aligned} \quad (14)$$

The practical form is obtained by integrating this equation over a subregion and replacing the integral on the right-hand side by a summation of the integrals over each subregion V_i , where $V_i (i=1 \sim N)$ is a set of subdivision of V appropriately taken under the condition:

$$\bigcup_{i=1}^N V_i = V, \quad V_i \cap V_j = \emptyset \quad \text{for } i \neq j \quad (15)$$

All the cross sections are spacially constant in each of V_i . As is well known, the mean value theorem of integral guarantees acceptability of the next expressions as to V_j -integral of (14)

$$\int_{V_j} \Sigma_t(\mathbf{r}, E) \phi(\mathbf{r}, E) dV(\mathbf{r}) = V_j \cdot \Sigma_{tj}(E) \cdot \phi_j(E) \quad (16)$$

$$\begin{aligned} & \int_{V_j} dV(\mathbf{r}) \int_V dV(\mathbf{r}') P(E, \mathbf{r}' \rightarrow \mathbf{r}) \left[\frac{1}{4\pi} S(\mathbf{r}', E, \Omega) + \int_0^\infty dE' \phi(\mathbf{r}', E') \Sigma(\mathbf{r}', E' \rightarrow E, \Omega) \right] \\ &= \sum_{i=1}^N V_i [P_{ij}^S(E) \cdot S_i(E) + P_{ij}^\phi(E) \int_0^\infty dE' \phi_i(E') \Sigma_i(E' \rightarrow E)] \quad (17) \end{aligned}$$

Here

$$\phi_i(E) \equiv \frac{1}{V_i} \int_{V_i} \phi(\mathbf{r}', E) dV(\mathbf{r}') \quad (18)$$

$$S_i(E) \equiv \frac{1}{4\pi V_i} \int_{V_i} S(\mathbf{r}', E, \Omega) dV(\mathbf{r}') \quad (19)$$

$$P_{ij}^S(E) \equiv \int_{V_i} dV(\mathbf{r}) \frac{\int_{V_j} dV(\mathbf{r}') P(E, \mathbf{r}' \rightarrow \mathbf{r}) S(\mathbf{r}', E, \Omega)}{\int_{V_i} dV(\mathbf{r}') S(\mathbf{r}', E, \Omega)} \quad (20)$$

$$P_{ij}^\phi(E) \equiv \int_{V_i} dV(\mathbf{r}) \frac{\int_{V_j} dV(\mathbf{r}') P(E, \mathbf{r}' \rightarrow \mathbf{r}) \int_0^\infty dE' \phi(\mathbf{r}', E') \Sigma(\mathbf{r}', E' \rightarrow E, \Omega)}{\int_{V_i} dV(\mathbf{r}') \int_0^\infty dE' \phi(\mathbf{r}', E') \Sigma(\mathbf{r}', E' \rightarrow E, \Omega)} \quad (21)$$

$$\Sigma_i(E' \rightarrow E) \equiv \frac{\int_{V_i} \phi(\mathbf{r}', E) \Sigma(\mathbf{r}', E' \rightarrow E, \Omega) dV(\mathbf{r}')}{\int_{V_i} \phi(\mathbf{r}', E') dV(\mathbf{r}')} \quad (22)$$

Note that the volume element $dV(\mathbf{r}')$ is given by $d\ell$ and $d\Omega$ as the relation (6) and the position vector \mathbf{r}' is given by ℓ and Ω as

$$\mathbf{r}' = \mathbf{r} - \mathbf{l} \cdot \Omega \quad (23)$$

It is seen, therefore, that the $V(\mathbf{r}')$ integral of any quantity $X(\mathbf{r}', \Omega)$,

$$\int_V X(\mathbf{r}', \Omega) dV(\mathbf{r}')$$

is a constant independent of both \mathbf{r}' and Ω . By applying the principle to the right-hand sides of eq. (18), (22), it is obvious the expressions on the left hand sides are quite reasonable.

Thus, a practical form of the integral transport equation may be given by equating the right hand sides of (16) and (17) as

$$\begin{aligned} & V_j \cdot \Sigma_{tj}(E) \cdot \phi_j(E) \\ &= \sum_{i=1} V_i [P_{ij}^S(E) \cdot S_i(E) + P_{ij}^\phi(E) \int_0^\infty dE' \phi_i(E') \Sigma_i(E' \rightarrow E)] \quad (24) \end{aligned}$$

It is easily seen that $P_{ij}^S(E)$ and $P_{ij}^\phi(E)$ must be given to solve eq. (24) as to $\phi_i(E)$. Strictly $P_{ij}^S(E)$ depends on spacial distribution of S and $P_{ij}^\phi(E)$ on that of ϕ , but if the subregion V_i is suitably chosen so that the spacial distribution of S and ϕ in V_i can be regarded as acceptably flat, the next relation holds:

$$P_{ij}^S(E) = P_{ij}^\phi(E) = P_{ij}(E) \equiv \frac{1}{V_i} \int_{V_i} dV(\mathbf{r}) \int_{V_i} dV(\mathbf{r}') P(E, \mathbf{r}' \rightarrow \mathbf{r}) \quad (25)$$

With aid of the relation (13), the relation (25) gives $P_{ij}(E)$ independently of both S and ϕ . The relation (25) is the so-called flat flux approximation. Concerning this approximation, the important conclusion is as follows. If the relation (25) holds strictly, the total flux (the isotropic component of angular flux) can be obtained in rigorous sense by eq. (24). Physical meaning of this conclusion is clear from the definitions (20), (21), and (25). It is also seen that a symmetry condition exists between $P_{ij}(E)$ and $P_{ji}(E)$:

$$V_j \Sigma_{tj} \cdot P_{ji} = V_i \Sigma_{ti} P_{ij} \quad (26)$$

APPENDIX IX Details of the reactor constant formulae

Here, derivation of the standard value formulae will be described.

A static form of the Boltzmann equation is written as

$$\text{div}[\Omega \cdot \phi(r, u, \Omega)] + \Sigma_t(r, u) \phi(r, u, \Omega) = S \quad (1)$$

with

$$S \equiv Q(r, u, \Omega) + \frac{\chi(u)}{4\pi} \int_{4\pi} d\Omega' \int_0^\infty du' v \Sigma_f(r, u') \phi(r, u', \Omega') \\ + \int_{4\pi} d\Omega' \int_0^\infty du' \Sigma_s(r, u' \rightarrow u, \Omega' \rightarrow \Omega) \phi(r, u', \Omega') \quad (2)$$

where

- Σ_t : macroscopic total cross section
- $v \Sigma_f$: macroscopic fission cross section multiplied by v value
- Σ_s : differential scattering cross section
- ϕ : angular flux
- Q : fixed source
- χ : fission spectrum
- r : space variable
- u' : incident neutron lethargy
- u : emergent neutron lethargy
- Ω' : incident neutron direction vector
- Ω : emergent neutron direction vector

If the neutron source Q is isotropic and the angular flux is approximated as

$$\phi(r, u, \Omega) = \bar{\phi}(r, u) + 3\Omega \cdot J(r, u) \quad (3)$$

with

$$\bar{\phi}(r, u) \equiv \int_{4\pi} \phi(r, u, \Omega) d\Omega / 4\pi \quad (4)$$

$$J(r, u) \equiv \int_{\pi} \phi(r, u, \Omega) \Omega d\Omega / 4\pi$$

substitution of relation (3) into eq. (1) and integration of both hand sides of the resultant equation E over Ω yields the next equation

$$\begin{aligned}
& \text{div } \mathbf{J}(\mathbf{r}, u) + \Sigma_t(\mathbf{r}, u) \bar{\phi}(\mathbf{r}, u) \\
&= Q(\mathbf{r}, u) + \chi(u) \int_0^\infty v \Sigma_f(\mathbf{r}, u') \bar{\phi}(\mathbf{r}, u') du' \\
&\quad + \int_0^\infty f_0(u' \rightarrow u) \Sigma_s(\mathbf{r}', u') \bar{\phi}(\mathbf{r}, u') du' \quad (6)
\end{aligned}$$

Further, Ω -integration of E multiplied through by Ω yields $\frac{1}{3}$

$$\begin{aligned}
& \frac{1}{3} \text{grad } \bar{\phi}(\mathbf{r}, u) + \Sigma_t(\mathbf{r}, u) \bar{\phi}(\mathbf{r}, u) = \int_0^\infty f(u' \rightarrow u) \Sigma_s(\mathbf{r}', u') \bar{\mathbf{J}}(\mathbf{r}, u') du' \\
&= \int_0^\infty f(u' \rightarrow u) \Sigma_s(\mathbf{r}', u') \mathbf{J}(\mathbf{r}, u') du' \quad (7)
\end{aligned}$$

Here, f_0 , f_1 , $\Sigma_s(\mathbf{r}, u)$ are defined as

$$\begin{aligned}
\Sigma_s(\mathbf{r}, u' \rightarrow u, \Omega' \rightarrow \Omega) &\equiv f(u' \rightarrow u, \mu) \cdot \Sigma_s(\mathbf{r}, u') \\
f(u' \rightarrow u, \mu) &\equiv \sum_{n=0}^{\infty} \frac{2n+1}{2} f_0(u' \rightarrow u) P_n(\mu) \\
\mu &\equiv \Omega' \cdot \Omega
\end{aligned}$$

Eq. (7) can be converted into the next scalar (or divergent) form in any spacial region r , with all coefficients being piece-wise constant.

$$\begin{aligned}
& \frac{1}{3} \nabla^2 \bar{\phi}(\mathbf{r}, u) + \Sigma_t(u) \text{div } \mathbf{J}(\mathbf{r}, u) \\
&= \int_0^\infty f_1(u' \rightarrow u) \Sigma_s(u') \text{div } \mathbf{J}(\mathbf{r}, u') du' \quad (8)
\end{aligned}$$

In the region r , eqs. (6) and (8) can be represented in discrete form concerning lethargy variable as

$$\text{div } \mathbf{J}^g(\mathbf{r}) + \Sigma_t^g \phi^g(\mathbf{r}) = Q^g(\mathbf{r}) + \chi^g \sum_{g'} \Sigma_f^{g' \rightarrow g} \phi^{g'}(\mathbf{r}) + \sum_{g'} \Sigma_s^{g' \rightarrow g} \phi^{g'}(\mathbf{r}) \quad (9)$$

$$\frac{1}{3} \nabla^2 \phi^g(\mathbf{r}) + \Sigma_{tr}^g \text{div } \mathbf{J}^g(\mathbf{r}) = \sum_{g' \neq g} \Sigma_{s1}^{g' \rightarrow g} \text{div } \mathbf{J}^{g'}(\mathbf{r}) \quad (10)$$

Here,

$$\phi^g(\mathbf{r}) \equiv \int_g \bar{\phi}(\mathbf{r}, u) du \quad (11)$$

$$\mathbf{J}^g(\mathbf{r}) \equiv \int_g \mathbf{J}(\mathbf{r}, u) du \quad (12)$$

$$Q^g(r) \equiv \int_g Q(r, u) du \quad (13)$$

$$\chi^g \equiv \int_g \chi(u) du \quad (14)$$

$$\Sigma_t^g \equiv \int_g \Sigma_t(u) \bar{\phi}(r, u) du / \phi^g(r) \quad (15)$$

$$v \Sigma_f^g \equiv \int_g v \Sigma_f(u) \phi(r, u) du / \phi^g(r) \quad (16)$$

$$\Sigma_s^{g' \rightarrow g} \equiv \int_g du \int_{g'} du' f(u' \rightarrow u) \Sigma_s(u') \phi(r, u') / \phi^{g'}(r) \quad (17)$$

$$\Sigma_{sl}^{g' \rightarrow g} \equiv \int_g du \int_{g'} du' f_1(u' \rightarrow u) \Sigma_s(u') \text{div } J(r, u') / \text{div } J^{g'}(r) \quad (18)$$

$$\Sigma_{tr}^g \equiv \int_g \Sigma_t(u) \text{div } J(r, u) du / \text{div } J^g(r) - \Sigma_{sl}^{g' \rightarrow g} \quad (19)$$

By eliminating $J_g(r)$ from eqs. (9) and (10), the diffusion equation is derived:

$$-D^g \nabla^2 \phi^g(r) + \Sigma_{rem}^g \phi^g(r) = S^g + \Sigma_{se}^{g-1 \rightarrow g} \phi^{g-1}(r) \quad (20)$$

where

$$D^g \equiv D_0^g - \Sigma_\ell^g \cdot \frac{\phi^g}{\nabla^2 \phi^g(r)} \quad (21)$$

$$D_0^g \equiv 1/3 \Sigma_{tr}^g \quad (22)$$

$$\Sigma_{rem}^g \equiv \Sigma_a^g + \Sigma_{sr}^{g \rightarrow g+1} - \Sigma_n^g \quad (23)$$

$$\Sigma_s^g \equiv \Sigma_e^g + \Sigma_i^g + 2 \Sigma_n^g \equiv \text{SUM}_{g'} \Sigma_s^{g \rightarrow g'} \quad (24)$$

$$\Sigma_\ell^g \equiv \text{SUM}_{g' \neq g} \left\{ \text{SUM}_{g''} (\chi^{g'} v \Sigma_f^{g''} \frac{\Sigma_{sl}^{g' \rightarrow g}}{\Sigma_{tr}^g} + \Sigma_{sn}^{g'' \rightarrow g' \rightarrow g}) \frac{\phi^{g''}(r)}{\phi^g(r)} \right. \\ \left. + \Sigma_{tm}^{g' \rightarrow g} \cdot \frac{\phi^{g'}(r)}{\phi^g(r)} \right\} \quad (25)$$

$$\Sigma_{se}^{g \rightarrow g+1} \equiv R_d^g \cdot \Sigma_s^{g \rightarrow g+1} \quad (26)$$

$$\Sigma_{sr}^{g \rightarrow g+1} \equiv R_r^g \cdot \Sigma_s^{g \rightarrow g+1} \quad (27)$$

$$R_d^g \equiv 1 + \sum_{\substack{g' \neq g \\ g' \neq g+1}} \frac{\sum_s \frac{g' \rightarrow g+1}{s} \phi^{g'}(r)}{\sum_s \frac{g \rightarrow g+1}{s} \phi^g(r)} \quad (28)$$

$$R_r^g \equiv 1 + \sum_{\substack{g' \neq g \\ g' \neq g+1}} \frac{\sum_s \frac{g \rightarrow g'}{s}}{\sum_s \frac{g \rightarrow g+1}{s}} \quad (29)$$

$$\sum_{tm} \frac{g' \rightarrow g}{s} \equiv \sum_t \frac{g'}{t} \sum_{sl} \frac{g' \rightarrow g}{sl} / \sum_{tr} \frac{g}{tr} \quad (30)$$

$$\sum_{sm} \frac{g'' \rightarrow g' \rightarrow g}{s} \equiv \sum_s \frac{g'' \rightarrow g'}{s} \sum_{sl} \frac{g' \rightarrow g}{sl} \sum_f \frac{g'}{f} \phi^{g'}(r) \quad (31)$$

$$S^g \equiv Q^g + \chi^g \sum_{g'} \sum_f \frac{g'}{f} \phi^{g'}(r) \quad (32)$$

Eq. (21) is consistent with discrete form of the Boltzmann equation (1) within the restriction of allowance for the approximations (9) and (10). Therefore if the Boltzmann equation (1) is solved in a unit cell geometry under appropriate cell boundary conditions, the unit cell average value of the constants may be obtained by averaging the necessary quantities defined by the above relations.

Using these cell average constants, a macroscopic neutron balance condition over a large power reactor core may be described by the next diffusion equation

$$-D^g \nabla_L^2 \phi^g + \sum_{rem} \frac{g}{s} \phi^g = S^g + \sum_{se} \frac{g-1 \rightarrow g}{se} \phi^{g-1} \quad (33)$$

Here, the Laplacian operator ∇_L^2 is defined as a difference operator for horizontal mesh width equal to one rod pitch or more, with other coefficients defined as described in (2.8.1).

Some additional explanation must be given about the cross section \sum_l^g and diffusion constant D^g . Physical meaning of the quantity \sum_l^g is obvious from eqs. (9) and (10); that is, real leakage should be represented by $\text{div } J^g(r)$, whereas diffusion equation represents it in terms of $-D^g \nabla_L^2 \phi^g(r)$. Therefore, the correction between these two expressions is required such as

$$\text{div } J_g(r) = -D_0^g \nabla^2 \phi^g(r) + \sum_l \frac{g}{l} \phi^g(r) \equiv -D^g \nabla_L^2 \phi^g(r)$$

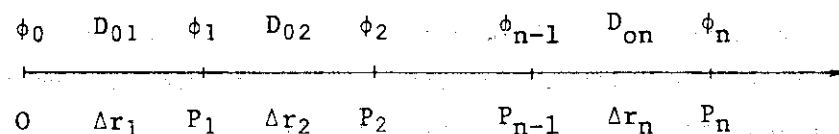
yielding the corrected diffusion constants

$$D^g = D_0^g - \Sigma_{\ell}^g \frac{\phi^g(r)}{\nabla^2 \phi^g(r)}$$

where Σ_{ℓ}^g is defined by the relation (25) and $\phi^g(r)/\nabla^2 \phi^g(r)$ is given by the unit cell calculation described above.

The diffusion constant is locally isotropic as are the cross sections, but the rod cell average value D^g is anisotropic because the material of a rod cell is not uniform radially; that is D^g may be a tensorial quantity. Practically, however, D^g may be regarded as composed of two components, viz., radial and axial for the ordinary light water reactor core structure.

These two components may be given by the following consideration. Let the radial distribution constant be as shown in the figure below.



The continuity condition at the mesh points $P_i (i=1 \sim n-1)$ of neutron current induced by total flux gradient may approximately be represented as

$$D_{01} \frac{\phi_1 - \phi_0}{\Delta r_1} = D_{02} \frac{\phi_2 - \phi_1}{\Delta r_2} = \dots = D_{on} \frac{\phi_n - \phi_{n-1}}{\Delta r_n}$$

Hence, if these be equated to the macroscopic neutron current cross over the half rod cell pitch, i.e., $\bar{D}_r \cdot (\phi_n - \phi_0)/R$, the formula for \bar{D}_r is obtained:

$$\bar{D}_r = \frac{R}{\Delta r_1/D_{01} + \Delta r_2/D_{02} + \dots + \Delta r_n/D_{on}}$$

which gives the isotropic terms of \tilde{D}_r . The materials of any rod cell are axially uniform, and the axial current in each material zone may be proportional to the flux density. It is thus reasonable that isotropic part \bar{D}_a of \tilde{D}_a is given as

$$\bar{D}_a = \frac{\sum_i D_{oi} \phi_i V_i}{\sum_i \phi_i V_i}$$

APPENDIX X Diffusion calculation based on multi-coordinate system

1. Basic concept

In general, any complete coordinate system can be used for expressing any spacial operator included in an equation. Then if the equation is such that describes balance condition on a physical quantity in unit volume at an arbitrary position, it is clear that:

- (1) The equation may be written in a convenient form by using the most suitable coordinate system in each of spacial subdomains which should be suitably chosen in the geometry considered.
- (2) The relative positions of the origins of the coordinate systems used may be arbitrary in the sense that the equation describes only a balance condition on a quantity at an arbitrary position. It is obvious that the continuity condition on each subdomain boundary is the necessary and sufficient condition assuring the conservativity of any multi-coordinate -system expression

Especially when the equation is written in difference form for the numerical solution, the treatment of this condition is important, since the convergence of the operator inversion may largely depend on assurance degree of the conservativity.

2. An example of the multi-coordinate-system expression

Here, an example of two-coordinate-system expression applied to a two-dimensional geometry is introduced. This is a typical problem encountered at the calculation of horizontal distribution of the neutron flux in a usual LWR core. For this problem, x-y system and r- θ system were used under the following calculation scheme.

- (1) Inversion⁽⁷⁾ of the spacial operator

The spacial operator is separated into some suboperators corresponding to the subdomains, then each sub-operator is inverted under the guess boundary conditions determined on sub-domain boundary by the method described afterwards or under the external boundary condition given.

- (2) Determination of the subdomain boundary condition

Let the domain of the geometry be V which is enclosed by the

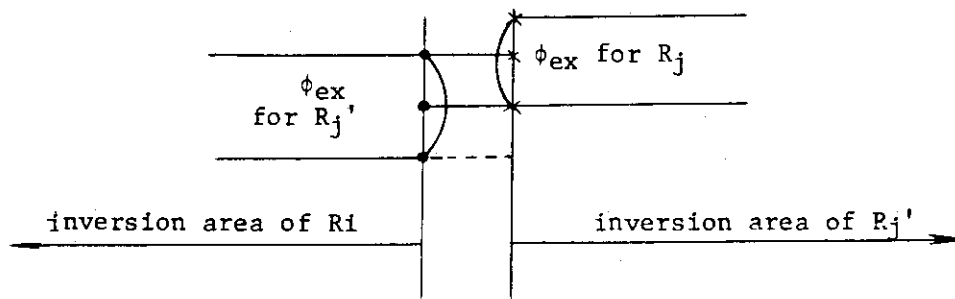
external boundaries $\Gamma_k (k=1 \sim K)$ and V be separated into subdomains $R_j (j=1 \sim J)$ with the numbering in ascending order from outer side, and R_j be enclosed by the boundaries $\Gamma_{ij} (i=1 \sim I_j)$

- (a) If $\Gamma_{ij} \in \{\Gamma_k\}$

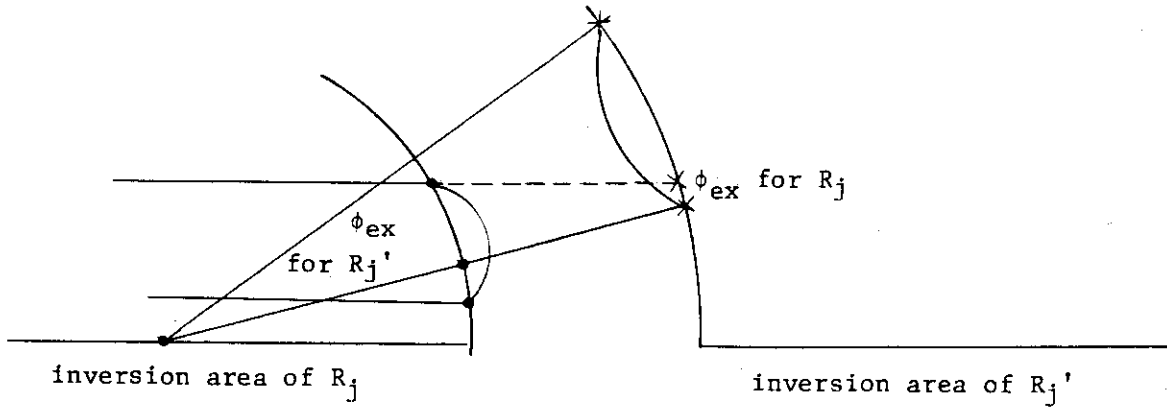
An extrapolated boundary value ϕ_{ex} is given for Γ_{ij} as

$$\phi_{ex} = (1 - \Delta n \cdot C_k) \phi$$

- (b) If two subdomains R_j and $R_{j'}$ ($j < j'$) are interconnected by Γ_{ij} , and the same coordinate system is used in R_j and $R_{j'}$, ϕ_{ex} for each of R_j and $R_{j'}$ is given by interpolation shown in the figure below



- (c) If the coordinate system used in R_j and $R_{j'}$ are different in case of (b), ϕ_{ex} is given by the manner illustrated below.



(3) Inversion scheme

Spatial inversion is performed every subregion by SOR scheme, etc., under the boundary value ϕ_{ex} determined as above.

APPENDIX XI Derivation of a macroscopic form of the thermo-hydraulic equation

Thermo-hydraulic balance conditions⁽¹¹⁾ in microscopic sense are described by equations (1.2), (1.3) and (1.4).

Here, a set of macroscopic thermo-hydraulic equations is derived from the rigorous microscopic equations above. A basic procedure used through is to integrate the microscopic equations over V the volume of sub-channel per unit length and smooth away microscopic dependency of every quantity on lateral coordinates for changing the equations into one-dimensional space dependent ones about a set of lateral average quantities for practical purposes. By the procedure described above, each equation may be changed into a macroscopic form as follows.

1. Mass balance equation

V -integral of the first term of equation (1.2) may be written as

$$\int_V \frac{\partial \rho}{\partial t} = S_z \cdot \frac{\partial \bar{\rho}}{\partial t} \quad (1)$$

while the leakage term may be represented as

$$\begin{aligned} \int_V \operatorname{div} \rho \mathbf{W} dV &= \int_{S_z} \frac{\rho \partial v_z}{\partial z} dS_z + \int_{S_y} \rho \bar{v}_y^t dS_y + \int_{S_x} \rho \bar{v}_x^t dS_x \\ &\equiv S_z \frac{\partial \overline{\rho v_z}}{\partial z} + W_y + W_x \end{aligned} \quad (2)$$

where

S_z : cross section of the subchannel flow area

$$\bar{\rho} = \frac{\int_{S_z} \rho dS_z}{S_z} \quad (3)$$

$$\overline{\rho v_z} = \frac{\int_{S_z} \rho v_z dS_z}{S_z} \quad (4)$$

\bar{v}^t : time average of diversion component of v

v' : turbulent component of v

W_x, W_y : x- and y-component of diversion cross flow rate

In terms of these notations, the integral form of the equation is written as

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho v_z}}{\partial z} + (W_x + W_y)/S_z = 0 \quad (5)$$

which may be specialized for a subchannel i with flow area A_i as

$$A_i \frac{\partial \rho_i}{\partial t} + \frac{\partial m_i}{\partial z} + \sum_j W_{ij} = 0 \quad (6)$$

where

$$m_i \equiv A_i \bar{\rho v_z}$$

$$\sum_j W_{ij} \equiv W_x + W_y$$

2. Momentum balance

The first term of eq. (1.3) may be integrated as

$$\begin{aligned} \int_V \frac{\partial \rho W}{\partial t} dt &= \frac{\partial}{\partial t} \int_V \rho W dV \\ &= S_z \left\{ \frac{\partial}{\partial t} (i \bar{\rho v_x} + j \bar{\rho v_y} + k \frac{\partial \rho v_z}{\partial t}) \right\} \end{aligned} \quad (7)$$

with

$$\begin{aligned} \bar{\rho v_x} &\equiv \int_{S_z} \rho v_x dS_z / S_z \\ \bar{\rho v_y} &\equiv \int_{S_z} \rho v_y dS_z / S_z \end{aligned} \quad (8)$$

The second term giving momentum loss rate by convection may be integrated as

$$\begin{aligned} \int_V [\nabla \cdot \rho W W] dV &= \int_S \rho W (W \cdot dS) \\ &= \int_{S_z} \frac{\partial \rho W v_z}{\partial z} + \int_{S_x} \rho W v_y dS_y + \int_{S_x} \rho W v_x dS_x \\ &= k \left\{ \int_{S_z} \frac{\partial \rho v_z^2}{\partial z} dS_z + \int_{S_y} \rho v_z v_y dS_y + \int_{S_x} \rho v_z v_x dS_x \right\} \\ &= j \left\{ \int_{S_z} \frac{\partial \rho v_y v_z}{\partial z} dS_z + \int_{S_y} \rho v_y^2 dS_y + \int_{S_x} \rho v_y v_x dS_x \right\} \\ &= i \left\{ \int_{S_z} \frac{\partial \rho v_x v_z}{\partial z} dS_z + \int_{S_y} \rho v_x v_y dS_y + \int_{S_x} \rho v_x^2 dS_x \right\} \end{aligned}$$

The third term becomes

$$\begin{aligned}
 \int_V \text{grad } P \, dV &= \int_V \left(i \frac{\partial P}{\partial x} + j \frac{\partial P}{\partial y} + k \frac{\partial P}{\partial z} \right) dV \\
 &= i \int_y \Delta_x P \, dy + j \int_x \Delta_y P \, dx + k \int_{S_z} \frac{\partial P}{\partial z} \, dS_z \\
 &= i \Delta_x P \cdot y + j \Delta_y P \cdot x + k S_z \cdot \frac{\partial \bar{P}}{\partial z}
 \end{aligned} \tag{10}$$

with

$$\overline{\Delta_x P} \equiv \int_{S_z} \Delta_x P \, dS_z / S_z \tag{11}$$

$$\overline{\Delta_y P} \equiv \int_{S_z} \Delta_y P \, dS_z / S_z \tag{12}$$

$$\bar{y} \equiv \int_y \Delta_x P \, dy / \overline{\Delta_x P} \tag{13}$$

$$\bar{x} \equiv \int_x \Delta_y P \, dx / \overline{\Delta_y P} \tag{14}$$

$$\bar{P} \equiv \int_{S_z} P \, dS_z / S_z \tag{15}$$

The fourth term representing momentum loss rate by viscous transfer becomes

$$\begin{aligned}
 \int_V [\nabla \cdot \tau] \, dV &= \int_S [\tau \cdot dS] \\
 &= k \left\{ \int_{S_z} \frac{\partial \tau_{zz}}{\partial z} \, dS_z + \int_{S_y} \tau_{yz} \, dS_y + \int_{S_x} \tau_{xz} \, dS_x \right\} \\
 &\quad + j \left\{ \int_{S_z} \frac{\partial \tau_{zy}}{\partial z} \, dS_z + \int_{S_y} \tau_{yy} \, dS_y + \int_{S_x} \tau_{xy} \, dS_x \right\} \\
 &\quad + i \left\{ \int_{S_z} \frac{\partial \tau_{zx}}{\partial z} \, dS_z + \int_{S_y} \tau_{yx} \, dS_y + \int_{S_x} \tau_{xx} \, dS_x \right\}
 \end{aligned} \tag{16}$$

The last term becomes

$$- \int_V \rho g \, dV = -(k \bar{\rho} g_z + j \bar{\rho} g_y + i \bar{\rho} g_x) S_z \tag{17}$$

Now, preparation is completed for the macroscopic treatment, hence the equation is treated as two scalar equations separately of axial and lateral components thereafter.

2.1) Axial component

It is easily seen from relations (7) ~ (17) that the V-integrated axial momentum balance is described as

$$\begin{aligned} S_z \frac{\partial \bar{p}}{\partial z} + \int_{S_z} \frac{\partial \rho v_z^2}{\partial z} dS_z + \int_{S_y} \rho v_z v_y dS_y + \int_{S_x} \rho v_z v_x dS_x \\ + S_z \frac{\partial \bar{p}}{\partial z} + \int_{S_z} \frac{\partial \tau_{zz}}{\partial z} dS_z + \int_{S_y} \tau_{yz} dS_y + \int_{S_x} \tau_{xz} dS_x - \bar{p} g_z S_z = 0 \end{aligned} \quad (18)$$

The second term of the left hand side may be represented as

$$\begin{aligned} \int_{S_z} \frac{\partial \rho v_z^2}{\partial z} dS_z &= \int_{S_z} (2v_z \frac{\partial \rho v_z}{\partial z} - v_z \frac{\partial \rho}{\partial z}) dS_z \\ &= S_z \{ 2\hat{v}_z \cdot \frac{\partial \rho v_z}{\partial z} - \bar{v}_z^2 \frac{\partial \rho}{\partial z} \} \end{aligned} \quad (19)$$

where

$$\hat{v}_z \equiv \int_{S_z} v_z \frac{\partial \rho v_z}{\partial z} dS_z / \int_{S_z} \frac{\partial \rho v_z}{\partial z} dS_z \quad (20)$$

$$\bar{v}_z^2 \equiv \int_{S_z} v_z^2 \frac{\partial \rho}{\partial z} dS_z / \int_{S_z} \frac{\partial \rho}{\partial z} dS_z \quad (21)$$

Using relation (5), the R.H.S. of (19) may be rewritten as

$$\int_{S_z} \frac{\partial \rho v_z^2}{\partial z} dS_z = -S_z \{ 2\hat{v}_z \frac{\partial \rho}{\partial t} + \bar{v}_z^2 \frac{\partial \rho}{\partial z} \} - 2\hat{v}_z W \quad (22)$$

The third and the fourth terms of equation (18) may be separated into two parts; diversion term and turbulent term. That is, substitution of the next expressions

$$\begin{aligned} v_x &= \bar{v}_x^t + v_x' \\ v_y &= \bar{v}_y^t + v_y' \end{aligned} \quad (23)$$

into the sum of the third and the fourth terms yields

$$\begin{aligned} \int_{S_y} \rho v_z v_y dS_y + \int_{S_x} \rho v_z v_x dS_x \\ = \hat{v}_z^x \int_{S_x} \rho \bar{v}_x^t dS_x + \hat{v}_z^y \int_{S_y} \rho \bar{v}_y^t dS_y \end{aligned} \quad (24)$$

$$\begin{aligned}
& + \overline{\rho v_z'} \cdot \widehat{\Delta x v_z} \cdot S_x + \overline{\rho v_y'} \cdot \Delta y v_z \cdot S_y \\
& = \widehat{v_z^x} W_x + \widehat{v_z^y} W_y + \widehat{\Delta x v_z} W_x' + \Delta y v_z W_y'
\end{aligned}$$

where

$\overline{v_x^t}, \overline{v_y^t}$: diversion component of v_x and v_y respectively

v_x', v_y' : Turbulent component of v_x and v_y respectively

$$\left. \begin{aligned}
\widehat{v_z^x} & \equiv \int_{S_x} \rho \overline{v_x^t} v_z dS_x / \int_{S_x} \rho \overline{v_x^t} dS_x \\
\widehat{v_z^y} & \equiv \int_{S_y} \rho \overline{v_y^t} v_z dS_y / \int_{S_y} \rho \overline{v_y^t} dS_y
\end{aligned} \right\} \quad (25)$$

$$\left. \begin{aligned}
\rho v_x' & \equiv \int_{S_x} \rho v_x' dS_x / S_x \\
\rho v_y' & \equiv \int_{S_y} \rho v_y' dS_y / S_y
\end{aligned} \right\} \quad (26)$$

$\widehat{\Delta x v_z}$: S_x - average of the difference between inside and outside values of speed v_z in the vicinity of S_x

$\Delta y v_z$: analogous to above concerning S_y in place of S_x

$$\left. \begin{aligned}
W_x & \equiv \int_{S_x} \rho \overline{v_x^t} dS_x \\
W_y & \equiv \int_{S_y} \rho \overline{v_y^t} dS_y
\end{aligned} \right\} \quad (27)$$

$$\left. \begin{aligned}
W_x' & \equiv \overline{\rho v_x'} \cdot S_x \\
W_y' & \equiv \overline{\rho v_y'} \cdot S_y
\end{aligned} \right\} \quad (28)$$

Substitution of relations (22) and (24) into equation (18) yields

$$\begin{aligned}
& \left\{ \frac{\partial \overline{\rho v_z}}{\partial t} - \widehat{2 v_z} \frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}}{\partial z} \right\} S_z = - \int_{S_x} \tau_{xz} dS_x \\
& - \int_{S_y} \tau_{yz} dS_y - \int_{S_z} \frac{\partial \rho_{zz}}{\partial z} dS_z + S_z \overline{v_z^2} \frac{\partial \overline{\rho}}{\partial z} \\
& + (2 \widehat{v_z} W - \widehat{v_z^x} W_x - \widehat{v_z^y} W_y)
\end{aligned}$$

$$- (\widehat{\Delta_x v_z W_x'} + \widehat{\Delta_y v_z W_y'}) + \rho g_z S_z \quad (29)$$

The first and the second terms in the R.H.S. of (29) are friction forces inflicted on V by channel wall areas S_x and S_y , while the third term is net viscous stress inflicted through S_z , either of them being directed toward z-axis. The fourth term is net incoming rate of z-directional momentum by density gradient through S_x .

The fifth term is net incoming rate of z-directional momentum through S_x and S_y by diversion cross flow, while the seventh term is that by turbulent cross flow. The first, the second and the third terms in the R.H.S. of (29) are to be approximated by a simple empirical correlation in total, because the dependency of τ_{xz} , τ_{yz} and τ_{zz} on velocity components, pressure and temperature, etc., may be horribly complicated. In general, the next correlation

$$\int_{S_x} \tau_{xz} dS_x + \int_{S_y} \tau_{yz} dS_y + \int_{S_z} \frac{\partial \tau_{zz}}{\partial z} dS_z = \overline{\rho v_z^2} \cdot C \cdot S_z \quad (30)$$

may be used, where the coefficient C is to be determined by a gross measurement at the given system.

It is to be noted that the various average velocities \hat{v}_x , $\sqrt{\overline{v_x^2}}$, \hat{v}_z^x , etc. contained in equation (29) should not be equated to the mass transfer velocity $\overline{\rho v_z / \rho} (= \bar{v}_z)$, because \bar{v}_z cannot always represent correct momentum transfer rate especially in case of two phase flow.

Therefore, it follows that an equivalent density for momentum transfer and the corresponding velocity are defined by the following consideration. Generally, momentum transfer rate M, mass velocity, i.e., momentum density m_0 and quality x are defined as

$$M = \alpha \rho_g v_g^2 + (1 - \alpha) \rho_e v_e^2 \quad (31)$$

$$m_0 = \alpha \rho_g v_g + (1 - \alpha) \rho_e v_e = m/A \quad (32)$$

$$x = \frac{\alpha \rho_g v_g}{\alpha \rho_g v_g + (1 - \alpha) \rho_e v_e} \quad (33)$$

where

- α : volume fraction of void
- ρ_g, ρ_e : gas and liquid density respectively
- v_g, v_e : gas and liquid velocity respectively
- A : subchannel flow area ($= S_z$)

Thus if M be equated to m_0^2/ρ' , a quantity ρ' is given with the aid of relation (31), (32) and (33) as

$$1/\rho' = \frac{x^2 (1-x)^2}{\alpha \rho_g \rho_e (1-\alpha)} \quad (34)$$

This is the equivalent density for momentum transfer giving the corresponding momentum transfer velocity u by equating m_0 to $\rho' u$ as

$$u = m_0/\rho' \equiv m_0 V' = m V'/A \quad (35)$$

where V' is the equivalent specific volume for momentum transfer. By the notices above, it may be obvious that the fourth term in the R.H.S. of eq. (29) should be represented by u and ρ' as

$$\begin{aligned} S_z \cdot \hat{v}_z^2 \cdot \frac{\partial \rho}{\partial z} &= A \cdot u^2 \cdot \frac{\partial \rho'}{\partial z} = A \cdot \left(\frac{m}{A}\right)^2 \cdot V'^2 \cdot \frac{\partial (1/V')}{\partial z} \\ &= -A \left(\frac{m}{A}\right)^2 \cdot \frac{\partial V'}{\partial z} \end{aligned} \quad (36)$$

Upon substituting the relations (30), (36) into equation (29) using u for \hat{v}_z , \hat{v}_z^x , etc., the next equation for subchannel i is obtained

$$\begin{aligned} \frac{1}{A_i} \frac{\partial m_i}{\partial t} - 2u_i \frac{\partial \rho_i}{\partial t} + \frac{\partial P_i}{\partial z} &= -\left(\frac{m_i}{A_i}\right)^2 \left(C_i + \frac{\partial V_i'}{\partial z}\right) \\ &+ \sum_j (2u_i - u^*) W_{ij}/A_i - \sum_j (u_i - u_j) W'_{ij}/A_i - \rho_i g \cos \theta \end{aligned} \quad (37)$$

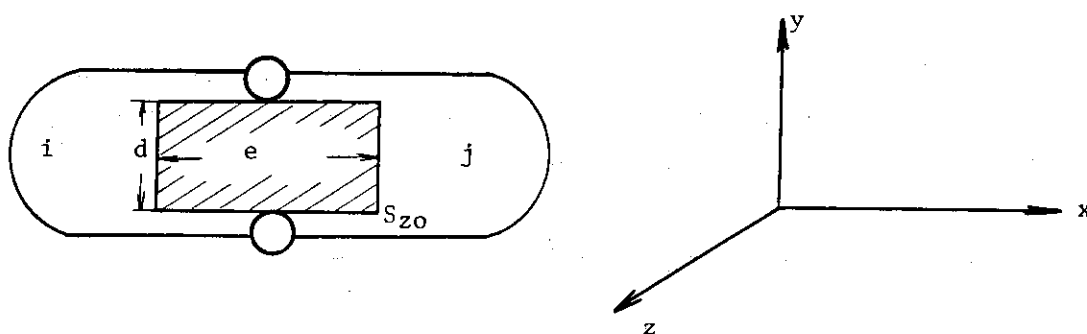
where the constant C_i includes all frictional pressure loss effects caused from viscosity.

2.2) Lateral component^(25,28)

In macroscopic point of view, the lateral momentum transfer phenomenon may be properly represented by an equation about the rates of gross momentum transfer from a subchannel to another, where the macroscopic directional distribution of lateral momentum in a subchannel is represented by the rates above, the number of which is equal to the number of adjacent subchannels. Such an equation may be derived by considering about only one lateral component of the integral momentum equation. For instance, i -component of the integral momentum equation is given by (7) ~ (17) as

$$\begin{aligned}
& S_z \frac{\partial}{\partial t} \overline{\rho v_x} + \int_{S_z} \frac{\partial \rho v_x v_z}{\partial z} dS_z + \int_{S_y} \rho v_x v_y dS_y + \int_{S_x} \rho v_x^2 dS_x \\
& + \overline{\Delta_x P} \cdot \bar{y} + \int_{S_z} \frac{\partial \tau_{zx}}{\partial z} dS_z + \int_{S_y} \tau_{yx} dS_y + \int_{S_x} \tau_{xx} dS_x - S_z \bar{\rho} g_x = 0
\end{aligned} \quad (38)$$

The physical meaning of every term in this equation may be comprehended by the next figure



Let i and j be two subchannels mutually adjacent at the broken line and the region ($\ell \times d$) with hatching be such a region in which gross lateral momentum transfer exists whereas the vectorial sum of lateral momentum in the region S_{z0} may be nearly equal to zero.

Then, if unit length of the two subchannels is taken as the integral domain V in equation (38), the resultant equation may be regarded as of gross lateral momentum balance condition between i and j by the following consideration.

The first term may conveniently be separated into two parts as

$$\begin{aligned}
S_z \frac{\partial}{\partial t} \overline{\rho v_x} &= S_{z0} \frac{\partial}{\partial t} \overline{\rho v_x} + \ell (d \frac{\partial}{\partial t} \overline{\rho v_x}) \\
&= S_{z0} \frac{\partial \bar{W}}{\partial t} + \ell \frac{\partial W_{ij}}{\partial t}
\end{aligned} \quad (39)$$

where, \bar{W} is average cross flow density in S_{z0} while W_{ij} the cross flow rate as defined previously. The second term may also be represented as

$$\begin{aligned}
\int_{S_z} \frac{\partial \rho v_x v_z}{\partial z} dS_z &= \int_{S_{z0}} \frac{\partial \rho v_x v_z}{\partial z} dS_z + \int_{d \times \ell} \frac{\partial \rho v_x v_z}{\partial z} dS_z \\
&= S_{z0} \cdot \widehat{W} \cdot \frac{\partial \widehat{v_{z0}}}{\partial z} + \ell \cdot \frac{\partial \widehat{v_{zc} W_{ij}}}{\partial z}
\end{aligned} \quad (40)$$

where the physical meaning of \widehat{W} , $\widehat{v_{zo}}$ and $\widehat{v_{zc}}$ may be self-evident from the previous explanation

The third term is y-directional net divergence of x-directional momentum hence if exists should necessarily be estimated in relation to the other subchannels adjacent to these two subchannels, thereby this term has not to be considered here. The fourth term may be represented as

$$\int_{S_x} \rho v_x^2 dS_x = d \cdot \rho^* \cdot \overline{v_x^2} \quad (41)$$

with appropriate mean value $\overline{v_x^2}$ and

$$\rho^* = \begin{cases} \rho_i & \text{for } v_x > 0 \\ \rho_j & \text{for } v_x < 0 \end{cases} \quad (42)$$

It may be clear from the definitions (11) and (13) that the fifth term can be written as

$$\overline{\Delta_x P} \cdot \overline{y} = (P_j - P_i) \cdot d \quad (43)$$

The sixth term may be represented as

$$\int_{S_x} \frac{\partial \tau_{zx}}{\partial z} S_z = S_{zo} \left(\frac{\partial \tau_{zx}}{\partial z} \right) + l \cdot d \cdot \left(\frac{\partial \tau_{zx}}{\partial z} \right)^* \quad (44)$$

for the appropriate mean values of $(\partial \tau_{zx} / \partial z)$ over the domains S_{zo} and $l \times d$. The seventh term need not be considered here for the same reason as that of the third term. The eighth term may be represented as

$$\int_{S_x} \tau_{xx} dS_x = d \cdot \tau_{xx}^* \quad (45)$$

with

$$\tau_{xx}^* = \tau_{xxi} - \tau_{xxj} \quad (46)$$

Collecting all terms above, the next equation is obtained

$$\begin{aligned} & l \left(\frac{\partial W_{ij}}{\partial t} + \frac{\partial \widehat{v_{zc}} W_{ij}}{\partial z} \right) + d \cdot \{ P_j - P_i + \rho^* \overline{v_i^2} + l \left(\frac{\partial \tau_{xx}}{\partial z} \right)^* + \tau_{xx}^* \} \\ & - (S_{zo} + l \cdot d) \overline{\rho g_x} + S_{zo} \left\{ \frac{\partial \overline{W}}{\partial t} + \overline{W} \frac{\partial \widehat{v_{zo}}}{\partial t} + \left(\frac{\partial \tau_{xx}}{\partial z} \right) \right\} = 0 \end{aligned} \quad (47)$$

This equation may be broken down into a simpler form by neglecting the last term for the prescribed reason:

$$\frac{\partial W_{ij}}{\partial t} + \frac{\partial u^* W_{ij}}{\partial z} = \{(P_j - P_i) - C_{ij}^f W_{ij}\} \times \frac{d}{\ell} \quad (48)$$

where the next correlation

$$\rho^* v_x^2 + \ell \left(\frac{\partial \tau_{zx}}{\partial z} \right)^* + \tau_{xx}^* = C_{ij}^f W_{ij} \quad (48)$$

is assumed to hold with an empirical coefficient C_{ij}^f and further use is made of

$$\hat{v}_{z0} \approx u^*$$

3. Energy balance equation

The energy balance equation (1.4) is rewritten as the next form using enthalpy h in place of internal energy e

$$\begin{aligned} \rho \frac{\partial h}{\partial t} + \text{div } h \rho \mathbf{v} - h \text{div } \rho \mathbf{v} + \text{div } \mathbf{q} + (\boldsymbol{\tau} : \nabla \mathbf{v}) \\ - \mathbf{v} \cdot \text{grad } P - \frac{\partial P}{\partial t} = 0 \end{aligned} \quad (51)$$

V-integral therefore, of every term may be represented as follows.

The first term:

$$\int_V \rho \frac{\partial h}{\partial t} dV = S_z \bar{\rho} \frac{\partial \bar{h}}{\partial t} \quad (52)$$

The sum of the second and the third terms:

$$\begin{aligned} \int_V (\text{div } h \rho \mathbf{v} - h \text{div } \rho \mathbf{v}) dV \\ = S_z \left\{ (\hat{h} - \bar{h}) \frac{\partial \overline{\rho v_z}}{\partial z} + \overline{\rho v_z} \frac{\partial \hat{h}}{\partial z} \right\} + \widehat{\Delta y h} W_y + \widehat{\Delta x h} W_x \\ + \widehat{\Delta y h'} W_{y'} + \widehat{\Delta x h'} W_{x'} \end{aligned} \quad (53)$$

where

\bar{h} : $\text{div } \rho \mathbf{v}$ - weighted average of h over V

\hat{h} : ρv_z - weighted average of h over V

\bar{h} : ρ - weighted average of h over V

$\widehat{\Delta y h}, \widehat{\Delta x h} : \overline{\rho v_y}^t$ and $\overline{\rho v_x}^t$ - weighted average of $(h-\tilde{h})$ over V
respectively

$\widehat{\Delta y h}', \widehat{\Delta x h}' : \rho v_y' -$ and $\rho v_x' -$ weighted average of $(h-\tilde{h})$ over V

The fourth term:

$$\int_V \text{div } q \, dV = S_z \cdot \frac{\partial \bar{q}_z}{\partial z} + Q_y + Q_x \quad (54)$$

where

$$\bar{q}_z \equiv \int_{S_z} q_z dS_z / S_z$$

$$Q_y \equiv \int_{S_y} q_y dS_y$$

$$Q_x \equiv \int_{S_x} q_x dS_x$$

The fifth term:

$$\int_V (\tau : \nabla \mathbf{v}) \, dv = \frac{1}{2} S_z \bar{\rho} \cdot v_z^3 \cdot e_v \quad (55)$$

with an empirical factor e_v co-related for example as

$$e_v = \begin{cases} 2.7(1-\beta)(1-\beta)/\beta^2 & \text{for orifice} \\ 0.45(1-\beta) & \text{for contraction} \\ (1/\beta - 1) & \text{for expansion} \end{cases}$$

$\beta \equiv \text{smaller area/larger area}$

The sixth term:

$$\int_V \mathbb{W} \text{grad } \rho \, dv = R \quad (56)$$

The last term:

$$\int_V \frac{\partial P}{\partial t} \, dv = S_z \cdot \frac{\partial \bar{P}}{\partial t} \quad (57)$$

Collecting all terms above, the next equation is obtained

$$\begin{aligned}
& S_z \bar{\rho} \frac{\partial \bar{h}}{\partial t} + S_z \bar{\rho} v_z \frac{\partial \hat{h}}{\partial z} - (\hat{h} - \tilde{h})(W_x + W_y + S_z \frac{\partial \bar{\rho}}{\partial t}) \\
& + (\Delta_y \hat{h} W_y + \Delta_x \hat{h} W_x) + (\Delta_y \hat{h}' W_y' + \Delta_x \hat{h}' W_x') \\
& + (Q_x + Q_y) + S_z \frac{\partial \bar{q}_z}{\partial z} + \frac{1}{2} S_z \bar{\rho} v_z^3 e_z + R \\
& + S_z \frac{\partial \bar{P}}{\partial t} = 0
\end{aligned} \tag{58}$$

For usual phenomena taking place in any large power LWR, the following assumption may be applied.

Heat flux vector is horizontal:

$$\frac{\partial \bar{q}_z}{\partial z} = 0 \tag{59}$$

Supersonic phenomena are not necessary to be considered:

$$\frac{\partial \rho}{\partial t} = 0 \quad \text{and} \quad \frac{\partial \rho}{\partial t} = 0 \tag{60}$$

Energy dissipation by viscosity is negligibly small:

$$\frac{1}{2} S_z \bar{\rho} v_z^3 e_v \approx 0 \tag{61}$$

The contribution of pressure gradient to energy dissipation by expansion is negligibly small.

$$R \approx 0 \tag{62}$$

Furthermore the assumption

$$\hat{h} - \tilde{h} \approx 0 \tag{63}$$

may be admissible to an extent.

Under these assumptions, equation (58) may be broken down into

$$\begin{aligned}
& A_{i \rho i} \frac{\partial h_i}{\partial t} + m_i \frac{\partial h_i}{\partial z} \\
& = q_i - (t_i - t_j) c_{ij}^t + (h_i - h^*) w_{ij} + (h_i - h_j) w'_{ij}
\end{aligned} \tag{64}$$

in gross notations for subchannel i.

Here, it is to be noted that⁽²⁷⁾

$$\bar{\rho}_i \frac{\partial h_i}{\partial t}$$

represents increasing rate of energy density, but energy density E for two phase flow is generally given by

$$E = \alpha \rho_v h_v + (1 - \alpha) \rho_e h_e \equiv \rho h - \psi h_{ev} \quad (65)$$

where

$$h \equiv h_e + x h_{ev}$$

$$\psi \equiv (1 - \alpha)x \rho_e - \alpha(1 - x)\rho_v \quad (67)$$

Hence it follows that

$$\begin{aligned} \bar{\rho}_i \frac{\partial h_i}{\partial t} &= \frac{\partial E}{\partial t} = \frac{\partial}{\partial t} (\rho h - \psi h_{ev}) \\ &= \rho \frac{\partial h}{\partial t} + h \frac{\partial \rho}{\partial t} - h_{ev} \frac{\partial \psi}{\partial t} \\ &\approx \rho \frac{\partial h}{\partial t} - h_{ev} \frac{\partial \psi}{\partial t} \quad [\text{by (54)}] \\ &= \rho \frac{\partial h}{\partial t} - h_{ev} \frac{\partial h}{\partial t} \cdot \frac{\partial \psi}{\partial h} \\ &= (\rho - h_{ev} \frac{\partial \psi}{\partial h}) \frac{\partial h}{\partial t} \end{aligned}$$

This result means that if h_i is defined by relation (66), then h_i the effective density of energy transfer should not be equal to the simple volume average density ρ_i , but it should be given as

$$\bar{\rho}_i = \rho_i - h_{ev} \frac{\partial \psi}{\partial h}$$

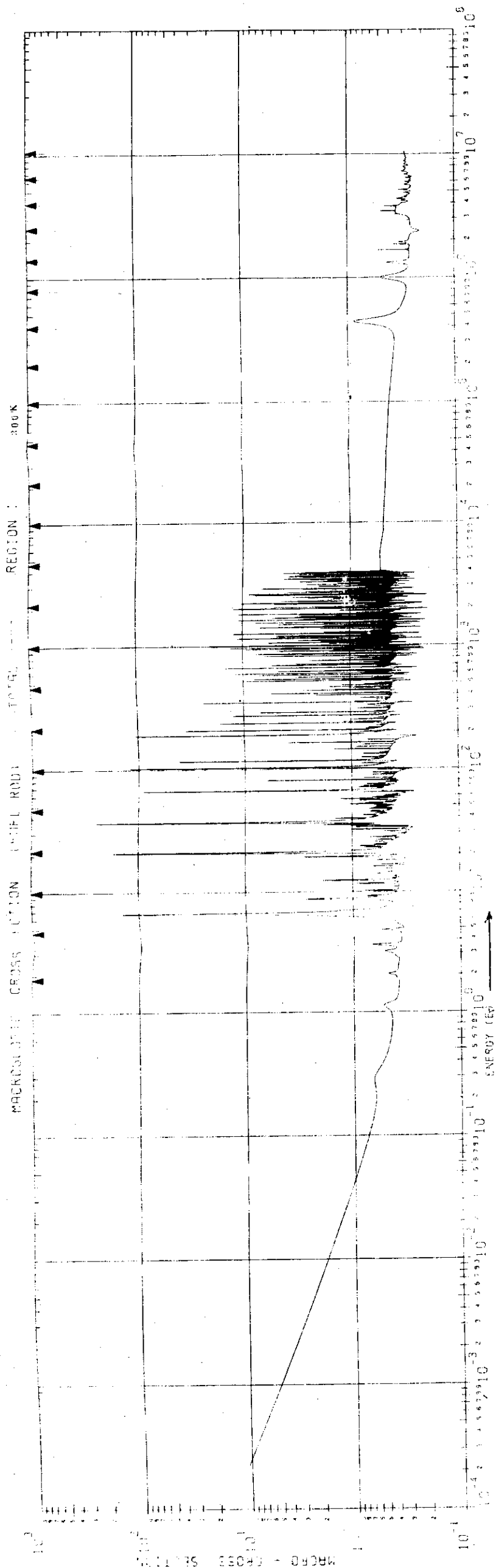
APPENDIX XII A set of examples obtained by applicating the code system to a PWR

Here, only the typical examples of the results obtained by test calculations of a PWR core using the code system are illustrated.

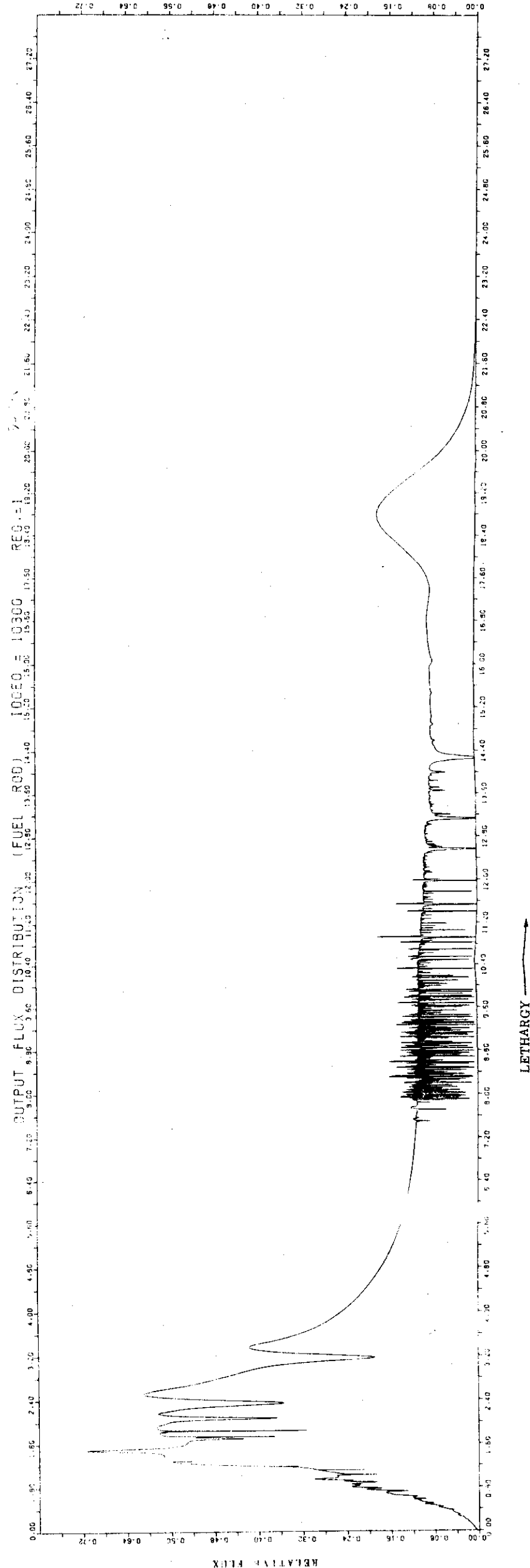
The examples are as follows:

- (1) Macroscopic total cross section curve of UO_2 reproduced from ENDF-B.
- (2) Fine spectrum in a fuel rod cell.
- (3) One-dimensional data of the multigroup constants for U-238 produced from ENDF-B.
- (4) Multigroup spectrum in a fuel rod cell.
- (5) A set of rod cell average reactor constants.
- (6) Axial and horizontal distribution of three group flux in a PWR core.

(1) Macroscopic total cross section curve of UO_2 reproduced from ENDF-B



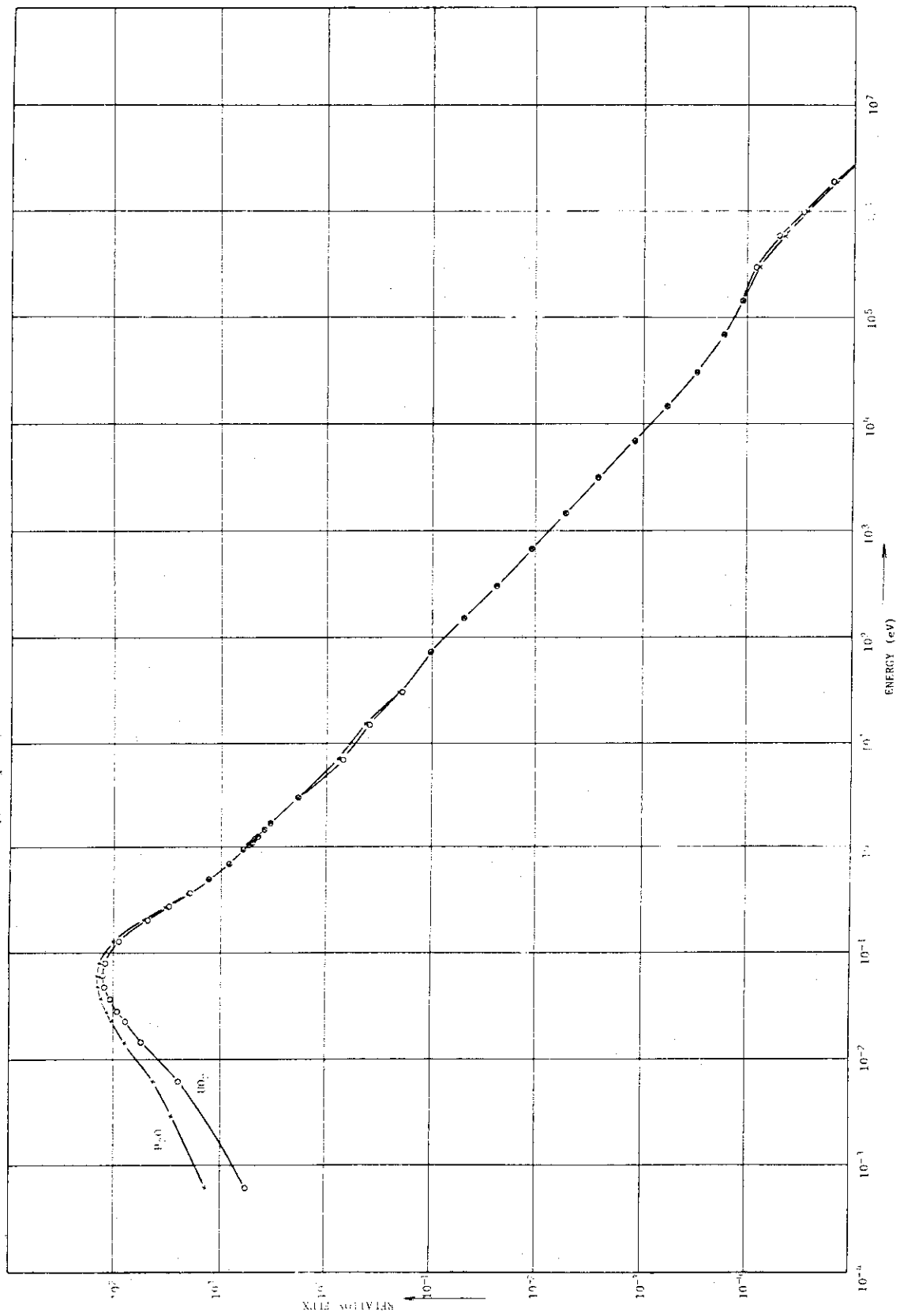
(2) Fine spectrum in a fuel rod cell



(3) One-dimensional data of the multigroup constants for U-238 produced from ENDF-B

GROUP	UPPER ENERG	ABSORPTION	NUCLEON	ELASTIC	INELASTIC	(N,2N)	FISSION	TOTAL	CAPTURE
1	1.64372E+07	1.21535E+00	5.62803E+00	2.72235E+00	6.03503E-01	5.58258E-01	1.21333E+00	5.10633E+00	1.72234E-03
2	1.45499E+07	1.07135E+00	4.67841E+00	2.70241E+00	6.37033E-01	1.07215E+00	1.06931E+00	5.43976E+00	2.04453E-03
3	1.28403E+07	9.78781E-01	4.03506E+00	2.73052E+00	7.02994E-01	1.31526E+00	9.75354E-01	5.72705E+00	2.42692E-03
4	1.13315E+07	9.83384E-01	3.85061E+00	2.81305E+00	7.72974E-01	1.27459E+00	9.80504E-01	5.84395E+00	2.87982E-03
5	1.00302E+07	9.91346E-01	3.69670E+00	2.94376E+00	8.36590E-01	1.18787E+00	9.87927E-01	5.95956E+00	3.41964E-03
6	8.82497E+06	1.00017E+00	3.56495E+00	3.11789E+00	1.04013E+00	9.90154E-01	9.95103E-01	6.14835E+00	4.05283E-03
7	7.78501E+06	9.84097E-01	3.36391E+00	3.34790E+00	1.65362E+00	4.84214E-01	9.79271E-01	6.47009E+00	4.82577E-03
8	6.87289E+06	7.78348E-01	2.55877E+00	3.59770E+00	2.43940E+00	7.16532E-02	7.72615E-01	6.85712E+00	5.73312E-03
9	6.05531E+06	5.56287E-01	1.75700E+00	3.82132E+00	2.85855E+00	0.0	5.49474E-01	7.29616E+00	6.81263E-03
10	5.35261E+06	5.42681E-01	1.65245E+00	4.14040E+00	2.93394E+00	0.0	5.34534E-01	7.61702E+00	8.05634E-03
11	4.72367E+06	5.66702E-01	1.66133E+00	4.26511E+00	2.98300E+00	0.0	5.57079E-01	7.81780E+00	9.62323E-03
12	4.16862E+06	5.72127E-01	1.61803E+00	4.28099E+00	3.05531E+00	0.0	5.60647E-01	7.91842E+00	1.14776E-02
13	3.67879E+06	5.50585E-01	1.50257E+00	4.17785E+00	3.17250E+00	0.0	5.36656E-01	7.90094E+00	1.39803E-02
14	3.24652E+06	5.46281E-01	1.44129E+00	3.99672E+00	3.26161E+00	0.0	5.29215E-01	7.80461E+00	1.70668E-02
15	2.86505E+06	5.60925E-01	1.44714E+00	3.78017E+00	3.31615E+00	0.0	5.39930E-01	7.65724E+00	2.10248E-02
16	2.52849E+06	5.76098E-01	1.46263E+00	3.59088E+00	3.32441E+00	0.0	5.50270E-01	7.49133E+00	2.58276E-02
17	2.23130E+06	5.78616E-01	1.44152E+00	3.46925E+00	3.28669E+00	0.0	5.46385E-01	7.33477E+00	3.22316E-02
18	1.96912E+06	5.46901E-01	1.32904E+00	3.43132E+00	3.22291E+00	0.0	5.07072E-01	7.20113E+00	3.92217E-02
19	1.73774E+06	4.70039E-01	1.09403E+00	3.45446E+00	3.16320E+00	0.0	4.19879E-01	7.08769E+00	5.01512E-02
20	1.53355E+06	3.29700E-01	6.89066E-01	3.51956E+00	3.15065E+00	0.0	2.65766E-01	6.99990E+00	6.39340E-02
21	1.35335E+06	1.44094E-01	1.60265E-01	3.72550E+00	3.08994E+00	0.0	6.20934E-02	6.95953E+00	8.19958E-02
22	1.19433E+06	1.38702E-01	8.22625E-02	4.09141E+00	2.80991E+00	0.0	3.20144E-02	7.04001E+00	1.06687E-01
23	1.05399E+06	1.40465E-01	4.20997E-02	4.62889E+00	2.43855E+00	0.0	1.64465E-02	7.20790E+00	1.24019E-01
24	9.30145E+05	1.37840E-01	2.70704E-02	5.02758E+00	2.23747E+00	0.0	1.06067E-02	7.40289E+00	1.27234E-01
25	8.20350E+05	1.26506E-01	8.78630E-03	5.54192E+00	1.97094E+00	0.0	3.45272E-03	7.63936E+00	1.23054E-01
26	7.24398E+05	1.20166E-01	3.87585E-03	6.05706E+00	1.72300E+00	0.0	1.52713E-03	7.90022E+00	1.18638E-01
27	6.39279E+05	1.15155E-01	2.09494E-03	6.43014E+00	1.63078E+00	0.0	8.27315E-04	8.17607E+00	1.14328E-01
28	5.64161E+05	1.11323E-01	1.27971E-03	6.78059E+00	1.56169E+00	0.0	5.06375E-04	8.45360E+00	1.10917E-01
29	4.97871E+05	1.09372E-01	8.99759E-04	7.11148E+00	1.50093E+00	0.0	3.56663E-04	8.72178E+00	1.09015E-01
30	4.39369E+05	1.08950E-01	5.70086E-04	7.43201E+00	1.44429E+00	0.0	2.26345E-04	8.98525E+00	1.08724E-01
31	3.87742E+05	1.08896E-01	5.21028E-04	7.75442E+00	1.38867E+00	0.0	2.07146E-04	9.25398E+00	1.10689E-01
32	3.42181E+05	1.13829E-01	3.11808E-04	8.08470E+00	1.33429E+00	0.0	1.24109E-04	9.53283E+00	1.13705E-01
33	3.01974E+05	1.17976E-01	2.20833E-04	8.41582E+00	1.28741E+00	0.0	8.80005E-05	9.81620E+00	1.17888E-01
34	2.66491E+05	1.21604E-01	2.24620E-04	8.75721E+00	1.23275E+00	0.0	8.95943E-05	1.01116E+01	1.21514E-01
35	2.35177E+05	1.25456E-01	2.46004E-04	9.10206E+00	1.18238E+00	0.0	9.82051E-05	1.04099E+01	1.25358E-01
36	2.07543E+05	1.30739E-01	2.47813E-04	9.45531E+00	1.12245E+00	0.0	9.90901E-05	1.07085E+01	1.30640E-01
37	1.83156E+05	1.37431E-01	2.47652E-04	9.80293E+00	1.05357E+00	0.0	9.95002E-05	1.09940E+01	1.37332E-01
38	1.61535E+05	1.44424E-01	1.95030E-04	1.01534E+01	9.90165E-01	0.0	7.80665E-05	1.13180E+01	1.44345E-01
39	1.42642E+05	1.52509E-01	1.05476E-04	1.05471E+01	9.16049E-01	0.0	4.21902E-05	1.16157E+01	1.52457E-01
40	1.25881E+05	1.62996E-01	1.05153E-04	1.08339E+01	8.42641E-01	0.0	4.21003E-05	1.18395E+01	1.62953E-01
41	1.11090E+05	1.75112E-01	1.05109E-04	1.11336E+01	7.66455E-01	0.0	4.20978E-05	1.20751E+01	1.75070E-01
42	9.80365E+04	1.89831E-01	7.18689E-05	1.14145E+01	7.01710E-01	0.0	2.87938E-05	1.23060E+01	1.89802E-01
43	8.65169E+04	2.08230E-01	7.92457E-05	1.17055E+01	6.06433E-01	0.0	3.17618E-05	1.25201E+01	2.08198E-01
44	7.63509E+04	2.27143E-01	1.34303E-04	1.19993E+01	5.12752E-01	0.0	5.38412E-05	1.27392E+01	2.27092E-01
45	6.73794E+04	2.51714E-01	2.06298E-04	1.23095E+01	3.94972E-01	0.0	8.27231E-05	1.29563E+01	2.51632E-01
46	5.94622E+04	2.82922E-01	2.39089E-04	1.25830E+01	2.63202E-01	0.0	9.58916E-05	1.31291E+01	2.82826E-01
47	5.24752E+04	3.23287E-01	3.12446E-04	1.26953E+01	1.15586E-01	0.0	9.27531E-05	1.31342E+01	3.23194E-01
48	4.63092E+04	3.72442E-01	1.55241E-04	1.27300E+01	3.66473E-03	0.0	6.22335E-05	1.31061E+01	3.72379E-01
49	4.08677E+04	4.00227E-01	1.05769E-04	1.28163E+01	0.0	0.0	4.24411E-05	1.32166E+01	4.00163E-01
50	3.60566E+04	4.19455E-01	7.13233E-05	1.29142E+01	0.0	0.0	2.86244E-05	1.33377E+01	4.19437E-01
51	3.18278E+04	4.40328E-01	1.32777E-04	1.29937E+01	0.0	0.0	5.32925E-05	1.34341E+01	4.40275E-01
52	2.80879E+04	4.64496E-01	1.90968E-04	1.30555E+01	0.0	0.0	7.66592E-05	1.35200E+01	4.64419E-01
53	2.47875E+04	4.89824E-01	2.34020E-04	1.31187E+01	0.0	0.0	9.39463E-05	1.36038E+01	4.89730E-01
54	2.18749E+04	5.15756E-01	2.66050E-04	1.31852E+01	0.0	0.0	1.06513E-04	1.37010E+01	5.15649E-01
55	1.93045E+04	5.43811E-01	2.94321E-04	1.32588E+01	0.0	0.0	1.18171E-04	1.38026E+01	5.43692E-01
56	1.70362E+04	5.74346E-01	3.19248E-04	1.33329E+01	0.0	0.0	1.28188E-04	1.39073E+01	5.74217E-01
57	1.50344E+04	6.21334E-01	2.67191E-04	1.34549E+01	0.0	0.0	1.07305E-04	1.40763E+01	6.21226E-01
58	1.17088E+04	6.36421E-01	1.53225E-04	1.39157E+01	0.0	0.0	6.15327E-05	1.45521E+01	6.36359E-01
59	9.11882E+03	6.34996E-01	4.07001E-04	1.51836E+01	0.0	0.0	1.61454E-04	1.58186E+01	6.34831E-01
60	7.10174E+03	7.32998E-01	5.03498E-05	1.53221E+01	0.0	0.0	2.02207E-05	1.60551E+01	7.32978E-01
61	5.53084E+03	7.77810E-01	1.00146E-07	1.41561E+01	0.0	0.0	4.02212E-08	1.49439E+01	7.77810E-01
62	4.30742E+03	8.31833E-01	1.00774E-07	1.67372E+01	0.0	0.0	4.04749E-08	1.75690E+01	8.31833E-01
63	3.35463E+03	9.94455E-01	1.02327E-07	1.55963E+01	0.0	0.0	4.10388E-08	1.65907E+01	9.94455E-01
64	2.61259E+03	1.07379E+00	1.06862E-07	1.67128E+01	0.0	0.0	4.29215E-08	1.77866E+01	1.07379E+00
65	2.03459E+03	1.04635E+00	1.26027E-07	1.67348E+01	0.0	0.0	5.06290E-08	1.77812E+01	1.04635E+00
66	1.58461E+03	1.04589E+00	5.85396E-05	1.37604E+01	0.0	0.0	2.35154E-05	1.48053E+01	1.04587E+00
67	1.23410E+03	1.41777E+00	2.75560E-03	1.56339E+01	0.0	0.0	1.10721E-03	1.70517E+01	1.41666E+00
68	9.61116E+02	1.62195E+00	2.22511E-04	1.31894E+01	0.0	0.0	8.93800E-05	1.48114E+01	1.62136E+00
69	7.48518E+02	1.70110E+00	8.94050E-03	1.39911E+01	0.0	0.0	3.59098E-03	1.56922E+01	1.69751E+00
70	5.82947E+02	1.64850E+00	6.53987E-05	1.22404E+01	0.0	0.0	2.62697E-05	1.38837E+01	1.64347E+00
71	4.53999E+02	1.39445E+00	2.25000E-06	1.24934E+01	0.0	0.0	9.03892E-07	1.33879E+01	1.39445E+00
72	3.53575E+02	1.51242E+00	1.37391E-05	1.38110E+01	0.0	0.0	5.16001E-06	1.53234E+01	1.51241E+00
73	2.75364E+02	1.99793E+00	4.03669E-06	1.47924E+01	0.0	0.0	1.62152E-06	1.67903E+01	1.99793E+00
74	2.14454E+02	2.61585E+00	1.59465E-05	2.15297E+01	0.0	0.0	6.40516E-06	2.41655E+01	2.61583E+00
75	1.67017E+02	1.53592E+00	4.08574E-07	1.08505E+01	0.0	0.0	1.64144E-07	1.23855E+01	1.53592E+00
76	1.30073E+02	5.68535E+00	4.55446E-06	2.48313E+01	0.0	0.0	1.82950E-06	3.05665E+01	5.68534E+00
77	1.01301E+02	2.53087E+00	1.32109E-05	8.00292E+00	0.0	0.0	5.30724E-06	1.05313E+01	2.53085E+00
78	7.88932E+01	5.07390E+00	2.87814E-05	1.57633E+01	0.0	0.0	1.15619E-05	2.03377E+01	5.07389E+00
79	6.14421E+01	1.39843E+01	1.01066E-06	1.03074E+01	0.0	0.0	4.06037E-07	1.05272E+01	1.39842E+01
80	4.78512E+01	2.00750E+00	2.82080E-06	2.03414E+01	0.0	0.0	1.13318E-06	2.23487E+01	2.00750E+00
81	3.72665E+01	1.27899E+01	1.39438E-05	1.78884E+01	0.0	0.0	5.60277E-06	3.01783E+01	1.27899E+01
82	2.90232E+01	6.84450E+01	3.95531E-06	1.05289E+01	0.0	0.0	1.58891E-06	1.12134E+01	6.84448E+01
83	2.26033E+01	2.02288E+01	1.19298E-04	1.55125E+01	0.0	0.0	4.79219E-05	3.57413E+01	2.02288E+01
84	1.76035E+01	4.52885E+01	3.12303E-06	7.55408E+00	0.0	0.0	1.25450E-06	8.00696E+00	

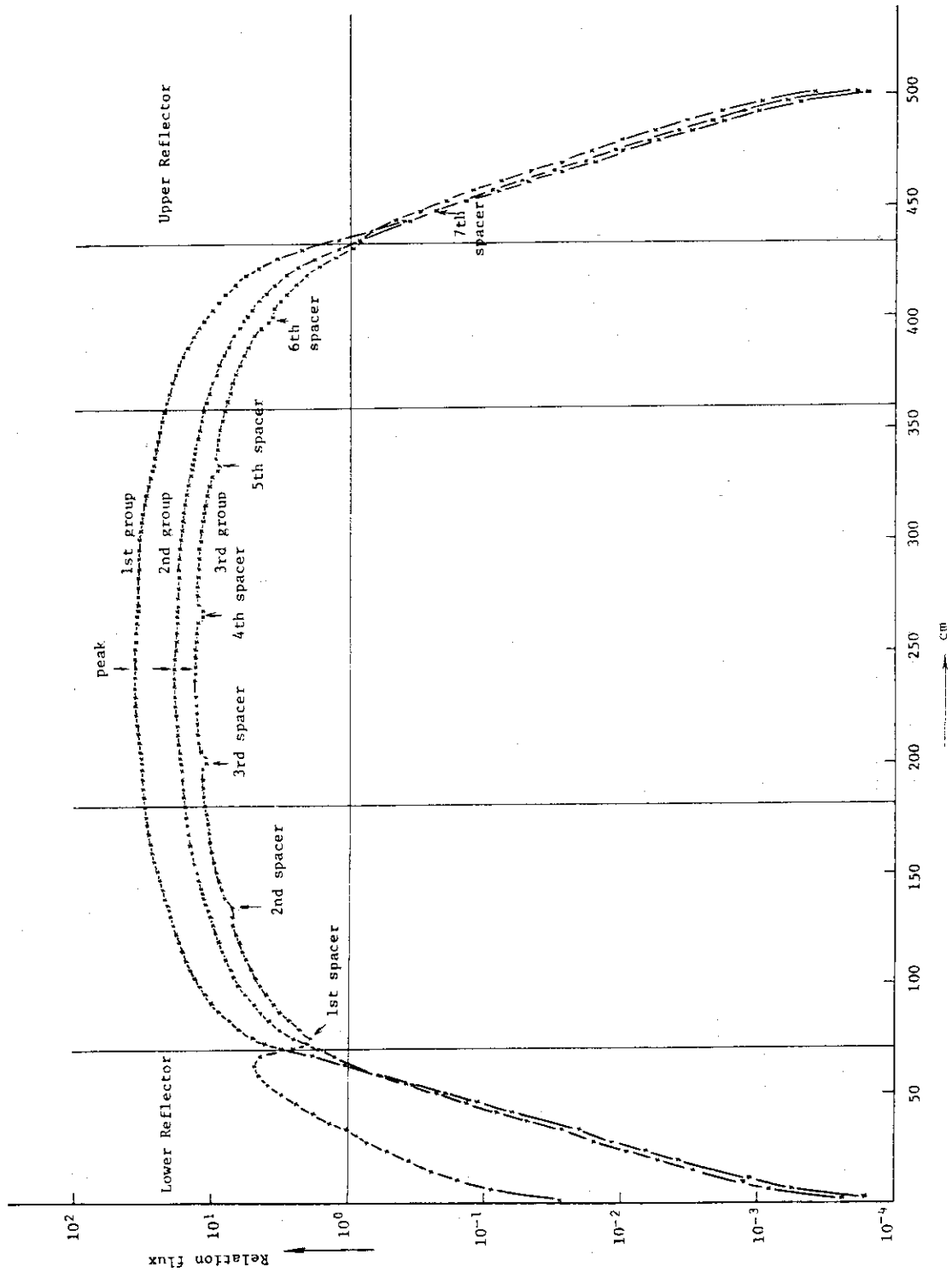
(4) Multigroup spectrum in a fuel rod cell



(5) A set of rod cell average reactor constants

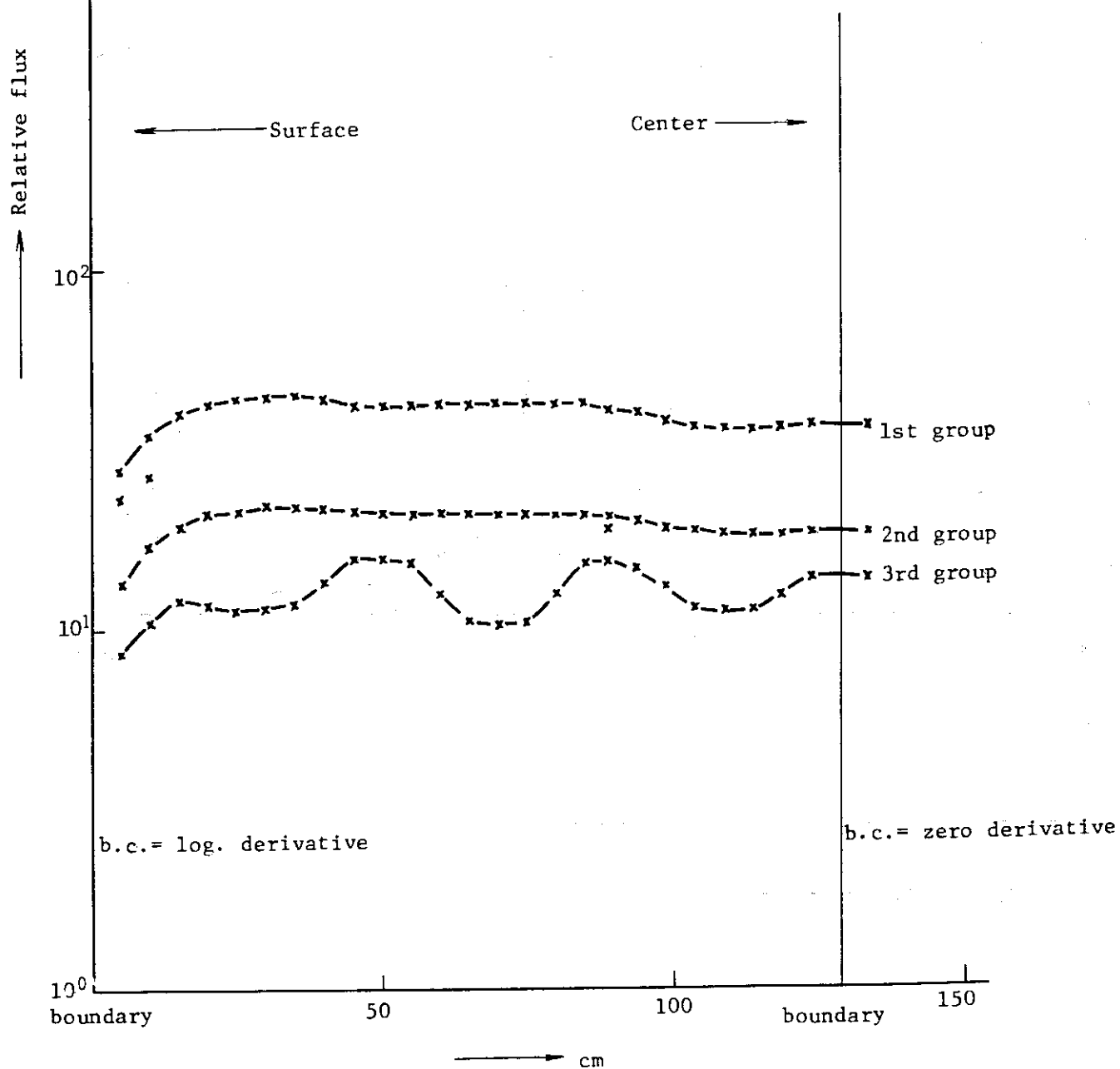
	Dradial	Daxial	Σ_a	$\nu \Sigma_f$	Σ_{re}	Σ_n	Σ_i	Σ_{se}	ρ
Fuel rod (2.27 w/o)									
Group 1	1.49593	1.83094	2.85212E-3	3.68966E-3	3.64700E-2	4.52713E-5	0.0	0.0	2.72684
Group 2	0.739769	0.785612	2.40904E-2	8.79887E-3	4.75699E-2	0.0	-1.03990E-4	3.65093E-2	2.42304
Group 3	0.392381	0.437551	7.15036E-2	9.64998E-2	0.0	0.0	1.02976E-3	4.75827E-2	2.42300
Fuel rod (3.03 w/o)									
Group 1	1.50151	1.83713	2.94034E-3	3.89856E-3	3.64047E-2	4.50004E-5	0.0	0.0	2.7141
Group 2	0.735139	0.783540	2.56335E-2	1.16480E-2	4.68859E-2	0.0	-7.63005E-5	3.64425E-2	2.42304
Group 3	0.382630	0.423461	8.23581E-2	1.20751E-1	0.0	0.0	1.31306E-3	4.68990E-2	2.42300
Fuel rod (3.40 w/o)									
Group 1	1.50422	1.84015	2.98333E-3	4.00029E-3	3.63729E-2	4.48711E-5	0.0	0.0	2.70847
Group 2	0.732839	0.782528	2.63754E-2	1.30183E-2	4.65590E-2	0.0	-6.23804E-5	3.63729E-2	2.42304
Group 3	0.378225	0.418011	8.7263 E-2	1.31648E-1	0.0	0.0	1.45792E-3	4.65590E-2	2.42300
Control rod (Ag-In-Cd)									
Group 1	1.74487	1.99205	4.92081E-3	0.0	2.78257E-2	9.52647E-7	0.0	0.0	0.0
Group 2	0.472529	0.622118	7.67083E-2	0.0	1.57818E-2	0.0	-7.74791E-3	2.78256E-2	0.0
Group 3	0.0980185	0.471535	6.38910E-1	0.0	0.0	0.0	2.29107E-1	1.57985E-2	0.0
Control rod (Al ²⁶ O ₃)									
Group 1	2.65025	3.33289	2.79363E-4	0.0	2.87649E-2	3.07882E-7	0.0	0.0	0.0
Group 2	0.955627	0.984643	1.83822E-3	0.0	4.59352E-2	0.0	-6.75896E-4	2.88175E-2	0.0
Group 3	0.539359	0.805961	2.70354E-2	0.0	0.0	0.0	6.53171E-5	4.59435E-2	0.0
Burnable Poison									
Group 1	6.99007	6.48759	7.20226E-4	0.0	2.82852E-2	3.29036E-7	0.0	0.0	0.0
Group 2	0.949471	0.599593	3.07613E-2	0.0	2.99351E-2	0.0	-7.06666E-4	2.83005E-2	0.0
Group 3	0.357994	0.378023	3.14975E-1	0.0	0.0	0.0	3.91621E-2	2.99459E-2	0.0
Water hole									
Group 1	2.5568	2.53894	1.35732E-4	0.0	5.08525E-2	5.29902E-7	0.0	0.0	0.0
Group 2	0.91774	0.934394	1.65783E-3	0.0	9.52210E-2	0.0	-8.53174E-4	5.09145E-2	0.0
Group 3	0.275610	0.349681	2.96000E-2	0.0	0.0	0.0	4.05127E-6	9.52391E-2	0.0

6.1 Z-directional flux distribution at center assembly



6.2 Flux distribution (principal direction)

(Node No. = 6)



6.3 Flux distribution (diagonal direction)

