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INTRODUCTION TO REACTOR LATTICE CALCULATIONS BY THE WIMSD CODE

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Teresa Kulikowska: Introduction to Reactor Lattice Calculations by the WIMSD Code. The present report is based on lectures delivered at the Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety hold in the International Centre of Theoretical Physics, Trieste, in March 1998. The main goal of the set of lectures was to give the basis of reactor physics calculations for participants working on nuclear data. The last lectures, devoted to the WIMS including the WIMSD code users. Following this general line the material is divided into three parts: The first part includes a short description of neutron transport phenomena limited to those definitions that are necessary to understand the approach to practical solution of the problem given in the second part on reactor lattice transport calculations. The detailed discussion of the neutron cross sections has been skipped as this subject has been treated in detail by other lecturers. In the third part those versions of the well-known WIMSD code which are distributed by NEA. Data Bank are described. The general structure of the code is given supplied in a more detailed description of aspects being the most common points of misunderstanding for the code users.

Teresa Kulikowska: Wprowadzenie do zastosowania kodu WIMSD w obliczeniach siatek reaktorowych. Raport oparty jest na wykładach wygłoszonych na kursie na temat danych jądrowych i reaktorów jądrowych zorganizowanym przez Międzynarodowy Ośrodek Fizyki Teoretycznej i MAEA w Trieście w marcu 1998 r. Celem serii wykładów było zaznajomienie uczestników zajmujących się przygotowaniem danych jądrowych z obliczeniami, w których te dane są stosowane. Ostatnie wykłady, dotyczące kodu WIMSD, były przeznaczone również dla fizyków reaktorowych włącznie z tymi, którzy już byli użytkownikami tego kodu. Zgodnie z powyższym ukierunkowaniem raport składa się z trzech części: w pierwszej zebrano podstawowe pojęcia teorii transportu neutronów ograniczając się do tych, które są niezbędne do zrozumienia części drugiej, poświęconej obliczeniom transportowym siatek reaktorowych. Część trzecia zawiera opis tych wersji kodu WIMSD, które są rozprowadzane przez NEA Data Bank. Podano opis kodu oraz położono nacisk na aspekty będące najczęściej przedmiotem błędów użytkowników wynikajcych z niezrozumienia przybliżeń stosowanych w kodzie.

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1. INTRODUCTION TO THE NEUTRON TRANSPORT PHENOMENA

1.1. Definitions

1.1.1. Description of the medium

The medium is described by its isotopic composition and its nuclear properties. The composition is given in terms of *number densities* of isotopes defined as the numbers of respective nuclei in a cubic centimetre:

$$ND = \frac{\rho \cdot N_A}{A}, \tag{1.1}$$

with the Avogadro Number N_A=6.022×10^{23}, ρ - the isotope density in grams per cubic centimetre, and A the Atomic Number.

The nuclear properties are described by *microscopic cross sections*, σ_x, for reactions of type x.

The *macroscopic cross sections*, $\Sigma^x(r,E)$ of an isotope i, is a product of its microscopic cross section and its number density, ND^i, at position r:

$$\Sigma^{x,i}(r,E) = ND^i(r) \cdot \sigma^{x,i}(E). \tag{1.2}$$

If the medium is composed of more than one isotope then the total macroscopic cross section of the medium is equal to the sum of cross sections for each isotope:

$$\Sigma^x{}_{medium}(r,E) = \sum_i \Sigma^{x,i}(r,E) = \sum_i (\sigma^{x,i}(E) \cdot ND^i(r)). \tag{1.3}$$

The sum of the partial cross sections for all possible types of neutron-nucleus collisions is the *total cross section.* It is defined as the total collision (or interaction) cross section of a neutron at position r having energy E (in the laboratory system). It is the probability of neutron interaction per unit distance travelled by a neutron and has the dimension of a reciprocal length, e.g., cm^{-1}:

$$\Sigma_m{}^{tot}(r,E) = \sum_x \Sigma_m{}^x(r,E). \tag{1.4}$$

The reciprocal of the total cross section, λ, is called a *mean free path* and is an average distance of neutron travel between two consecutive collisions.

$$\lambda = 1/\Sigma_m{}^{tot}(r,E). \tag{1.5}$$

A form of *differential cross section,*

$$\Sigma^x(r,E')f^x(r;\Omega',E' \rightarrow \Omega,E), \tag{1.6}$$

is defined for collisions, from which neutrons emerge, as the cross sections for initial direction Ω' and energy E' emerging in a collision in the interval $d\Omega$ about Ω with energy dE about E. The cross section for a reaction of type x, for neutrons of energy E',

is Σ^x and $f^x(r;\Omega',E'\rightarrow\Omega,E)d\Omega\,dE$ is the probability that if a neutron of direction Ω' and energy E' has a collision of type x, there will emerge from the collision a neutron in the direction interval $d\Omega$ about Ω with energy dE about E. For elastic scattering, integration of f^x over all directions and energies gives unity. For elastic scattering of neutrons from initially stationary nuclei f^x is a function only of $\Omega'\cdot\Omega$ which is a cosine of the scattering angle between the directions of motion of the neutron before and after the collision. For fission it is a good approximation to assume that the neutrons are emitted isotropically in the laboratory system. Then it is possible to write:

$$f^x(r;\Omega',E'\rightarrow\Omega,E)d\Omega\,dE = 1/(4\pi)\cdot\kappa(r;E'\rightarrow E)\,d\Omega\,dE, \qquad (1.7)$$

where $\cdot\kappa(r;E'\rightarrow E)dE$, referred to as the spectrum of the fission neutrons, is the probability that a fission caused by a neutron at r with energy E' will lead to a neutron within dE about E. It is normalised so that after integration over full angle it gives $\kappa(r;E')$ which is the average number of neutrons produced by a fission at r caused by a neutron of energy E'.

Instead of the neutron energy, E, the neutron velocity, v, may be used represented as:

$$\mathrm{v} = v\cdot\Omega$$

where $v = |\mathrm{v}|$ is the neutron speed and is connected to the energy by a standard equation

$$E = mv^2/2.$$

with m the neutron mass.

The rate, in neutrons per unit volume and time at r and t, at which neutrons are transferred by interactions of type x into final directions within $d\Omega$ about Ω and final energies dE about E is:

$$v'\,\Sigma^x(r,E')f^x(r;\Omega',E'\rightarrow\Omega,E)\,N(r,\Omega',E',t)\,d\Omega'dE'\,d\Omega\,dE. \qquad (1.8)$$

The total rate at which neutrons are transferred is obtained by integrating the above quantity over all initial neutron directions and energies, and summing over all reactions.

1.1.2. Description of neutrons

A population of neutrons is described by a quantity called the *neutron angular density* denoted by

$$N(r,\Omega,E,t),$$

and defined as the probable (or expected) number of neutrons at the position r with direction Ω and energy E at time t, per unit volume per unit solid angle per unit energy, e.g., per cm^3 per steradian per MeV. Thus

$$N(r,\Omega,E,t)dVd\Omega dE$$

is the expected number of neutrons in the volume element dV about r, having directions within $d\Omega$ about Ω and energies in dE about E at time t. Such a number of neutrons in an infinitesimal volume is sometimes referred to as a *packet* of neutrons.

In the definition the expression 'probable' or 'expected' number of neutrons is meant to imply that fluctuations from the mean neutron population are not taken into account.

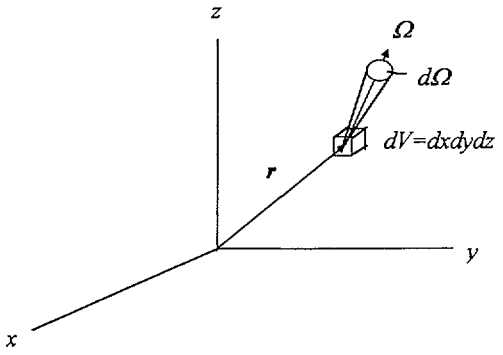

Figure 1: A packet of neutrons.

The integral of the neutron angular density over all directions is the energy dependent *neutron density* $n(r,E,t)$:

$$n(r,E,t) = \int_{4\pi} N(r,\Omega,E,t)d\Omega\,, \tag{1.9}$$

where the integral is taken over all directions. Hence $n(r,E,t)$ is the expected number of neutrons at r, with energy E at time t, per unit volume per unit energy.

The product of the neutron speed v and the neutron angular density is called vector flux:

$$\Phi(r,\Omega,E,t)=v\cdot N(r,\Omega,E,t), \tag{1.10}$$

and its magnitude is called the *neutron angular flux*. The integral over all directions of the neutron angular flux is called *total neutron flux*, often referred to simply as the *neutron flux*, and is equal to:

$$\phi\,(r,E,t). = v\cdot n(r,E,t). \tag{1.11}$$

The neutron flux has been introduced as a quantity much more useful for the description of reactor properties than the neutron number density. The product of the neutron flux and the macroscopic cross section:

$$\Sigma^{x,}\,(r,E)\cdot\phi\,(r,E,t) \tag{1.12}$$

gives, by definition, the number of reactions suffered by neutrons per second, per cubic centimetre and per eV. This quantity is called a *reaction rate* of type *x*. In particular, the fission reaction rate integrated over energy is used to calculate the energy production.

The net number of neutrons crossing a surface element per unit energy in unit time is called the neutron current:

$$J(r,E,t) = v \int_{4\pi} \Omega N(r,\Omega,E,t) d\Omega \,. \tag{1.13}$$

The above introduced quantities are expressed in units given in Table 1.

Table 1: Summary of introduced quantities.

Quantity	Symbol	Unit
Neutron angular density	N	neutrons/(cm^3· steradian·eV)
Neutron density	n	neutrons/(cm^3 ·eV)
Neutron angular flux	Φ	neutrons/(cm^2· steradian·eV·sec)
Neutron flux	ϕ	neutrons/(cm^2 ·eV·sec)
Neutron net current	J	neutrons/(cm^2 ·eV·sec)

It can be seen that the neutron current and the neutron total flux have the same units. The difference between these two quantities can be better understood if we compare their definitions, derived from Eqs. (1.9-11) and Eq.(1.13), but expressed in terms of the angular flux:

$$\begin{aligned} \phi(r,E,t) &= \int_{4\pi} \Phi(r,\Omega,E,t) d\Omega \,, \\ J(r,E,t) &= \int_{4\pi} \Omega \cdot \Phi(r,\Omega,E,t) d\Omega \,. \end{aligned} \tag{1.14}$$

Equations (1.14) show that the neutron flux and current are, respectively, the zero's and first moment of the neutron angular flux.

By the *neutron sources* we understand neutrons which emerge in the system from events other than neutron collision and, therefore, they are independent of the neutron density. They are usually denoted by $Q(r,\Omega E,t)$, which expresses the probability per unit time that a neutron of energy E will appear at r per unit volume per unit solid angle per unit energy. Sometimes they are referred to as external or independent neutron sources.

1.2. The neutron transport equation

1.2.1. Two basic forms of the neutron transport equation

The neutron transport equation is derived from the neutron balance inside a neutron packet (cf. Fig.1). It takes into account the number of neutrons remaining in the packet, the number of neutrons entering the packet as a result of collision and the number of neutrons entering the packet from external sources. The final result is:

$$\frac{\partial N}{\partial t} + v\Omega\nabla N + \Sigma vN = \iint \Sigma' fv' N' dE' d\Omega' + Q, \tag{1.15}$$

where $N = N(r,\Omega,E,t)$, $N' = N(r,\Omega',E',t)$, $\Sigma = \Sigma(r,E)$, $\Sigma' = \Sigma(r,E')$, $f = f(r;\Omega',E' \rightarrow \Omega,E)$, $Q = Q(r,\Omega,E,t)$.

The neutron transport equation may be also expressed in terms of the angular flux Φ, which is equal to $v \cdot N$. By a direct substitution of its definition one gets:

$$\frac{1}{v}\frac{\partial \Phi}{\partial t} + \Omega\nabla\Phi + \Sigma\Phi = \iint \Sigma' f\Phi dE' d\Omega' + Q. \tag{1.16}$$

1.2.2. Interface conditions

The solutions to the neutron transport equation are frequently sought in spatial regions including interfaces between different materials. At such interfaces, the cross sections are discontinuous and it is necessary to consider how the transport equation is to be used in these circumstances. The number of neutrons in a packet is not changed, merely by crossing a physical interface. This means that the neutron angular density must be continuous in r as the interface is crossed. Thus the continuity condition is to be used at the interface. This refers to the neutron angular density but is equally applicable to the angular flux.

1.2.3. Boundary conditions

In general the region of interest is surrounded by a convex surface. A neutron leaving the region through the surface cannot intersect the surface again. If neutrons enter the region from external sources, then the incoming neutron flux must be specified. If no neutrons enter from external sources and if a neutron, once it leaves the surface, cannot return, then the surface is called a free surface and we have the condition:

$$N(r,\Omega,E,t) = 0 \qquad \text{if} \quad n \cdot \Omega < 0, \tag{1.17}$$

where n is a unit vector in the direction of the outward normal at a position r on the surface. Such situation appears if the region is surrounded by vacuum or a perfect absorber.

In practical applications we deal quite often with another type of boundary conditions. We speak about a specular reflection boundary condition if all the neutrons approaching the boundary from within are reflected back to the region with angles preserving the general reflection rule, and about a white boundary condition if they are reflected back with an isotropic distribution. The schematic explanation of the difference between the two boundary conditions is given in Fig. 2. It can be seen that if a packet of neutrons born in the middle of square region reaches the consecutive boundaries without collision they have a good chance to reach the central region under

both types of boundary conditions. The same packet born in the middle of a circular region has a good chance to reach the central region under the white boundary condition but practically no chance under the reflective one. This fact will be used in the application of the transport theory to the solution of practical reactor problems.

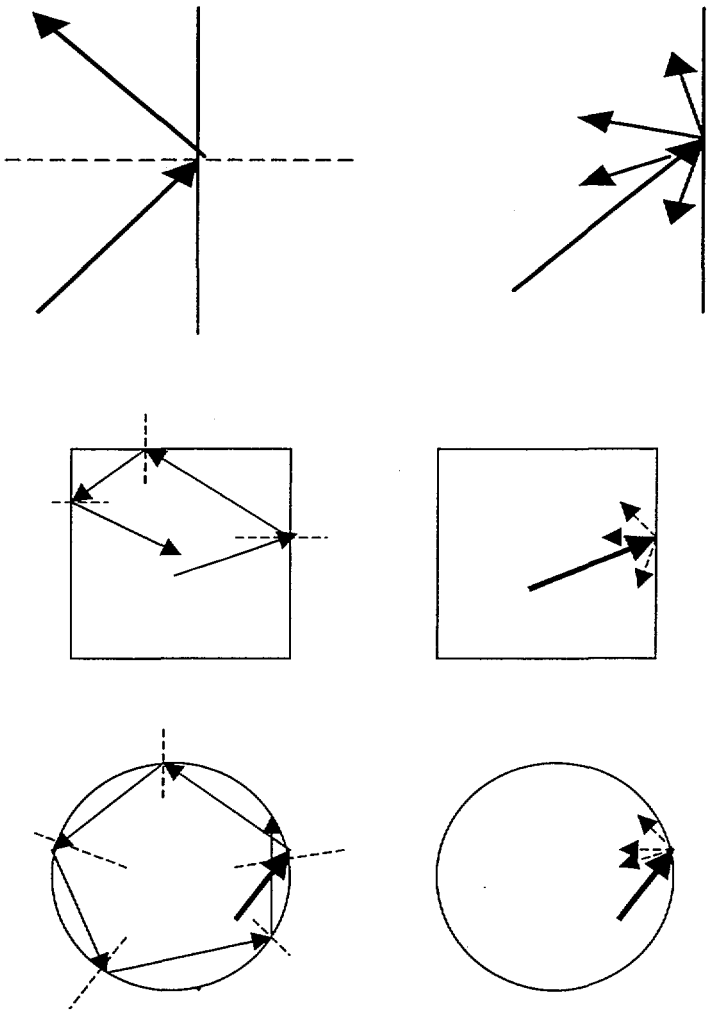

Figure 2: Effect of reflective (on the left hand side) and white (on the right hand side) boundary conditions for plane, square and circular boundaries.

1.2.4. Neutron conservation

The neutron transport equation is simply a statement of neutron conservation as applied to an infinitesimal element of volume, direction and energy. If it is integrated over all directions, the result will be a statement of neutron conservation for a small element of volume and energy. Integration of the neutron transport equation (1.15) over all values of Ω gives with the previous notation (cf. Eqs. (1.9) and (1.13)):

$$\frac{\partial n}{\partial t} + \nabla J + \Sigma v n = \int \Sigma(r; E' \rightarrow E) v' n' dE' + Q, \tag{1.18}$$

where also Q and Σ have been integrated over the angle and

$$\Sigma(r;E'\rightarrow E)=\int\Sigma(r;E')f(r;\Omega',E'\rightarrow\Omega,E)d\Omega\,, \tag{1.19}$$

which is the cross section at r for collisions which result in a neutron of energy E' being replaced by one of energy E.

Integration over a finite region of volume, V, and energy gives:

$$\begin{aligned}&\frac{\partial\iint ndVdE}{\partial t}+\iint\nabla JdVdE+\iint vn\Sigma dVdE\\&=\iiint\Sigma(r;E'\rightarrow E)v'n'dE'dVdE+\iint QdVdE\end{aligned}\,. \tag{1.20}$$

Each of the five terms in the equation has clear physical meaning. The quantity

$$\iint ndVdE$$

is the total number of neutrons in the space-energy region under consideration. Hence the first term is the time rate of change of the total number of neutrons in this region. The second term can be written with application of the divergence theorem:

$$\iint_V\nabla J\cdot dVdE=\iint_A Jn\cdot dAdE\,, \tag{1.21}$$

where dA refers to an element of area, on the boundary surface of the region, V, under consideration and n is a unit normal to the surface element, directed outward from the region. Hence, the second term is the net number of neutrons flowing out of the space-energy region per unit time. The third term

$$\iint v\Sigma ndVdE$$

is the rate at which neutrons are entering into collisions in the given region, i.e., the total collision rate, and the fourth term

$$\iiint\Sigma(r;E'\rightarrow E)v'n'dE'dVdE$$

is the rate at which they emerge from these collisions. The fifth term gives the rate at which neutrons from independent sources are introduced into the region.

Thus the direct representation of particular terms gives:

Rate of change of neutrons = Net rate of generation of neutrons in collisions
+ Rate of introduction of source neutrons
- Net rate of outflow of neutrons.

1.2.5. *Integral equation for neutron transport*

The neutron transport equation is an integro-differential one for the neutron angular density or flux. By the application of the method of characteristics to the neutron transport equation, it can be converted into an integral equation:

$$\Phi(r,\Omega,E,t) = \int_0^\infty exp\left[-\int_0^{s'} \Sigma(r - s''\Omega; E)ds'' \right] q(r - s'\Omega;\Omega, E, t - \frac{s'}{v})ds', \qquad (1.22)$$

with

$$q(r;\Omega, E, t) = \int dE' \int \Sigma(r; E')f(r;\Omega', E' \to \Omega, E)\Phi(r,\Omega,\Omega',E)d\Omega\Omega + Q(r,\Omega, E, t).$$

Thus q is the total rate with which neutrons appear at r, Ω, E and t as a result of both collisions and the independent source.

The integral equation in the simple case of the total cross section independent of position, isotropic scattering and source and no time dependence of the neutron flux becomes:

$$\Phi(r,E) = \int \frac{e^{-\Sigma(E)R}}{4\pi \cdot R^2} dV' \left[-\int \Sigma(r'; E' \to E)\Phi(r', E')dE' + Q(r', E) \right], \qquad (1.23)$$

with $R = |r - r'|$.

The assumption of a cross section independent of the spatial variable is not fulfilled in any realistic reactor system. However, if the system can be divided into subregions with constant material properties Eq. (1.23) can be used for effective reactor calculations.

1.2.6. *Multigroup approach to the neutron transport equation solution*

There is no possibility of obtaining exact solutions to the energy-dependent neutron transport equation for general reactor problems. It is necessary, therefore, to adopt approximate methods for solving the transport equation. The most important are the multigroup methods in which the neutron energy interval of interest is divided into a finite number of intervals, ΔE_g (called groups). It is then assumed that the cross section in each group is constant, e.g., equal to an average over energy. Within each group it is then independent of energy, although arbitrarily dependent on position:

$$\Sigma^x(r,E) \Rightarrow \Sigma_g^x(r), \quad \text{for } g=1,2,...G,$$

$$\int_{\Delta E_{g'}} \int_{\Delta E_g} f(r;\Omega', E' \to \Omega, E)dE'\,dE = c_g(r) \cdot f_{g'g}(r;\Omega' \to \Omega). \qquad (1.24)$$

The neutron angular flux and sources are integrated over respective energy intervals of groups:

$$\Phi_g(r,\Omega) = \int_{\Delta E_g} \Phi(r,\Omega,\Omega)dE$$
$$Q_g(r,\Omega r = \int_{\Delta E_g} Q(r,\Omega,E)dE \qquad (1.25)$$

For a time independent case, using definitions from Eqs. (1.24-25), the energy dependent equation is replaced by a set of coupled one-speed equations which are then solved by approximate methods

$$\Omega\nabla\Phi_g(r,\Omega r + \Sigma_g(r)\Phi_g(r,\Omega r = c_g(r)\sum_{g'}\Sigma_{g'}(r)\int f_{g'g}(r;\Omega'\to\Omega)\Phi_{g'}(r,\Omega')d\Omega + Q_g(r,\Omega). \qquad (1.26)$$

The quantity $c_{g'}(r)$ introduced in Eq. (1.24) has a meaning of the mean number of neutrons with energy in ΔE_g emerging per collision at r. For scattering collision $c = 1$ and for fission $c = \kappa$ (cf. Eq. (1.7)).

1.3. Criticality

From physical consideration, it is to be expected that system containing fissile nuclides can be subcritical, critical or supercritical, based on the behaviour of the neutron population as a function of time.

A system is said to be subcritical if for any nonzero initial neutron population, the expected population dies out with time unless it is sustained by an external neutron source.

A system is said to be supercritical when the expected neutron population diverges with time, starting from any nonzero population.

A system is said to be critical as one in which a steady, time independent neutron population can be maintained in the absence of a source.

The neutron transport equation with boundary conditions defines an initial value problem. If the neutron angular density at $t = 0$ is given, the expected density at any later time can be found, in principle by solving the neutron transport equation. It has been shown that such a solution exists and is unique, provided some mathematical conditions are satisfied for actual physical situations.

The homogeneous (source free) neutron transport equation may be written in the operator form:

$$\frac{\partial N}{\partial t} = -v\Omega\nabla N - \Sigma vN + \iint \Sigma' fv' N' dE' d\Omega' = LN, \qquad (1.27)$$

where L is the transport operator. The boundary condition of no incoming neutrons is assumed. We consider the solution of the equation expressed in the form

$N = N(r,\Omega,E)e^{\alpha t}$ from which $\alpha N(r,\Omega,E) = \boldsymbol{L}N(r,\Omega,E)$. There may exist many eigenvalues α of the operator $\boldsymbol{L}$, represented by α_j with corresponding eigenfunctions N_j:

$$\alpha_j N_j = \boldsymbol{L}\, N_j. \tag{1.28}$$

In practical cases there exist a real eigenvalue greater than the real part of any other eigenvalue. It will be denoted α_0 and the eigenfunction associated with it $N_o(r,\Omega,E)$. If the sign of α_0 is negative the solution of Eq. (1.27) will decrease asymptotically and the system is subcritical. If the sign is positive the solution will tend asymptotically to infinity and the system is supercritical.. More rigorous considerations consisting in applying the Laplace transform lead to the asymptotic solution in the form:

$$N(r,\Omega,E,t) = A\, exp(\alpha_o t)\, N_o\,(r,\Omega,E), \quad \text{as } t\to\infty, \tag{1.29}$$

where A is a constant determined by the initial conditions. Thus, the criticality problem is that of finding the conditions for which $\alpha_o = 0$. A rigorous analysis has shown that for certain conditions (satisfied in practice) on the scattering kernel there is at least one discrete eigenvalue.

The homogeneous neutron transport equation will have a time independent solution when $\alpha_o = 0$ or the system is critical:

$$\boldsymbol{L}N_0 = 0.$$

The criticality problem may be approached by introducing auxiliary characteristic values. In particular, the spectrum of the fission neutrons $\kappa(r,E'\to E)$ we replace by $\kappa(r,E'\to E)/k$, and k can be varied to obtain the stationary solution, with $k = k\text{-}eff$, called effective multiplication factor. This amounts to multiplying the number of neutrons emitted per fission by the factor $1/k\text{-}eff$.

By definition $k\text{-}eff$ is a characteristic value of the equation:

$$v\Omega\nabla N_k + \Sigma v N_k = \iint \sum_{x\neq f} \Sigma^x{}' f^x \nu' N_k{}' d\Omega' dE' + \frac{1}{k_{eff}} \iint \frac{1}{4\pi}\kappa(r; E'\to E)\Sigma^f{}' \nu' N_k{}' d\Omega' dE' \tag{1.30}$$

where the summation over x unequal f refers to collisions other than fission in which neutrons are produced and N_k are eigenfunctions independent of time.

In elementary reactor theory $k\text{-}eff$ is treated as a ratio between the numbers of neutrons in successive generations, with the fission process being regarded as the birth event which separates generations of neutrons.

For a critical system, i.e., when $\alpha_o = 0$ and $k\text{-}eff = 1$, the corresponding eigenfunctions satisfy the same equation, for any other system, however, the two eigenfunctions are different. This can be seen when writing the homogeneous eigenvalue equation in the form:

$$v\Omega\nabla N_{\alpha_o} + (\Sigma + \frac{\alpha_o}{v})\nu N_{\alpha_o} = \iint \Sigma' f\nu' N'_{\alpha_o}\, d\Omega' dE'. \tag{1.31}$$

The term α_o/v appears as an additional absorption and it is sometimes referred to as 'time absorption' (or production).

1.4. Solution of the one-speed transport equation by the spherical harmonics method

1.4.1. Limitation to a time independent one-speed transport equation

The method is demonstrated for the time-independent, one-speed neutron transport equation in plane geometry. It has been shown that the application of the multigroup approach leads to a set of coupled one speed equations and, therefore, the assumption of one speed is not a real limitation of the method.

For a one speed case scattering is a function only of the cosine of the scattering angle, i.e., $\mu_o = \Omega \cdot \Omega'$, where Ω' and Ω are the neutron directions before and after scattering, respectively. A quantity $\Sigma_s(r,\Omega,\Omega')$ is then defined by:

$$\Sigma_s(r,\Omega,\Omega') = \Sigma(r)c(r)f(r;\ \Omega \rightarrow \Omega'), \tag{1.32}$$

which will be referred to as scattering cross section. With this notation the one-speed Eq. (1.26) may be written:

$$\Omega \nabla \Phi(r,\Omega) + \Sigma(r)\Phi(r,\Omega) = \int \Sigma_s(r,\Omega \cdot \Omega')\Phi(r,\Omega')d\Omega' + Q(r,\Omega). \tag{1.33}$$

1.4.2. Choice of geometry

To apply any effective method of solution to the neutron transport equation one has to specify the streaming term given by Eq. (1.21), i.e., to have expressions for the quantity $\Omega \nabla N$ or $\Omega \nabla \Phi$. For that purpose a system of co-ordinates has to be chosen and the geometry defined. The expression can be derived for co-ordinate systems where the position vector r is given in terms of rectangular, spherical, or cylindrical co-ordinates. Two angular co-ordinates are required to specify the neutron direction and these are chosen to be polar and azimuthal angles. Here the method is demonstrated using the simplest possible geometry, i.e., the plane geometry, for which spherical harmonics reduce to Legendre polynomials.

For plane geometry, in which the neutron angular density (for a specific energy) is a function of x and the azimuthal angle, θ, the streaming term can be expressed:

$$\Omega \nabla \Phi = \frac{d\Phi}{ds} = \frac{\partial \Phi}{\partial x}\frac{dx}{ds} = \frac{\partial \Phi}{\partial x}\cos\theta = \mu \frac{\partial \Phi}{\partial x} \tag{1.34}$$

with $\mu = \cos\theta$, where θ is the azimuthal angle corresponding to the direction Ω.

Hence Eq. (1.32) becomes:

$$\mu\frac{\partial\Phi(x,\mu)}{\partial x}+\Sigma(x)\Phi(x,\mu)=\int_0^{2\pi}d\theta'\int_{-1}^{1}\Sigma_s(x,\mu_0)\Phi(x,\mu')d\mu'+Q(x,\mu), \tag{1.35}$$

1.4.3. Expansion of the scattering cross section

The scattering cross section is expanded in Legendre polynomials and associated Legendre functions:

$$\Sigma_s(x,\mu_0)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\Sigma_{sl}(x)P_l(\mu_0) \tag{1.36}$$

and then $P_l(\mu_o)$ is expressed in terms of Legendre polynomials and associated Legendre functions of the directional cosines μ and μ'. The integration over the azimuthal angle is carried out giving:

$$\mu\frac{\partial\Phi(x,\mu)}{\partial x}+\Sigma(x)\Phi(x,\mu)=\sum_{l=0}^{\infty}\frac{2l+1}{2}\Sigma_{sl}(x)P_l(\mu)\int_{-1}^{1}\Phi(x,\mu')P_l(\mu')d\mu'+Q(x,\mu) \tag{1.37}$$

1.4.4. Expansion of the flux

The next step is to represent the angular dependence of the neutron flux as an expansion in terms of Legendre polynomials, $P_m(\mu)$

$$\Phi(x,\mu)=\sum_{m=0}^{\infty}\frac{2m+1}{4\pi}\phi_m(x)P_m(\mu) \tag{1.38}$$

where $\phi_m(x)$ are the expansion coefficients dependent on x. Because of the orthogonality of $P_m(\mu)$ the latter are given by

$$\phi_m(x)=\int\Phi(x,\mu)P_m(\mu)d\Omega=2\pi\int_{-1}^{1}\Phi(x,\mu)P_m(\mu)d\mu\,. \tag{1.39}$$

If the series is truncated after $N+1$ terms, the result is referred to as a P_N approximation.

For $m = 0$, $P_o(\mu) \equiv 1$; hence $\phi_0(x)$ is simply the total flux at x. For $m = 1$, $P_1(\mu) = \mu$ and Eq. (39) gives

$$\phi_1(x)=2\pi\int_{-1}^{1}\mu\Phi(x,\mu)d\mu\,, \tag{1.40}$$

which is the net current at x in the positive direction.

The general form of equations obtained by substituting expansion of Eq. (1.38) into Eq. (1.37) is:

$$(n+1)\frac{d\phi_{n+1}(x)}{dx}dx + n\frac{d\phi_{n-1}}{dx} + (2n+1)\Sigma_n(x)\phi_n(x) = (2n+1)Q_n(x), \qquad (1.41)$$

n=0, 1, 2, ...

where $\Sigma_n(x)=\Sigma(x)-\Sigma_{sn}(x)$ and the expansion coefficients are given by the orthogonality relations:

$$\phi_n(x) = 2\pi \int_{-1}^{1} \Phi(x,\mu)P_n(\mu)d\mu, \qquad (1.42a)$$

$$Q_n(x) = 2\pi \int_{-1}^{1} Q(x,\mu)P_n(\mu)d\mu. \qquad (1.42b)$$

1.4.5. The P_1 approximation

It is easy to see that the first two equations of the system (1.41), for $n = 0$ and $n = 1$ are:

$$\frac{dJ(x)}{dx} + \Sigma_0(x)\phi(x) = Q_0(x), \qquad (1.43a)$$

$$\frac{d\phi(x)}{dx} + 3\Sigma_1(x)J(x) = 3Q_1(x), \qquad (1.43b)$$

with appropriate definitions of $Q_0(x)$ and $Q_1(x)$.

By definition $\Sigma_0(x) = \Sigma(x)-\Sigma_{so}(x)$ and, therefore, is equal to the *absorption cross section* while Σ_1 is the *transport cross section.*.

1.4.6. Diffusion approximation

If the source is isotropic, $Q_1(x) = 0$ and Eq. (1.43b) becomes a so called Fick's law:

$$\phi_1(x) = J(x) = -D\frac{d\phi(x)}{dx}, \qquad (1.44)$$

where $D(x)=1/3\Sigma_1(x)$ is the *diffusion coefficient.*

Equation (1.44) combined with Eq. (1.43a) gives the *diffusion equation*:

$$-\frac{d}{dx}\left[D(x)\frac{d\phi(x)}{dx}\right] + \Sigma_0(x)\phi(x) = Q_0(x) \qquad (1.45)$$

With anisotropic scattering the equivalent equation can be obtained but with the diffusion coefficient defined as

$$D=(3\Sigma_s(1-\mu_0))^{-1}. \qquad (1.46)$$

The quantity $(1-\mu_0)\Sigma_s = \Sigma_{tr}$, is the transport cross section corrected for the first order of anisotropy.

1.5. Multigroup equations

1.5.1. P_l equations

The general form of the P_l equations in the multigroup approximation with the characteristic value introduced in section 1.3 is:

$$\nabla J_g(r) + \Sigma_{0,g}(r)\phi_g(r) = \sum_{g'} \Sigma^s_{g'\to g}(r)\phi_{g'}(r) + \frac{1}{k}\sum_{g'} \nu\Sigma^f_{g'\to g}(r)\phi_{g'}(r)$$

$$\nabla \phi_g(r) + 3\Sigma_{0,g}(r)J_g(r) = 3\sum_{g'} \Sigma_{1,g'\to g}(r)J_{g'}(r)\,; \qquad g,g'=1,2,...,G. \tag{1.47}$$

In Eqs. (1.47) the indices g and g' refer to the group number and represent the energy dependence, while the variable r refers to the spatial dependence.

1.5.2. Diffusion equations

With the same notation the multigroup diffusion equations are:

$$-\nabla D_g(r)\nabla\phi_g(r) + \Sigma_{0,g}\phi_g(r) = \sum_{g'} \Sigma^s_{0.g'\to g}(r)\phi_{g'}(r) + \frac{1}{k}\sum_{g'} \nu\Sigma^f_{g'\to g}(r)\phi_{g'}(r) \tag{1.48}$$

$$g=1,2,...,G,\ g'=1,2,...,G$$

1.6. The B_N approximation

1.6.1. Assumption on the spatial shape of the neutron flux

The method is demonstrated for the time independent neutron transport equation in plane geometry. The basis of the B_N method is that the spatial dependence of the angular flux can be often approximated by a cosine or exponential term. Thus, by assuming spatial distribution independent of neutron energy it is possible to write:

$$\Phi(x,\mu,E) = e^{-iBx}\Psi(\mu,E), \tag{1.49}$$

where B^2 for a bare reactor is the lowest eigenvalue of the wave equation, i.e., $\nabla^2\Phi = B^2\Phi$ with the zero flux boundary condition. For a reflected reactor, B is expected to be a real number in the core and an imaginary number in the reflector.

1.6.2. Expansion of the scattering cross section

If Eq. (1.49) is inserted to the neutron transport equation with scattering cross

section expanded in Legendre polynomials (Eq.(1.37) generalised to the energy dependent case), we get:

$$\Sigma\left(1-\frac{iB\mu}{\Sigma}\right)\Psi(\mu,E)=\sum_{l=0}^{\infty}\frac{2l+1}{2}P_l(\mu)\int\Sigma_l^s(E'\to E)\int_{-1}^{1}\Psi(\mu',E')P_l(\mu')d\mu'\,dE'+\frac{1}{2}F(E), \tag{1.50}$$

where Q(x,μ,E) has been replaced by an isotropic fission source, $\frac{1}{2}F(E)e^{-iBx}$.

1.6.3. Algebraic transformations

Equation (1.50) is divided by $1-(iB\mu/\Sigma)$, multiplied by $P_n(\mu)$, and then integrated to obtain for $n = 0, 1, 2, ...$

$$\Sigma(E)\phi_n(E)=\sum_{l=0}^{\infty}(2l+1)A_{ln}(E)\int\Sigma_l^s(E'\to E)\phi_l(E')dE'+A_{0n}(E)F(E), \tag{1.51}$$

with

$$A_{ln}(E)=\frac{1}{2}\int_{-1}^{1}\frac{P_l(\mu)P_n(\mu)}{1-\dfrac{iB\mu}{\Sigma(E)}}d\mu, \tag{1.51a}$$

$$\phi_n(E)=\int_{-1}^{1}\Psi(\mu,E)P_n(\mu)d\mu. \tag{1.51b}$$

The coefficients A_{ln} can be found by the fact that they satisfy the recurrence relation:

$$\frac{1}{y}(2l+1)A_{j,l}(y)-(l+1)A_{j,l+1}-lA_{j,l-1}=\frac{\delta_{jl}}{y} \tag{1.52}$$

where $y=\dfrac{iB}{\Sigma(E)}$.

Furthermore, $A_{jl}=A_{lj}$ and $A_{00}=\dfrac{\tanh^{-1}y}{y}$.

The set of coupled equations (1.51) can be solved numerically for ϕ_n provided the sum on the right-hand side is truncated. If the series is terminated by assuming $\phi_l = 0$ for $l>N$ the result is the B_N approximation. In practical lattice calculations the most often used is the B_1 approximation.

1.7. Leakage in diffusion approximation

In every realistic reactor system there exists the neutron leakage through the outer boundary. This leakage can be accounted for in an approximate way by applying the

formulas based on the Fick's law. Let us consider in infinitesimal cube defined in Fig.3.

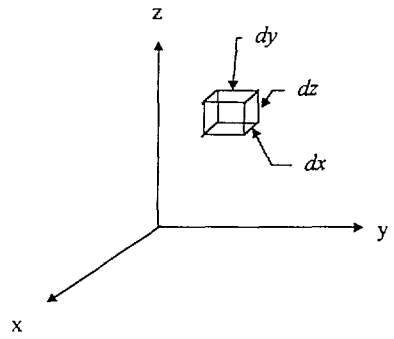

Figure 3: Infinitesimal cube in rectangular co-ordinate system.

Through each of the cube boundaries there exists a neutron flow connected with the net current:

$$J_{net} = J_+ - J_- \tag{1.53}$$

where the components, J_+ and J_-, describe the partial currents in positive and negative directions. Using the definition of the diffusion coefficient introduced in Eqs. (1.44,1.46):

$$J = D \cdot \frac{\partial \phi}{\partial z}$$

$$D = \lambda_{tr}/3,$$

the following formulas can derived for the magnitude of the partial currents in the z direction:

$$\begin{aligned} J_+ &= \frac{\phi}{4} - \frac{D}{2} \cdot \frac{\partial \phi}{\partial z} \\ J_- &= \frac{\phi}{4} + \frac{D}{2} \cdot \frac{\partial \phi}{\partial z} \end{aligned} \tag{1.54}$$

Hence for the z direction:

$$J_z = -D \frac{\partial \phi}{\partial z} = -\frac{\lambda_{tr}}{3} \frac{\partial \phi}{\partial z} \tag{1.55}$$

and

$$\begin{aligned} (J_{z+dz} - J_z)dxdy &= -D\left[\left(\frac{\partial \phi}{\partial z}\right)_{z+dz} - \left(\frac{\partial \phi}{\partial z}\right)_z\right]dxdy = \\ &= -D\frac{\partial^2 \phi}{\partial z^2} dxdydz = -D\frac{\partial^2 \phi}{\partial z^2} dV \end{aligned} \tag{1.56}$$

Similar expressions are obtained for x and y.

The leakage of neutrons out of an arbitrary volume will be composed of those in all partial directions and can be written as $-D\nabla^2\phi$. Assuming the spatial independence of the diffusion coefficient $D(x)=D$ in Eq. (1.45) the diffusion equation can be written:

$$D\nabla^2\phi - \Sigma^a\phi + Q = 0, \tag{1.57}$$

which expresses the neutron balance in diffusion approximation: leakage out of the system plus absorption equals the total sources, Q, including the external as well as internal sources.

2.1. Reactor lattice

2.1.1. A unit cell concept

In thermal reactors fuel is arranged in lumps of rods or plates separated by a material such as graphite, water or heavy water, in which neutrons are slowed to thermal energy with a minimum of capture. The fuel has a cladding separating the fission products from the cooling water. Thus, every thermal reactor, of research as well as of power type, is heterogeneous. The fuel elements are arranged in a regular manner. The cylindrical fuel elements with circular horizontal intersection are arranged in squares (cf.Fig. 4), hexagons or rings. The fuel plates are arranged in parallel bundles. In any case the fuel elements surrounded by moderator (coolant) form a *reactor lattice* which in the first step of reactor calculations is assumed infinite. We speak about the square lattice if fuel elements are arranged in squares, hexagonal if fuel elements are situated in corners of hexagons etc. In any type of reactor lattice we are able to identify a repetitive fragment composed of a single fuel element surrounded by a portion of adjacent moderator. Thus a fictitious boundary is introduced in the middle of moderator dividing the nearest fuel elements. The fuel rod (or plate) with its cladding and adjacent moderator portion form *a unit cell,* as shown in Fig. 4.

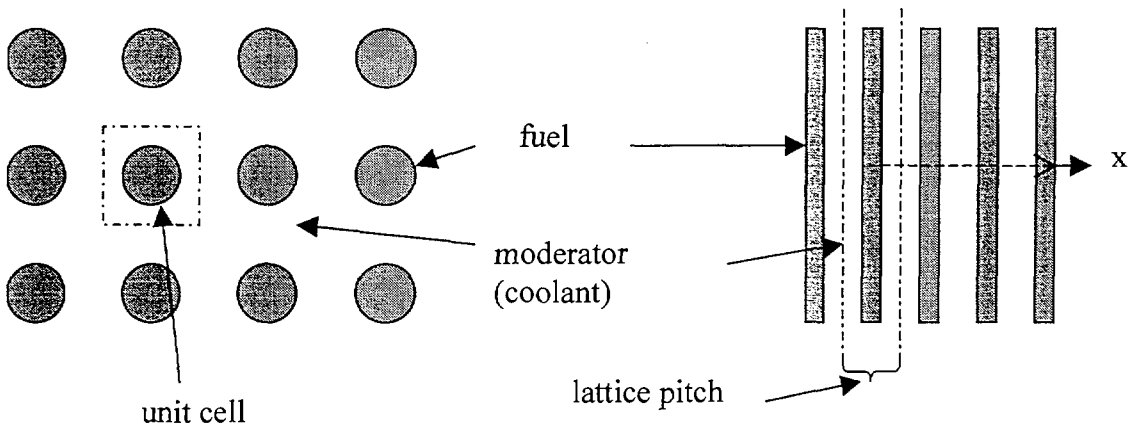

Figure 4: Fragment of a horizontal intersection of a square and plane lattice with a unit cell.

The form of the unit cell depends on the reactor type. For instance a typical unit cell of a PWR type reactor is square with a cylindrical fuel rod in its centre (cf. Fig. 4). The unit cell for TRIGA is most often hexagonal with a cylindrical rod, the MTR unit cell is a fuel plate, cladded on both sides and surrounded by water. Typical shapes of unit cells are shown in Fig. 5.

In the concept of the unit cell it is assumed that such a cell is a repetitive fragment of the large reactor lattice and under this assumption a zero current boundary condition can be imposed on its boundary. The outer boundary of the unit cell, in case of a cylindrical fuel rod, is transformed from the rectangle, hexagon etc. into a cylinder as shown in Fig. 5.

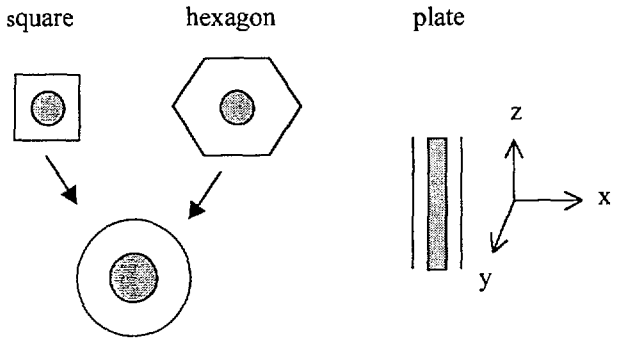

Figure 5: Typical shapes of unit cells.

The transformation of the outer boundary is carried out on the basis of preservation of the volumes of all materials. For a rectangle the outer radius of the equivalent unit cell is $R = a/\sqrt{\pi}$ with a denoting the *lattice pitch* (distance between centres of direct neighbours of fuel rods). The white boundary condition, introduced in section 1.2.3, at the cylindrical unit cell boundary is applied.

In the plate unit cell concept it is usually assumed that the plates are infinite in both y and z directions (cf. Fig.5), which reduces the problem of solution of the transport equation to a one-dimensional one with constant flux (or zero current) boundary condition. With this assumption the plane unit cell does not need to be transformed. Similarly, it is assumed that for a cylindrical unit cell, the cell is infinite in the vertical direction. This again reduces the transport equation to a one-dimensional case in cylindrical geometry.

2.1.2. Definition of a macrocell

Unfortunately, the fuel elements are not the only heterogeneity in the reactor core. In power reactors the fuel elements are combined into fuel assemblies. This is not a serious problem, as the number of fuel elements in the assembly is large enough to assume an infinite lattice of unit cells. The real difficulty is connected with the presence of strongly absorbing control elements. In research reactors besides control elements (plates or rods) there exist other types of heterogeneities as, e.g., various non-multiplying media inserted for irradiation.

To account for various types of strong heterogeneity a concept of a *macrocell* has been created. A macrocell is again a repetitive fragment of the reactor lattice but composed of several unit cells. By 'repetitive' it is understood that a constant flux (zero current) boundary condition is justified at the outer boundary of the macrocell. It is just left to the reactor physicist to decide which region of a given reactor core can be chosen as a macrocell. Typical shapes of macrocells are shown in Fig. 6.

The typical approach applied in reactor macrocell calculations is to solve first the neutron transport equation for a unit cell and then use the obtained results in the second solution of the transport equation over the macrocell. This two-step procedure can be carried out by one code or by two codes with automatic transfer of information. The two steps can use the same method of solution or different methods and/or different

approximations of the neutron transport equation. For instance, in case of a PWR assembly the second step can be carried out for the whole, or a quarter of, the fuel assembly using an improved diffusion theory approximation.

Sometimes for the macrocell the transport equation is solved in a rectangular geometry with the fuel cross section area transformed into a square with volume preservation. In that case there arise doubts if such a change of interface and outer boundary shapes does not introduce an additional error. The effect can be more pronounced for reactors with a large lattice pitch.

In order to clarify this point there have been considered four model cells composed of a homogeneous fuel element region and beryllium moderator with the lattice pitch equal 13 cm. The number densities for the homogenised fuel region are given in Table 2.

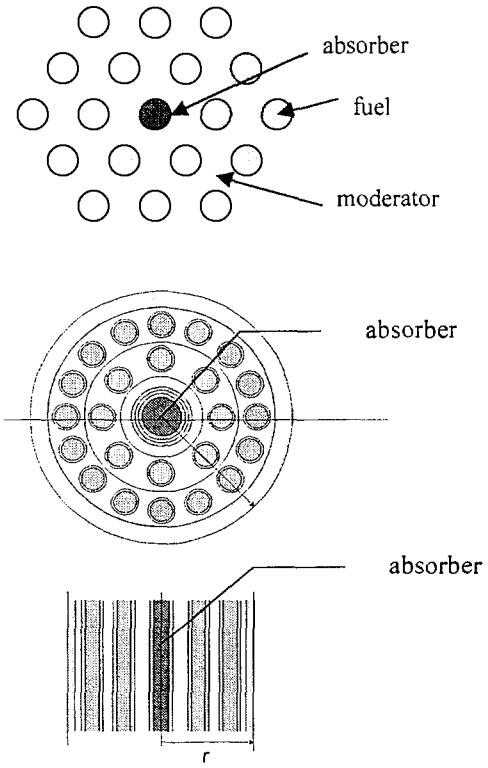

Figure 6: Possible macrocells with fuel rods and fuel plates with an absorber.

Table 2
Number densities of the homogenised fuel region.

Isotope	Number density x 1.0E-24
hydrogen	4.1271E-02
oxygen	2.0638E-02
uranium-235	1.5254E-04
uranium-238	3.7649E-05
aluminium	2.2310E-02

The MCNP-4A [4] calculations have been performed for all the four combinations of square and circular boundary as shown in Fig.7. The first case corresponds to the real geometry of the cell. The second is equivalent to the unit cell geometry, the third to macrocell or whole reactor geometry and the fourth has been added for completeness.

The results are given in Table 3. It may be concluded that the change of geometry from unit cell to square macrocell gives discrepancies of less than 2mk. However, the unit cell geometry introduces approximately 6mk discrepancy as compared to the actual one. Thus, calculations in rectangular geometry are closer to reality due to the error cancellation.

The transport equation over the unit cell should be solved to get the neutron flux distribution and eigenvalue. The diffusion approximation is not recommended here as it can be used only in case of low neutron flux gradients. At the fuel-moderator interface this is never the case, nor it is in the presence of strongly absorbing control elements.

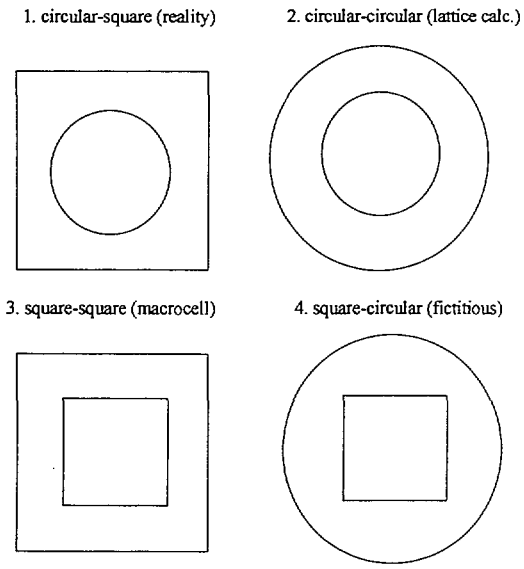

Figure 7: Possible schemes of fuel element and outer cell boundaries.

Table 3
MCNP k-inf values for a cell with homogenised fuel region
with different shapes of interfaces.

No	Type of boundaries	*k-inf*
1	cylindrical-square, reality	1.7090
2	cylindrical-cylindrical, (unit cell)	1.7031
3	square- square, (macrocell or whole reactor)	1.7094
4	square-cylindrical, fictitious	1.7054

2.1.3. Energy dependence

The energy dependence in lattice calculations is treated through the multigroup approach. The number of groups dipends strongly on the actual computer code but with

current computers it usually approaches hundred and, very often, even several thousands of groups are used to treat, eg., the resonance phenomena. However, in the analysis of the physics for a particular type of the reactor lattice it is convenient to distinguish several energy intervals characterised by special physical phenomena:

1. Fast energy region in which the fission neutrons emerge and the neutron energy dependence (spectrum) follows approximately the fission spectrum.
2. The slowing-down region with the energy dependence of $1/E$.
3. Resonance region in which the heavy nuclei exhibit a resonance character.
4. Thermal region where the thermalization of neutrons takes place and both up- and down-scattering of neutrons are possible.

The neutrons are born with energies corresponding to fast energy region. They interact with the medium nuclei and reduce their energy in collisions. Some of these neutrons produce fission as they are slowed down, but in a thermal reactor it happens (by definition) with a rather low probability. The total number of neutrons generated in fission, divided by the number of neutrons produced by the thermal fission is denoted by ε. In a thermal reactor ε slightly exceeds unity.

In the upper energy region where the slowing-down is the main process and no significant number of neutrons emerge from fission, it is convenient to introduce a variable called *lethargy*, related to energy:

$$u = ln(E_{max}/E) \quad \rightarrow \Phi(u)du = -\Phi(E)dE, \tag{2.1}$$

A maximum energy loss of a neutron suffering a collision is:

$$(1-\alpha)E_i \text{ , it is } E_f \geq E_f \geq \alpha E_i$$

where E_i is the initial and E_f final neutron energy, and $\alpha = (A-1)^2/(A+1)^2$, with A being the nucleus mass.

An *average energy loss*, or lethargy gain, *per collision,* ξ, is then defined and using the just introduced quantities can be expressed as:

$$\xi = 1 - \frac{\alpha}{1-\alpha}\ln\alpha \cong \frac{2}{A+\frac{2}{3}}. \tag{2.2}$$

As neutrons slow down through the resonance region, the resonance cross sections change their magnitude dramatically in a small energy interval of few eV. In this energy region special methods are employed in lattice calculations to take into account the rapid changes of the coefficients in the neutron transport equation. The basic quantity for the resonance region is the escape probability which has the meaning of the probability for a neutron to escape the resonance absorption and in the simplified form is equal to:

$$P = exp\ (-(\Sigma^r)_e/(\xi\Sigma^s)) \tag{2.3}$$

with $(\Sigma_r)_e$ the *effective resonance integral,* ξ defined by Eq. (2.2) and Σ_s the macroscopic scattering cross section.

There are several effects that should be taken into account in the resonance region, non-existent or negligible for other energies.

The most important effect is due to the fuel lumping. The neutron born in the fuel rod or plate has to get out of the fuel area to reach the moderator and to get a possibility of collision with its nuclei. On its way to the fuel-moderator interface it can enter into collision with a fuel nucleus and get absorbed. Thus the fuel lumping decreases the probability of neutrons of being slowed down. The probability of absorption in the fuel increases with the fuel dimensions and fuel number density. The effect is called *self-shielding*. The *Bell factor* is introduced, to relate a resonance integral of a lumped fuel to that for fuel and moderator forming a homogeneous mixture.

If a neutron leaves a fuel rod/plate of his birth it can still enter another rod/plate of the lattice without a collision (cf. Fig.4). The *Dancoff factor* is introduced to take into account the fact that the fuel element in the reactor lattice is not isolated. Namely, the resonance integral for the lattice of fuel rods of radius R is the same as that of an isolated fuel pin of radius γR, where γ is the Dancoff factor. It can be also defined [2] as the reduction factor of the fuel escape probability compared to that of an isolated fuel pin when all fuel pins are black. The correction to the resonance escape probability, responsible for this effect, is called the *Dancoff correction.*

Then still there exists a flux depression caused by a resonance and the interference of resonances of different resonance isotopes. The algorithms applied for all these corrections vary for various authors.

The thermal region is the one where the majority of fission reactions take place. It is characterised by existence of upscattering of neutrons as a slow neutron entering into a collision with a nucleus can not only loose but also gain the energy. The thermal neutron flux is a quantity of prime importance in the thermal reactor physics and several quantities are introduced useful for the description of physical properties of various lattices. Some of them are introduced below.

2.1.4. Thermal flux distribution in a unit cell

The neutron thermal flux in the fuel region is always lower than in the moderator because of a high absorption of neutrons by the fuel nuclei. Typical shape of the thermal flux is shown in Fig. 8, where the dotted lines represent the average flux levels in the fuel and in the moderator

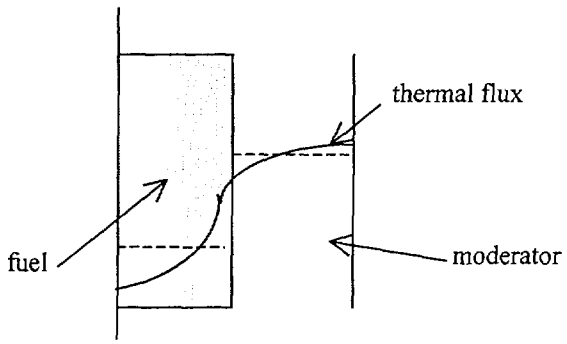

Figure: 8: Thermal flux distribution in a unit cell.

The quantity called *flux disadvantage factor* is used to compare the flux level in the fuel element to the average flux in the fuel cell and is calculated as a ratio of average flux values in the fuel and in the cell:

$$f_{dis} = \frac{\overline{\phi_{fuel}}}{\overline{\phi_{cell}}}. \tag{2.4}$$

2.1.5. *A 'four-factor formula' for the infinite multiplication factor*

In a thermal reactor it is convenient to divide the whole energy region into two parts: the slowing-down energy region, where only down-scattering takes place, and the energy region with up-scattering – the thermal region. The cross sections of any type, x, for each of those energy regions, G, are then understood as averages over respective energy groups, $g \in G$:

$$\Sigma_G^x = \frac{\sum_{g \in G} \Sigma_g^x \phi_g}{\sum_{g \in G} \phi_g}$$

where κ is the number of neutrons per fission. We introduce the number of neutrons per absorption in fuel (denoted by index U)

$$\eta = \frac{\left(\Sigma^f\right)_U}{\left(\Sigma^a\right)_U} \kappa . \tag{2.5}$$

Here the index a denotes the thermal absorption and f – thermal fission

We introduce also a quantity called the *thermal utilisation* factor that is equal to the fraction of all thermal neutrons absorbed that are absorbed in uranium. With the assumption of a negligible absorption in the moderator the thermal utilisation factor is given by a formula:

$$f = \frac{\left(\Sigma^a\right)_U}{\Sigma^a} \tag{2.6}$$

Otherwise Eq.(2.6) has to be multiplied by the fuel disadvantage factor defined in section 2.1.4. Thus, the number of fast neutrons produced by one thermal neutron absorbed in the lattice can be written as ηf. This quantity has to be corrected by the quantity ε to account for a possibility of fission caused by fast neutrons. In thermal reactors ε is very close to unity and is often neglected in rough estimations. The probability that neutrons are not captured during the slowing-down process is labeled p, and called the resonance escape probability defined in section 2.1.3.

Then the number of fission neutrons obtained from one thermal neutron absorbed in the lattice is $\varepsilon \eta f$ and the number of neutrons becoming thermal and ending the neutron generation is

$$k = \varepsilon p f \eta \tag{2.7}$$

This is by definition the infinite multiplication factor, k_∞, as no leakage has been taken into account.

2.1.6. *Neutron leakage and buckling concept*

The neutron cycle in the thermal reactor starts with fission, which proceeds at a rate

$$S = \phi \Sigma^f \kappa , \tag{2.8}$$

Combining Eqs. (2.5 , 2.6, 2.8) the fast source is

$$S = \phi \Sigma^a f \eta .$$

Of the fast neutrons a fraction F, which can be called the fast neutron non-leakage probability, will slow down in the reactor, without escaping from the core and of those the fraction εp will escape the fast and resonance absorption. Thus, of the S fast neutrons only $SF\varepsilon p$ get to thermal, and the resulting thermal source is equal

$$S_{th} = \phi \Sigma^a p \varepsilon f \eta F = \phi \Sigma^a k F \tag{2.9}$$

The diffusion equation derived in Chapter 1 is:

$$D\nabla^2 \phi - \Sigma^a \phi + Q = 0 , \tag{2.10}$$

where for the thermal reactor the source term can be substituted by Eq. (2.9) leading to:

$$D\nabla^2 \phi = \Sigma^a \phi (kF - 1). \tag{2.11}$$

The constants depending on reactor materials are usually grouped into a single one, called the *buckling:*

$$B^2 = \frac{\Sigma^a}{D}(kF - 1) , \tag{2.12}$$

so that Eq. (2.11) simplifies to a form of the so-called wave equation,

$$\nabla^2 \phi - B^2 \phi = 0 \tag{2.13}$$

The flux distribution with position is given by its solution. But to solve this equation it is necessary to select the reactor core shape. In spherical coordinates the general solution is a linear combination

$$\phi = A\frac{\sin Br}{r} + C\frac{\cos Br}{r}, \tag{2.14}$$

where A and C are arbitrary constants to be determined by information on the flux condition at the boundary and the centre of the core. Since an infinite flux is not allowed on physical grounds, C must be equal to zero, leaving

$$\phi = A\frac{\sin Br}{r} . \tag{2.15}$$

A reasonable condition is the flux going to zero at some distance d beyond the core boundary, i.e., at $R' = R+d$. Applying this boundary condition, Eq. (2.15) gives

$$A\frac{\sin BR'}{R'}=0\,.$$

Since R' is finite, A cannot be zero without incurring a meaningful solution, so that $\sin(BR')=0$, $BR'=\pi$, or

$$B^2=\left(\frac{\pi}{R'}\right)^2,$$
$$R=R'-d=\frac{\pi}{B}-d. \tag{2.16}$$

Thus the reactor size is determined by the constant B^2. The buckling from Eq.(2.12) is sometimes referred to as *'material buckling'*, $(B^2)_m$, as it is defined by the material properties of the medium. The expression for B^2 in Eq.(2.16) is usually called the geometric buckling $(B^2)_g$ dependent only on the size and shape of the core. The critical condition can be written as $(B^2)_m = (B^2)_g$.

2.1.7. The boundary with vacuum

It has been mentioned in the previous section that the typical boundary condition, introduced together with the diffusion approximation, is the neutron flux going to zero at some distance from the outer boundary of the system considered. Let us consider an idealised case of an infinite plane reactor core surrounded by vacuum. The distance at which the flux drops off to zero is called then the *extrapolation distance*, and it is shown in Fig. 9.

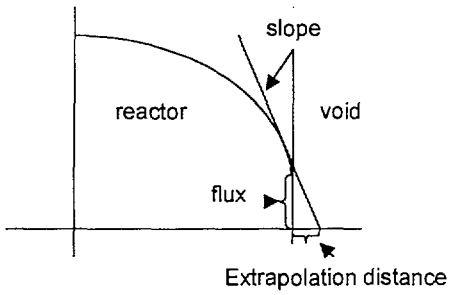

Figure 9: Extrapolation distance.

By diffusion theory, using Eqs. (1.55), the extrapolation distance, d, is found to be equal to:

$$d=\frac{2}{3}\lambda_{tr}\,. \tag{2.17}$$

A calculation based on the transport theory gives approximately:

$$d=-\frac{\phi}{d\phi/dx}=0.71\,\lambda_{tr}\,. \tag{2.18}$$

where λ_{tr} is the transport mean free path.

2.1.8. *Fuel burn-up*

The lattice calculations are made for a steady-state reactor and do not involve the time variable explicitly. Also the coefficients of the transport equation, i.e., the macroscopic cross sections are considered constant in time. But in practice, the slow time evolution has to be included to account for the fuel burn-up.

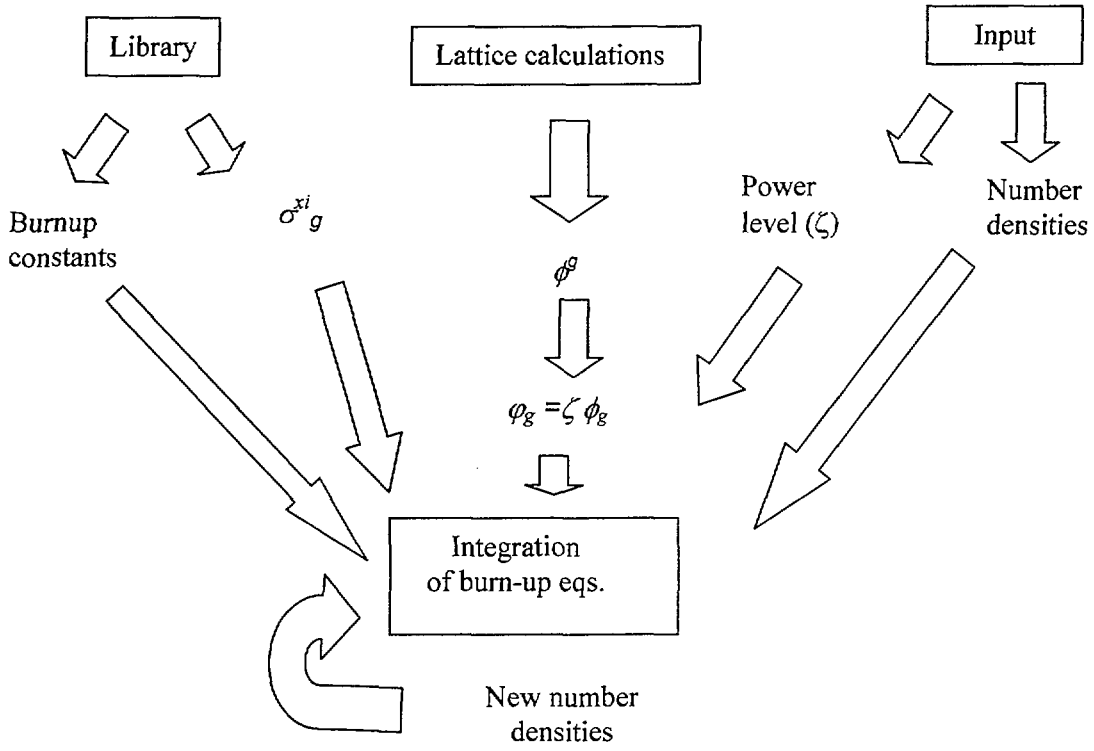

Figure 10: General flow of depletion calculations.

The burn-up changes the number densities, and hence the macroscopic cross sections of the nuclides undergoing the depletion or the build-up process. Thus, the neutron transport equation loses its linearity. To cope with the problem in an efficient way a repetition of the sequence shown schematically in Fig. 10 is applied:

1. Full solution of the transport equation with starting neutron densities or those from 3.
2. Normalisation of the neutron flux to a given power level (ζ – normalisation factor in Fig.10).
3. Solution of the equation for isotopic transformation, establishing new number densities.
4. Calculation of new macroscopic cross sections.
5. Go to 1.

Usually several burn-up steps can be carried out without accounting for the neutron spectrum modification, as shown in Fig. 10. However, after a sufficiently long time the change in macroscopic cross sections gets significant and the repetition of lattice spectrum calculations is necessary. Thus, the flow chart from Fig. 10 has to be repeated many times until the desired burn-up level is reached

In practice, the procedure gets much more complicated to make it more accurate, more efficient or take into account additional phenomena, as e.g., burnable poisons.

2.2. Discrete ordinates method

2.2.1. Discretisation of independent variables

The discrete ordinate method, referenced as S_N [6] or DSN [7], belongs to the most often used numerical methods for solving the steady state neutron transport equation. In this method the finite difference approach is applied in all three independent variables:

1. The multigroup approach is used for the energy dependence.
2. Angular integrals are replaced by sums over discrete directions.
3. Angular derivatives are transformed into finite differences.
4. Discrete space mesh is imposed on the spatial region.
5. Spatial derivatives are transformed into finite diffrences finite differences.

A number of discrete directions is introduced denoted by Ω_m to each of which a weight w_m is associated. Each weight represents a segment $\Delta\Omega_m$ on the unit directional sphere, in stereradians, with the normalisation condition:

$$w_m = \Delta\Omega_m / 4\pi; \quad \Rightarrow \quad \sum_m w_m = 1. \tag{2.19}$$

The subscript m on angular flux (source) means 4π times its value at Ω_m.

The neutron flux and neutron current are approximated by the basic equations of the method:

$$\begin{aligned} \phi_g(r) &= \sum_m w_m \phi_{mg}(r) \\ J_g(r) &= \sum_m w_m \Omega_m \phi_{mg}(r) \end{aligned} \tag{2.20}$$

for g=1,2,.....,G and m=1,2,...,M.

The effective realisation of the method has encountered a set of problems, which had to be solved. The most important of them are:

1. the choice of a particular discrete directions,
2. the approximation of the integrals over the direction variable,
3. the approximation of the derivatives of the neutron angular flux with respect to the components of Ω appearing in the transport equation in curved geometries.

Applying the approximation defined by Eqs. (2.20), to the multigroup neutron transport equations with linearly anisotropic scattering we get:

$$\Omega_m \cdot \nabla\phi_{mg}(r) + \Sigma_{mg}(r)\phi_{mg}(r) = S_{mg}(r) + \frac{1}{k}\chi_g(r)F(r), \tag{2.21}$$

where

$$F(r) = \sum_{g'} \kappa\Sigma^f_{g'}(r)\phi_{g'}(r),$$

$$S_{mg}(r) = \sum_{g'} \Sigma^s_{0,g'\to g}(r)\phi_g(r) + 3\Omega_m \cdot \sum_{g'} \Sigma^s_{1,g'\to g}(r)J_{g'}(r)$$

$$\phi_{mg} = \int_g \phi_m dE; \quad \phi_g = \int_g \phi dE; \quad J_g = \int_g J dE; \quad \chi_g = \int_g \chi dE,$$

$$\kappa\Sigma^f_g = \frac{\int_g \kappa\Sigma^f(E')\phi(E')dE'}{\phi_g},$$

$$\Sigma^s_{0,g'\to g} = \frac{\int_{g'}\int_g \Sigma^s_0(E'\to E)\phi(E')dE'\,dE}{\phi_{g'}},$$

$$\Sigma^s_{1,g'\to g} = \frac{\int_{g'}\int_g \Sigma^s_1(E'\to E)J(E')dE'\,dE}{J_{g'}},$$

There are several possibilities of defining the directional total cross section [6]. The simplest, often chosen definition is:

$$\Sigma_{mg} = \Sigma_g = \frac{\int_g \Sigma\phi dE}{\phi_g}.$$

2.2.2 *The discrete ordinate form of the neutron transport equation*

The streaming term has to be defined, separately for each geometry. In rectangular geometry it is:

$$\Omega\nabla\phi = \mu\frac{\partial\phi}{\partial x} + \eta\frac{\partial\phi}{\partial y} + \varsigma\frac{\partial\phi}{\partial z} \tag{2.22}$$

The spatial mesh is imposed which for a 2-dimensional case, (x,y), is shown in Fig.11.

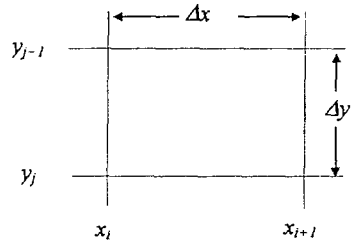

Figure 11. Spatial mesh in (x,y) geometry.

The finite difference equations based on that mesh become:

$$\mu_m \Delta y(\phi_{i+1,m} - \phi_{i,m}) + \eta_m \Delta x(\phi_{j+1,m} - \phi_{j,m}) = V(Q_m - \Sigma\phi_m), \qquad (2.23)$$

where $V=\Delta x \cdot \Delta y$, is the mesh area.

The Gauss quadrature set of directions and weights has been found an adequate choice, but various computer codes use different approaches to particular problems. More information on the method can be found, e.g., in Ref. 7.

2.3 Method of collision probabilities

2.3.1 Probability of a neutron to travel of a distance s without collision

The method of collision probabilities, or more adequately the method of the first flight collision probability, is applied for the solution of the neutron transport equation at least as frequently as the S_N one. Before defining the basic equation solved in this method, two basic quantities are introduced.

Let $\Sigma(E)$ be the total cross section, i.e., the probability of neutron interaction with a nucleus per unit distance, s the distance measured in the direction of the neutron travel, Ω, and $p(s)$ the probability of a neutron to travel of a distance s without collision. Then the decrease of $p(s)$ is:

$$d\,p(s) = -\,p(s)\,\Sigma(E)ds.$$

and hence:

$$p(s) = \exp[-\Sigma(E)s] \qquad (2.24)$$

2.3.2 Escape probability

Let us consider a square unit cell composed of a fuel rod surrounded by moderator.. Neutrons, which escape from the fuel, will be slowed down in the moderator. Let us consider a neutron produced at position $\boldsymbol{r}$ with direction Ω, and let $R(\boldsymbol{r}, \Omega)$ be the distance from the point of the neutron birth to the boundary of the region in the direction Ω. The probability that a neutron will escape from the region without making a collision by Eq. (2.24) is $\exp[-\Sigma(E)R(r,\Omega)]$.

Probability that a neutron will be generated in the direction $d\Omega$ about Ω and position in the volume element dV about $\boldsymbol{r}$ is $(d\Omega/(4\pi))\cdot(dV/V)$. Hence, the escape probability, P_{esc}, for neutrons born in the whole region V is:

$$P_{esc} = \frac{1}{4\pi}\iint exp(-\Sigma(E)R(r,\Omega))d\Omega dV\,. \qquad (2.25)$$

If dimensions of the body are large compared to the mean free path, $1/\Sigma$, then Eq.(2.25) can be approximated by $P_{esc}=1/(4\Sigma V)$. For small bodies P_{esc} must approach unity. A *rational approximation* proposed by Wigner for bodies of all sizes is $P_{esc} = 1/(1+4\Sigma V)$, or with a *mean chord,* $R=(4V)/A$, where A is a surface of the fuel intersection:

$$P_{esc} = 1/(1+\Sigma RA) \qquad (2.26)$$

2.3.3 *Transfer probabilities*

Let us consider now a region divided into a finite number of subregions, as shown in Fig. 12. It is assumed that neutrons are produced uniformly and isotropically in each of these subregions. The problem is then to determine the probability that neutrons born in one of the regions make their next collision in the source region or in one of the other regions.

All the probabilities from Fig. 12 can be calculated as functions of the macroscopic total cross sections and the P_c probability, which is a nonescape probability from an infinite cylinder and has been determined by Case, de Hoffman, Placzek [5]. Thus, under the assumption of constant material properties in each in the subregions, it is possible to calculate the transfer probabilities for all the subregions.

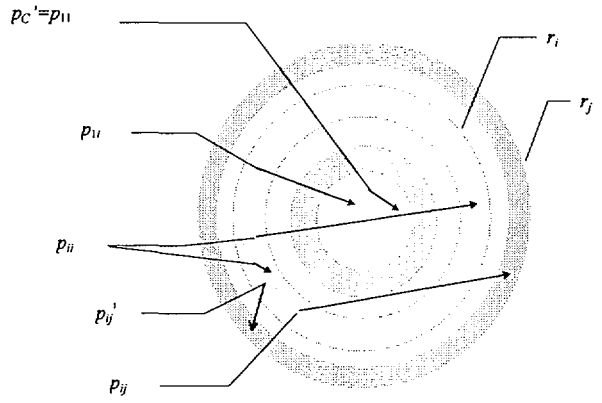

Figure 12: A circular region divided into a set of subregions.

2.3.4 *Equations solved in the collision probability method*

We recall the steady state transport equation in its integral form and with the assumption of isotropic scattering and a constant cross section in the region:

$$\phi(r,E) = \int \frac{e^{-\Sigma(E)R}}{4\pi R^2} \left[- \int \Sigma(r';E' \rightarrow E)\phi(r',E')dE' + Q(r',E) \right] dr',$$

with $R=|\boldsymbol{r}-\boldsymbol{r}'|$.

To this equation the multigroup approach is applied, which allows for substitution of the integral over energy by a sum over groups. Integrating over each subregion volume gives a set of equations, with i,j the region indices and g a group index:

$$\phi_{g,i} = \sum_j \frac{V_j}{V_i} M_{g,ij} \left(\Sigma^s_{g,j} \phi_{g,j} + Q_{g,j} \right), \tag{2.27}$$

where:

$$\phi_{g,i} = \frac{1}{V_i} \int_{V_i} \phi_g(r) dr ,$$

$$Q_{g,i} = \sum_{g'} \left(\Sigma^s_{g'g,i} \phi_{g',i} + \chi_g \frac{\left(\kappa \Sigma^f\right)_{g',i}}{k} \phi_{g',i} \right),$$

and $\mathbf{M}_g$ is a square matrix with the dimension equal to the number of subregions, $\mathbf{Q}_g$ and Φ_g are vectors for each energy group g. $\mathbf{Q}$ is here an energy transfer matrix including also any transfer of neutron energy due to fission.

Hence, with $\mathbf{P}$ the group collision probability matrix averaged over the emission spectrum we get a set of two equations for the emission rate of neutrons produced from all sources in group g:

$$\Psi_{g,i} = \sum_{g'=1}^{G} \mathrm{Q}_{gg',i} \Phi_{g',i} + \mathrm{S}_{g,j} , \tag{2.28a}$$

and for the total collision rate in group g, defined as $\Phi_{g,i} = V_i \Sigma_{g,i} \phi_{g,i}$:

$$\Phi_{g,i} = \sum_{j=1}^{J} P_{g,ij} \Psi_{g,j} \tag{2.28b}$$

These equations are effectively solved on the computer.

More details on both, DSN and Collision Probability methods, can be found in Ref.2.

3. REACTOR LATTICE CODES: WIMSD

3.1. What is a reactor lattice code?

3.1.1. The basic goal of a reactor lattice code in reactor physics computations

A reactor lattice code is used to calculate neutron flux distribution and an infinite medium multiplication factor. It takes as input the multigroup library of isotopic nuclear data and a description of the reactor lattice, and solves the neutron transport equation over a specified region of the reactor lattice. This region may be a unit cell or a macrocell. Therefore, the lattice codes include methods for solving an appropriate set of equations for neutron flux and infinite multiplication factor (*k-inf*) in a discrete energy and spatial mesh (energy groups and discrete spatial points). The calculated neutron flux may be used to get sets of macroscopic cross sections homogenised over chosen subregions and in a chosen broad energy group structure as can be seen in Fig. 13.

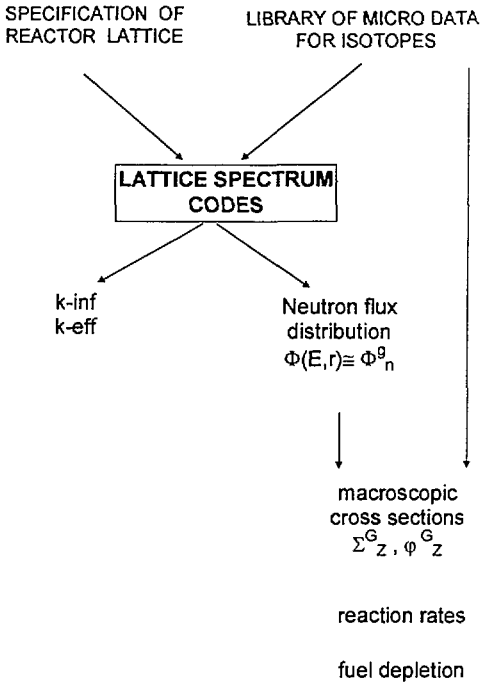

Figure 13: General diagram of the input and output of a reactor lattice code.

Those sets of macroscopic cross sections are then used as material data in the input for various codes solving the neutron transport equation or diffusion equation, over the whole reactor or its fragment. The calculated neutron flux can be also used for reaction rates calculation or in fuel depletion calculations.

3.1.2. Areas of application

Almost any physical arrangement of fissile and neutron absorbing materials can be modelled using Monte Carlo methods and the cost of calculating the effective

multiplication constant (*k-eff*) is more or less independent of the detail of representation. Still there are three principle areas of application of a code based on deterministic grounds [8,9], as shown in Fig. 14:

1. The analysis of experiments, usually critical lattices and usually with measurements of bucklings and reaction rates in specific nuclides.
2. Criticality determination.
3. Power reactor design, assessment and operation.

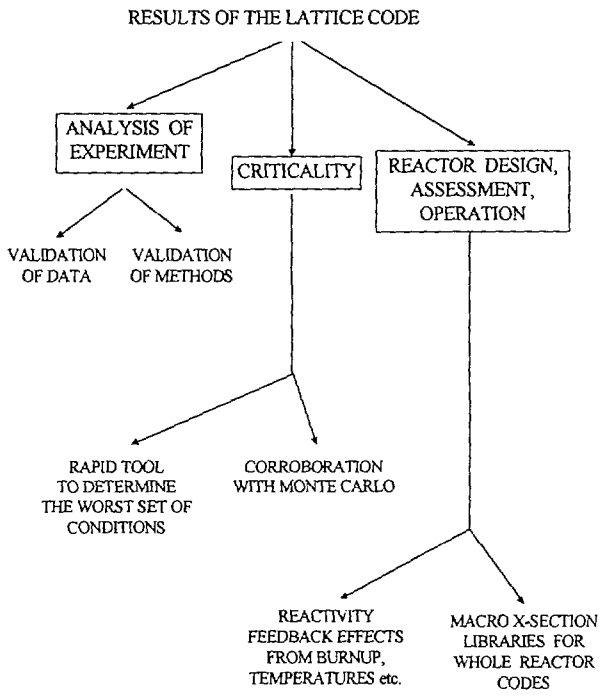

Figure 14: Areas of application of the lattice code results.

The first activity is usually associated with the validation of the data and methods, and is undertaken by the library and code developers. The second one is usually associated with Monte Carlo methods. The lattice code is used here as a rapid tool for determination of the worst set of conditions (e.g., water density, geometrical configuration, moderator to fissile material ratio, temperature effects, enrichment) in safety related analyses. It can be also used as a corroboration of a Monte Carlo calculation to give reassurance that no errors had been made in setting up geometry data. A criticality clearance should not be based on a single calculation.

The third activity is the one where the deterministic methods are the most appropriate. The lattice code is used in calculating fuel depletion and evaluating reactivity feedback effects from burn-up, fuel temperature and density. In this context a lattice code is used in setting up libraries of homogenised cross sections for use by whole reactor codes in fuel management/simulation studies.

3.2. The WIMSD lattice codes

3.2.1. Outline of the algorithm

The WIMSD codes belong to the family of lattice codes called WIMS. The original WIMS code developed by AEE Winfrith [10] has been modified and adjusted to special types of problems through years. There exist a set of commercial versions or versions with restricted distribution. The versions of the code available through the NEA Data Bank belong to the WIMSD class and we limit our description to these versions, namely to WIMSD-4 [11] and WIMSD-5 [9]. Nevertheless the general approach to the solution of the transport equation over a reactor lattice is common for all the WIMS versions.

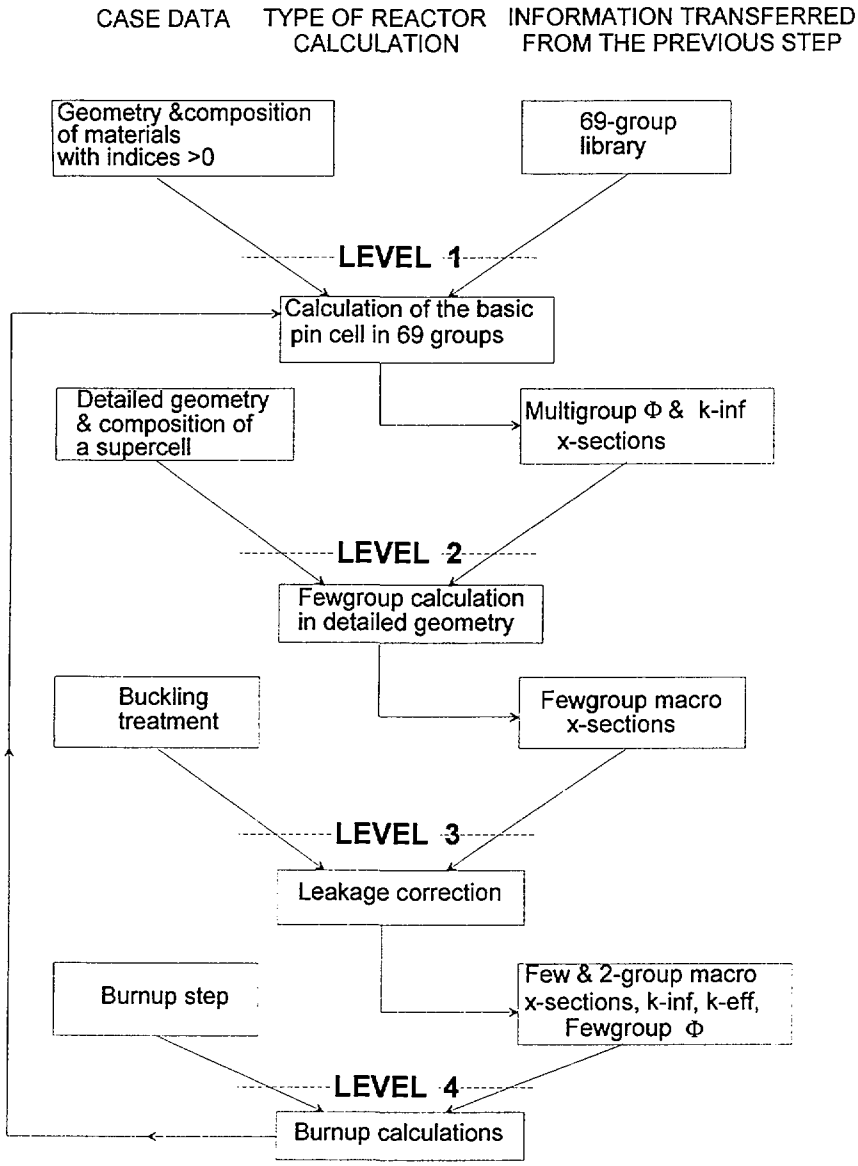

Figure 15: Simplified flowchart of WIMSD calculations.

The final solution of the transport equation in the WIMSD code is obtained in steps in which the energy treatment gets simplified and spatial effects are treated in more detail [9,12]. The general scheme of the WIMS code is presented in Fig. 15 where, on the left hand side the input data needed at each step are shown and on the right hand side the data transferred between the parts of the code are given.

At each step, called 'level' to avoid confusion with burn-up time steps, the transport equation is solved in one of its well-known approximations. However, regions over which the equation is solved differ for different levels.

3.2.2. A unit cell definition in WIMSD

In the first part of calculations (called 'level 1' in Fig. 15) a representative elementary cell with 3 or 4 regions is treated in cylindrical, slab or spherical symmetry. The concept of three- or four-region cell follows the general idea of a 'unit cell' described in section 2.1.1, but in detail it is characteristic for the WIMSD approach. It is referred sometimes as a 'basic', 'representative' or 'pin cell' of the calculated system.

The composition and radii of the representative cell are defined by the data prescribed to materials with corresponding spectral indices through input cards. The user has to define in the input the materials that are treated by the code as fuel (index 1), cladding (index 2), coolant (index 3), and possibly moderator (index 4), respectively (cf. Fig. 16).

All the materials with a given index are mixed together by the code and placed in the appropriate layer of the cylinder (plate or sphere). If the code user wants to exclude a material from calculations of the unit cell a negative spectrum index should be prescribed to this material. This possibility is recommended for a heavy absorber.

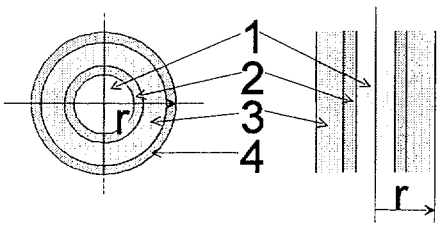

Figure 16: Spatial model of representative elementary cells:
fuel - index 1, can - index 2, coolant - index 3, moderator - index 4.

This definition implies that a tubular fuel element is not treated properly at the unit cell level and special tricks are needed to calculate that type of fuel by the WIMSD code.

For the unit cell the integral neutron transport equation is solved by a collision probability method defined in section 2.3 [13,14]. The flat flux assumption is made for each of the basic 4 regions. The latter has a meaning of treating each of these regions as a separate annulus of Fig. 12. The integral transport equation is solved only up to the coolant region. The bulk moderator region is treated by an approximate technique based on the diffusion theory [13,15]. For that purpose a separate balance equation is built for the moderator region and coupled by the neutron current at the outer boundary of the

coolant region: A negligible absorption in the moderator region is assumed and then the following relations for the currents hold at the coolant - moderator boundary:

$$Q_M = J_{net} = J_{in} - J_{out}$$
$$J_{out} = J_{in}(1 - p_N) + \sum_j \left(\Sigma_j^s V_j + Q_j\right) p_{jN} \tag{3.1}$$

leading to

$$J_{in} = \frac{Q_M}{P_N} + \frac{1}{p_N}\left\{\sum_j \left(\Sigma_j^s V_j \phi_j p_{jN}\right)\right\}, \tag{3.2}$$

where p_{jN} are the transfer probabilities introduced in Fig. 12 of section 2.3, p_N denotes a total collision probability on entry to the moderator region, Q_j is the total source in region j, the index j denoting respectively fuel, canning and coolant and M the moderator.

After the fluxes in regions j = 1,.., 3 have been found from the solution of the integral transport equation[1], the net current J_{net} obtained from Eqs. (3.1, 3.2) is used to find the average flux in the moderator. This is done using the diffusion boundary condition at the coolant – moderator boundary, $r = r_N$:

$$J_{net} = 2\pi r_N D_M \frac{\partial \phi}{\partial r}(r_N, E) \tag{3.3}$$

where the flux derivative is taken at $r = r_N$, and D_M is the diffusion coefficient of the moderator.

In the next step an equation is used formulated independently by G. W. Schaefer, by M. O. Tretiakoff and by D. C. Leslie [10, 15]. As shown by Tretiakoff the formula is the first term in an expansion of the flux in the moderator in a series of so called 'buckling eigenfunctions'

$$\phi(r,E) = \phi(r_N,E) + r_N \cdot \frac{\partial \phi}{\partial r}(r_N,E)\left\{\frac{{r_M}^2}{{r_M}^2 - {r_N}^2} \cdot ln\left(\frac{r}{r_N}\right) - \frac{r^2 - {r_N}^2}{2({r_M}^2 - {r_N}^2)}\right\} \tag{3.4}$$

where r_N is the inner and r_M the outer boundary of the diffusion region. It should be noted that equation (3.4) may represent a rather poor approximation for thin moderator regions [15].

Integrating Eq.(3.4) across the moderator, dividing by the moderator volume and using Eq. (3.3) we get the mean flux in the moderator region:

$$\overline{\phi_M} = \left\{\phi_N + \frac{h(y)}{2\pi} + 3\Sigma^{tr} J_{net}\right\}, \tag{3.5}$$

where $\phi_N = \phi(r_N)$,

[1] The full integral transport equation is solved only for the fuel and coolant regions while for the canning an approximate approach is applied.

$$h(y) = \frac{y^4 \ln(y)}{(y^2-1)^2} - \frac{3y^2-1}{4(y^2-1)}; \qquad y = \frac{r_M}{r_N}.$$

The current is eliminated using Eqs. (3.1, 3.2) combined with the solution in the fuel region. That way a formula is obtained yielding the mean flux in the moderator as a function of the solution for internal regions.

The multigroup flux of 3 or 4 regions of a pin cell is then used to obtain average macroscopic cross-sections for all materials in the few-group structure. The materials with negative indices are averaged over the spectrum calculated for the absolute value of their indices.

Thus, the results of the first 'level' of calculations, referred usually as multigroup calculations consist of

- multigroup fluxes for 3 or 4 regions of a representative cell,
- *k-inf* estimate for the unit cell,
- few-group macroscopic cross sections of all materials.

3.2.3. Approach to resonances

To carry out the effective solution of the integral transport equation for a unit cell the coefficients of equations have to be known. Those are expressed through macroscopic cross sections for respective 3 or 4 media present in the unit cell. The macroscopic cross sections are linear combinations of library microscopic cross sections and number densities of respective isotopes unless the isotope is a resonance one. In that case a special approach is applied to take into account all the effects substantial for the magnitude of the resonance.

The WIMSD library contains resonance integrals for a mixture of a resonance absorber with hydrogen [16]. These resonance integrals are tabulated as functions of potential scattering per absorber atom, σ_p, but in the form:

$$\sigma_b' = \lambda\sigma_p + (N_H / N)\sigma_p, \tag{3.6}$$

corresponding to various values of number densities, N, of the resonance isotope per hydrogen atom. To get a resonance integral for the material with an arbitrary isotopic composition an equivalent potential scattering per absorber atom is obtained:

$$\sigma_b = \sum_i (N_i / N)\lambda_i \sigma_{pi}, \tag{3.7}$$

with i denoting each isotope present in the material.

The values of σ_{pi} are given in the library for all isotopes in each resonance group. The library includes the resonance tabulation for few chosen temperatures and interpolation is performed by the code to take into account the Doppler effect. In the WIMSD-5 version of the code an alternative method for resonance integral interpolation developed by Segev [17] has been included as a separate option.

The actual reactor system is heterogeneous and to define properly resonance integrals for such a system WIMSD uses the approach based on the equivalence principle. It consists in replacement of a heterogeneous problem by an equivalent

homogeneous one. In WIMSD, for the purpose of calculating resonance integrals, the heterogeneous case is considered as equivalent to a linear combination of homogeneous cases. To do that a set of parameters has to be determined based on Bell and Dancoff factors (cf. Section 2.1.3). These can be either calculated in the code or supplied by the user through the input cards.

In the case of macrocell calculations the WIMSD algorithm for Dancoff factor calculations assumes a full isolation of the system defined in input as a macrocell. It means that the Dancoff factor of a macrocell is calculated with an assumption of the lack of outer neighbours for the outermost ring of fuel rods. A similar assumption holds for a system of fuel plates calculated with more than one plate. If, for physical reasons, such an approach is wrong a special option available in the WIMSD-5 version should be applied which ensures Dancoff factors for inner and outer fuel pins to be the same.

The resonance integral of a heterogeneous system I_{het} is calculated as a linear combination of integrals for homogeneous system, I_{hom}, with modified arguments through Bell and Dancoff factors combined with geometrical characteristics of the fuel:

$$I_{het}(I_{hom},\beta)=(1-\beta)I_{hom}(\sigma_b+a/l)+\beta I_{hom}(\sigma_b+(a\alpha)/l) \tag{3.8}$$

where

σ_b - potential scattering cross section in the fuel region,

a - Bell factor,

l - mean chord length of the fuel region,

$$\begin{aligned}\alpha&=\frac{1-\gamma}{a\gamma+(1-\gamma)}\\ \gamma&=\frac{1-D_n}{\beta}\end{aligned}, \tag{3.9}$$

where D_n is the Dancoff factor given in WIMSD input or calculated by the code. Index n=1 corresponds to the Dancoff factor for fuel pins internal in the fuel cluster, n=2 to that for fuel pins from the outermost cluster ring.

$$\beta=\{\prod_{j=2}^{NREG}(1-G_{1j})^2\}/\{\prod_{j=2}^{NREG}(1-G_{j-1,j})^2\}, \tag{3.10}$$

where G_{ij} is a probability that a neutron escaping from region i will suffer a collision in region j.

If slab geometry has been chosen β is taken equal to unity and Eq. (3.8) contains only one term. The Dancoff factor is then expressed through the E_3 Placzek function:

$$G_{ij}=1-2E_3(x_{ij}),$$

where x_{ij} is the optical path of a neutron going through coolant and cladding layers between the fuel plates, and the Placzek function is defined as:

$$E_3(x)=\int_1^{\infty}\frac{\exp(-xu)}{u^3}du, \tag{3.12}$$

and taken with an argument corresponding to a sum of macroscopic total cross sections multiplied by can and coolant widths. For other geometries G_{ij} are calculated by a more complicated algorithm [12].

The general expression for the resonance integral of a cluster composed of N rods (plates) with M rods (plates) in the outer ring (layer) is

$$I_{out}^{cl} = I_{het}^{pin} + \frac{M}{N}(I_{het}^{cl} - I_{het}^{pin}), \tag{3.10}$$

where:

M - number of fuel pins or plates in the outer ring,

N - total number of fuel pins or plates in the cluster,

pin and *cl*- pin cell and cluster indices,

hom and *het* refer to resonance integrals for homogeneous and heterogeneous systems.

The Dancoff factor, if calculated, may be obtained by a default routine [12] or by a subroutine due to Carlvik [18] with an extension for the cladding.

The Bell factor is calculated in the code (if required by the input option) following the formula obtained from Beardwood fit [19]:

$$a = \frac{1.0 + 2.71b}{1.0 + 2.34b}, \tag{3.13}$$

$$b = \frac{0.5D}{(3.2N^{238} + \Sigma_p)r_f},$$

where a is the Bell factor, D - the Dancoff factor, N^{238} - the U-238 number density, Σ_p - the macroscopic potential cross section, r_f - the fuel radius.

3.2.4. Macrocell concept in WIMSD

In the second part of the calculations ('level 2' in Fig. 15) the neutron transport equation is solved once more but in the full geometry described by the user on input cards. The number of groups may be reduced to few groups specified in the input. The coefficients of the transport equation are taken from the results of the previous step. At this level a macrocell can be calculated. The physical model applied as well as the method of solution can be this time chosen by the user. Five geometry models and two numerical methods: DSN [20] or collision probability called PERSEUS [21], are possible here.

The simplest and the most frequently used is the 'cluster' model shown in Fig. 17, where a set of fuel pins (plates) is situated in consecutive rings (layers) with a possibility of an absorber rod (plate), or another type of heterogeneity, in the middle of the macrocell.

The ring(s) of fuel pins may be surrounded by a ring of moderating material. The Dancoff factor for a cluster model is calculated separately for the outermost layer of fuel pins, following Eqs. (3.9-3.10). If the calculated macrocell is used to model a situation without a bulk moderator surrounding the cluster of pins, the code user is responsible for a choice of an option calculating the Dancoff correction for an infinite lattice of fuel pins.

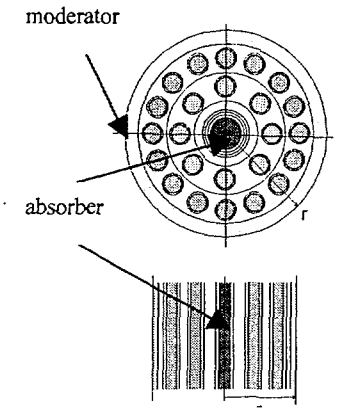

Figure 17: Model of a 'cluster' in cylindrical and plane geometry.

In the cluster model the few-group transport equations are solved by DSN or collision probability method with the application of so called smearing - unsmearing procedure. First the homogenisation of materials inside each ring, specified as annulus in input data, is done. The transport equation is solved over the macrocell composed of a system of homogeneous rings (layers) what allows for a 1D calculation. Then the unsmearing procedure is carried on, on the basis of macrocell few-group fluxes, φ_G, and multigroup fluxes, Φ_g It consists of the following steps:

(i) Condensation of the multigroup flux calculated for each spectrum type L of the unit cell at 'level 1' to the few-group structure:

$$\Phi_{G,L} = \sum_{g \in G} \Phi_{g,L} , \tag{3.14a}$$

(ii) Calculation of the average group flux for each annulus M from the few-group flux distribution calculated at 'level 2' in mesh points m:

$$\overline{\varphi_{G,M}} = \frac{\sum_{m \in M} (\varphi_{G,m} V_m)}{\sum_{m \in M} V_m}, \tag{3.14b}$$

(iii) Calculation of the few-group flux for materials with spectrum indices L and $-L$ contained in volumes V_K of the annulus M:

$$\varphi_{G,L,M} = \frac{\Phi_{G,L}}{\sum_K (V_K \Phi_{G,L})} \overline{\varphi_{G,M}} , \tag{3.14c}$$

Dividing both sides of Eq. (3.14c) by the mean flux in the annulus, $\overline{\varphi_{G,M}}$, we get the disadvantage factor of the materials K with spectrum indices L and $-L$ in the annulus M:

$$f_{G,K,M} = \frac{\varphi_{G,L,M}}{\overline{\varphi_{G,M}}} = \frac{\Phi_{G,L}}{\sum_K (V_K \Phi_{G,L})} \tag{3.15}$$

It is easy to see that the RHS of Eq. (3.15) is independent of the annulus *M*. Thus, the disadvantage factors are the same for all materials to whom the same spectrum index (negative or positive) has been prescribed.

A special option gives a possibility to calculate different multigroup flux and hence different disadvantage factors for pin cells belonging to different annuli. However, there is no possibility of introducing different fuel pins into the same annulus. The smearing - unsmearing process makes impossible a treatment of a strong heterogeneity as one of rods placed in an annulus of fuel pins. In the cluster option an absorber may be put only in the middle of a macrocell. The absorbers placed as one of rods of an annulus require the PIJ option where a two dimensional integral transport equation is solved [22].

Choosing the cluster option the user should remember that the neutron flux calculated at 'level 1' enters the final solution through Eqs. (3.14, 3.15). This flux is calculated from the pin cell, defined in section 3.2.2, and therefore, the proper definition of cross sectional areas of fuel, cladding and coolant materials per one rod is necessary. This requires a careful choice of spectrum type indexes and width of the annuli containing fuel rods.

The geometry models available in WIMSD-4 and WIMSD-5 versions are:

- pin cell representing an infinite lattice of identical cells,
- a cluster given in Fig. 17 with annular regions smeared during transport equation solution, and 'unsmeared' through application of disadvantage factors obtained from multigroup fluxes calculated for a representative cell,
- PIJ - a cluster shown in Fig. 18, with explicit two-dimensional transport solution in (r,θ) geometry, with a possibility of a square macrocell outer boundary,
- PRIZE - the (r-z) calculations introducing a possibility of taking into account an axial nonuniformity of the fuel rod in pin cell calculations, shown in Fig. 19,
- multicell calculations with cells or clusters coupled through input collision probabilities as shown in Fig. 20.

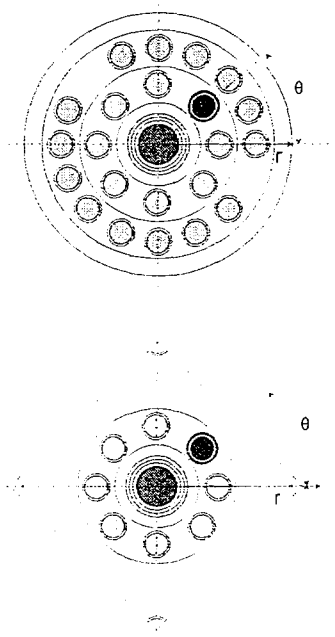

Figure 18. Examples of clusters treated by PIJ- PERSEUS.

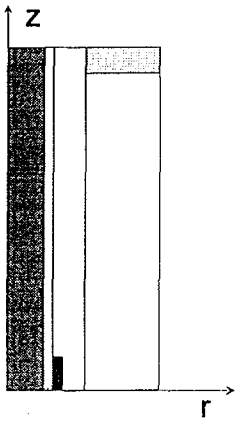

Figure 19. Example of a cell calculated in (r-z) geometry.

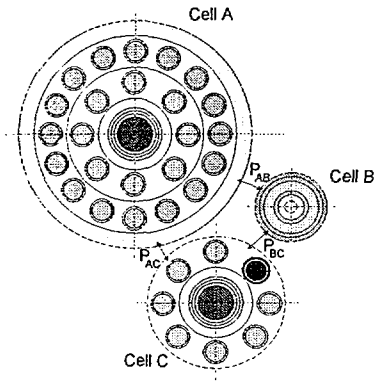

Figure 20. Example of a system calculated as 'multicell'.

It should be stressed that the WIMSD code can be used as well for unit cell calculations giving the homogenised single cell macroscopic cross sections to be used in macrocell calculations carried out by another code. The choice of the approach depends on the actual reactor and purpose of calculations, and as always, should be done by the reactor physicist.

3.2.5. Leakage calculation

Up to now all the results have been obtained in an asymptotic spectrum. The third step of WIMS calculations ('level 3' in Fig.15) introduces a correction for the buckling in both r, and z directions. The bucklings may be given in input. They can be also calculated as critical for a slab system. The slab introduced here is a uniform mixture of all materials present in the system with effective macroscopic cross sections obtained for the infinite medium. Criticality calculations are carried out with the bucklings in the diffusion approximation or in B_1 approximation with the first order correction for anisotropy. The calculation is done in the few-group and two-group structure, In case of the diffusion approximation equations solved for the groups $g = 1,2,...,G$ have the form:

$$\left\{\Sigma_g - \Sigma^s_{0,gg} + D_{g,r}B_r^2 + D_{g,z}B_z^2\right\}\cdot\phi_g = \\ = \sum_{g'\neq g}\Sigma^s_{0,g'g}\phi_{g'} + S^f_g \quad . \tag{3.16}$$

The quantity $\Sigma_g - \Sigma^s_{0,gg}$ describes the absorption and removal in the group g, since it is the total cross sections minus self-catering. The streaming term in Eq. (3.16) has been replaced by buckling multiplied by diffusion coefficients in r and z directions. Thus, the streaming out of the system has been expressed by additional absorption. The group diffusion coefficients, $D_{g,r}$ and $D_{g,z}$ can account for the additional streaming in the z direction if a special option is chosen in the input. The term S^f_g includes the fission source and the multiplication factor of the system:

$$S^f_g = \frac{1}{k_{eff}}\sum_{g'}\nu\Sigma^f_{gg'}(r)\phi_{g'}(r) \tag{3.17}$$

It is, therefore, a *k-eff* calculated with leakage treated in an approximate way through buckling correction. Therefore, the value of *k-eff* is meaningful only if the reactor core is regular enough to be approximated by macrocells defined in the calculations.

In the B_1 approximation Eq. (1.51) from section 1.6.3 is solved in the multigroup approach: The $\Sigma^s_{1,gg'}$ matrices in the standard WIMSD libraries are available only for hydrogen, deuterium, oxygen and graphite. In the special library for TRIGA reactors there exists the $\Sigma^s_{1,gg'}$ matrix for hydrogen in zirconium hydride.

3.2.6. Burn-up calculations

In the next step ('level' 4 in Fig.16) the time dependence is introduced, i.e., the fuel burn-up calculations are performed whose flowchart is given in Fig. 21. The main steps of calculations, namely, the lattice calculations, flux normalisation to the required power level (pt. (iv) in Fig. 21), solution of burn-up equations (pt. (v) in Fig. 21), can be easily distinguished. These points repeat the general diagram of burn-up calculations given in Fig. 10 of section 2.1.8. However, several additional calculations are here included.

The most important feature of the WIMSD burn-up calculations is an internal loop inside which the diffusion equation for a homogeneous mixture of materials is solved (pt. (iii) in Fig 21). It is introduced to save the repetitions of full lattice calculations, which constitute the most time consuming part of burn-up calculations. The change of number densities caused by fuel burn-up affects mainly the absorption macroscopic cross sections of the fuel materials, while the transport cross sections are disturbed very slowly. Using this physical property the inner loop has been constructed inside which only absorption cross sections are changed and instead of full lattice calculations the diffusion equation for a homogenised mixture is solved to correct the neutron flux spectrum. Usually several short steps may be done before the full lattice calculation has to be repeated. This leads to a substantial reduction of the computing time.

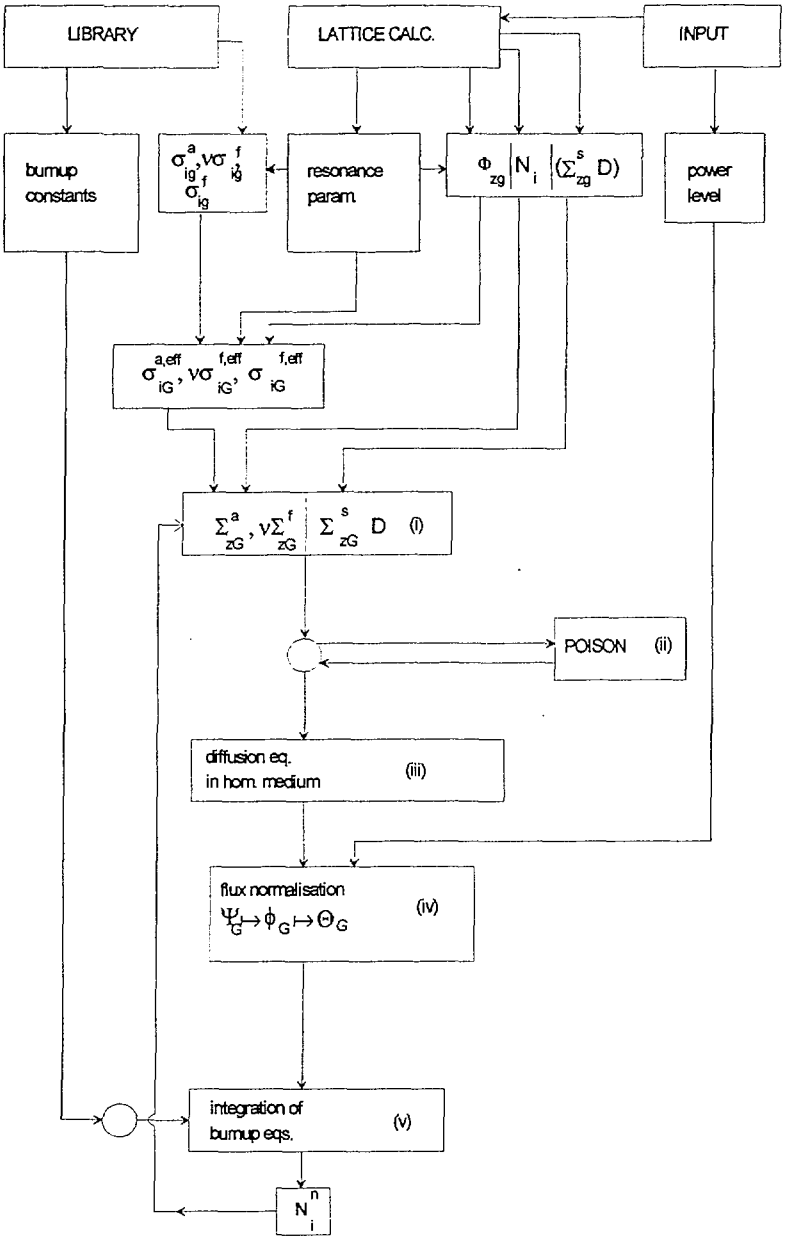

Figure 21: Diagram of WIMSD burn-up calculations.

The few-group fluxes, $\varphi_{G,z}$, (G - the group index in the few-group scheme, z – index of the zone containing material m) calculated in the main transport routine at 'level 2' are used in burn-up calculations. The few-group fluxes are averaged over mesh points l of each zone z:

$$\varphi^T_{G,z} = \frac{\sum_l (\varphi^T_{G,l} V_l)}{\sum_l V_l}, \tag{3.18}$$

where φ^T is the flux calculated in the main transport routine.

Under the cluster option the maximum power densities in cluster are calculated. Inside the loop over burnable materials a search is done for each material m, to be equal to the material of the innermost zone defined in all types of rods in the input data. As a result of this search the number of rods with each material m is calculated. If no rods with material m are found, an error message is printed.

Then the burn-up calculations are entered denoted by (i) through (v) in Fig. 21.

(i) Preparation of macroscopic cross sections.

The macroscopic absorption and production cross sections are recalculated in each short step using the isotopic densities, N, obtained in the previous burn-up step *(n-1)*. For the first step these are number densities used in the last full lattice calculation.

$$\Sigma_G^{x(n)} = \frac{\sum_z \left\{ V_z \varphi_{G,z}^{(n-1)} \left[\sum_i N_m^{i(n-1)} \sigma_{G,m}^{x,i} + \Sigma_{z'}^{a} \right] \right\}}{\sum_z \left(V_z \varphi_{G,z}^{(n-1)} \right)} \tag{3.19}$$

where x denotes the type of cross section: absorption or production, i the isotope index, n – the current number of the short step, G the group index in the few-group scheme and the summation over volumes, V_z, times group flux, is carried out for all zones, z. The first term represents the zones containing the burnable materials and the second the zones z' without the burnable materials for which the constant absorption cross section is added. The second term is not added in calculation of production cross section.

$$\varphi_{G,z}^{(n-1)} = \begin{cases} \varphi_{G,z}^{T} & n-1 \\ \theta_{G,z}^{(n-1)} & n>1 \end{cases}. \tag{3.20}$$

with φ^T coming from Eq. (3.18) and $\theta^{(n-1)}$ from the previous step solution expressed by Eq. (3.29).

The total flux is calculated as:

$$\varphi_G^c = \sum_z V_z \varphi_{G,z}^{(n-1)} / V_c, \tag{3.21}$$

where $V_c = \sum_z V_z$ with z –a zone index, is the total volume.

(ii) POISON option.

If the burnable poisons are present in the reactor the time steps have to be much shorter than for the fuel because of strong flux variation at the burnable poison boundary. A special possibility has been introduced (pt. (ii) in Fig. 21) that allows for a solution of the transport equation in the short time steps for the burnable poison cell surrounded by a homogeneous mixture of fuel 'paste' [11]. It is assumed that the flux in the paste region is invariant from one homogeneous flux solution to the next. This is a simplifying assumption allowing for treating the term with the paste flux as a constant source in the transport equation solved for the pin with the burnable absorber. This feature of the WIMSD algorithm allows again for less frequent repetition of full lattice calculations.

(iii) Solution over the homogenised system:

The few-group diffusion equations for a homogeneous medium with cross sections, calculated in (i) (absorption and production) and taken from the main transport routine (scattering), is solved in each short burn-up step.

$$\left\{\Sigma_G^{a(n)} + \sum_{G'\neq G}\Sigma_{GG'}^{s}\right\}\phi_G^{(n)} + D_G\left(B^2 + \lambda\Delta B^2\right)\phi_G^{(n)} = \\ = \sum_{G'\neq G}\Sigma_{G'G}^{s}\phi_G^{(n)} + (\rho + \lambda\rho')\chi_G\sum_{G'}\kappa_{G'}\Sigma_{G'}^{f(n)}\phi_{G'}^{(n)} \quad : \tag{3.22}$$

Equation is solved for the neutron group flux ϕ_G in the infinite medium and for the parameter λ. The previous notation has been kept for cross sections. The additional parameters depend on the input option:

- If $\Delta B^2 = 0$ in input then $\rho = 0$, $\rho' = 1$, and the equation is solved for $\lambda = 1/k\text{-}eff$ and neutron group flux $\phi_G^{(n)}$ in the n-th short step and all groups G. Leakage is then described by the input B^2 times the diffusion coefficient in group G. In particular, if $B^2 = 0$ there is no leakage and the calculated *k-eff* is really *k-inf*.
- If $\Delta B^2 > 0$ then $\rho = 1$, $\rho' = 0$ and a search for λ is carried out leading to the new value of the buckling equal $B^2+\lambda\Delta B^2$ which ensures *k-eff* = 1.

Thus, in the first case a flux spectrum corresponding to a given leakage, expressed through the input buckling, is found. In the second case the flux spectrum for a critical system is calculated.

The flux $\phi^{(n)}$ from Eq.(3.22) is then normalised to the total flux from Eq. (3.21) and then multiplied by the flux from Eq. (3.20):

$$\varphi_{G,z}^{(n)} = \varphi_{G,z}^{(n-1)}\frac{\phi_G^{(n)}}{\varphi_G^c}. \tag{3.23}$$

(iv) Flux normalisation.

First the fission reaction rate is calculated:

$$\{RR\}^{f(n)} = \sum_i\sum_{m,z}\left[V_z N_m^{i(n-1)}\sum_G\left(\sigma_{G,m}^{f,i}\varphi_{G,z}^{(n)}\right)\right] \tag{3.24}$$

where all indices have the previous meaning, i.e., i – isotope, G – group in few-group scheme, *(n)* –burn-up step, m – burn-up material index, and the summation for each material is carried out for all zones containing this material.

The mean energy per fission is calculated as

$$E^{(n)} = \frac{\sum_i\left\{\varepsilon^i\sum_{m,z}\left[V_z N_m^{i(n-1)}\sum_G\left(\sigma_{G,m}^{f,i}\varphi_{G,z}^{(n)}\right)\right]\right\}}{0.6025\cdot 1.6\cdot 10^{-13}\{RR\}^{(n)}} \tag{3.25}$$

where ε^i is the energy release per fission for isotope i.

The formula (3.25) is a modification introduced to WIMSD-4 by Aragones and Ahnert [23,24] which gives the energy release per fission in MeV/fission.

The isotopic content of fissionable material in the fuel is calculated as a number of grams of fissionable isotopes in the height of 1 cm of the cell or macrocell considered multiplied by the Avogadro number. It can be:

(A) calculated at the first entry into the code according to the formula:

$$c = \sum_{m,z} \left\{ V_z \sum_i N_m^{i(0)} A^i \right\} \tag{3.26}$$

where A^i- atomic weight of isotope i read from the library and the summation is taken over burnable materials m and for each material over zones containing that material.[2]

(B) if the input card FUEL -1 is present, the value of c is calculated from Eq. (3.26) in each burn up step using the actual number densities $N_m^{i(n-1)}$.

(C) if an input card FUEL c, $c>0$ is present, this value of c is used instead of the one calculated by Eq. (3.26).

In cases (A) and (C) the value of c is printed under the name 'initial inventory'. In any case the value c is used to get the flux level. For that purpose the power in the n-th burn-up step, $P^{(n)}$, is calculated on the basis of last number densities and fluxes:

$$P^{(n)} = \frac{1}{c} \sum_i \left\{ \varepsilon^i \sum_{m,z} \left[V_z N_m^{i(n-1)} \sum_G \left(\sigma_{G,m}^{f,i} \varphi_{G,z}^{(n)} \right) \right] \right\}, \tag{3.27}$$

where the previous convention on summation over materials m and zones containing those materials holds.

Hence the normalisation factor, ζ, is obtained as

$$\zeta^{(n)} = \frac{P^{(0)}}{P^{(n)}}, \tag{3.28}$$

where $P^{(0)}$ is the power defined in input data. The factor ζ is then used for flux normalisation. In case of required normalisation to a given power the normalisation is carried out following the formula:

$$\theta_{G,z}^{(n)} = \varphi_{G,z}^{(n)} \zeta^{(n)} \tag{3.29}$$

(v) Integration of burn-up equations:

Integration of burn-up equations for each material m and isotope i is done by trapezoidal method with the burn-up equation written in the form:

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[2] Since all zone volumes V_z are calculated, as sums over $(r_{l+1}^2 - r_l^2)$ for curvilinear and as $(r_{l+1} - r_l)$ in plane geometry, with r_l the distance to the l-th layer of the cell or macrocell from its centre, the factor π is missing in Eq. (3.26) in cylindrical and spherical geometry.

$$\frac{dN_m^i(t)}{dt} = -(\lambda^i + \{RR\}_m^{a,i})N_m^i(t) + \sum_k q_m^{i,k'}(t)N_m^k(t) = \sum_k q_m^{i,k}(t)N_m^k(t), \quad (3.30)$$

where λ^i is the decay constant of nuclide i, $\{RR\}^{a,i}$ is the absorption reaction rate of nuclide i, and coefficients q^{ik} and $q^{ik'}$ are expressed through yields of fission products i from fission of nuclide k, production fractions, capture and fission reaction rates. Solution of Eq. (3.30) gives the number densities of all isotopes i in the current step n.

In WIMSD-5 several additional possibilities have been introduced for burn-up calculations [9,25].

3.3. Results of lattice calculations

3.3.1. Types of lattice code results

The direct results of the solution of the neutron transport equation are *k-eff* or *k-inf* and the neutron flux. in as many energy groups as they were used in the calculation and in mesh intervals applied in the numerical solution.

These results can be then used in secondary calculations to deliver other needed quantities. Secondary quantities calculated from the multiplication factors are the reactivity effects of various types: temperature reactivity coefficients, effects of lattice pitch dimensions, burnable absorber number densities, etc.

The effective multiplication factor, if given in the results, may be only a rough approximation of this quantity. The result based on the buckling approach can be reasonable only if the reactor is of a very regular shape, and surrounded by a homogeneous reflector (no dry lattice above the critical stand).

The neutron flux is used in calculations of r*eaction rates.* They can be calculated directly from the regional neutron flux and cross sections.

Reaction rates are usually defined for a reaction of type x, where x can be absorption, fission or production, as:

$$\{RR\}_g^x = \frac{\sum_{i,z} V_z \sigma_g^{x,i} \varphi_{g,z}}{\sum_z V_z} \quad (3.31a)$$

and are effectively calculated as finite sums over materials and isotopes. The physical meaning of definition of Eq. (3.31a) is the number of interactions of type x per unit volume. The reaction rates may be calculated for a chosen isotope (i.e., without the summation over i) or for reactions caused by all isotopes present in the chosen material. They are usually calculated for a chosen energy interval, e.g., for the thermal region.

Sometimes a different definition is applied based on microscopic cross sections. In the WIMSD code *reaction rates* $\{RR\}^{x,i}_z$ in group g for isotope i, in the cell material or cell zone z, and for reaction of type x are calculated as:

$$\{RR\}_{g,M}^{x,i} = \frac{\sum_z V_z \sigma_g^{x,i} \varphi_{g,z}}{\sum_z V_z}. \tag{3.31b}$$

The quantity based on macroscopic cross sections is then called the *number of reactions* of a given type x, in group g for isotope i, and is defined as

$$\{RR\}_g^{x,i} = \sum_z N_z^i V_z \sigma_g^{x,i} \varphi_{g,z}, \tag{3.32}$$

with a sum taken over regions z containing the isotope i, with the number density N_z^i.

3.3.2. Homogenisation of macroscopic cross sections

The most important secondary results of the reactor lattice calculations are the macroscopic cross sections for use in calculations of the whole reactor. These cross sections have to be given in a smaller number of energy groups than that used in lattice calculations and in homogenised regions. Thus, the problem of homogenisation is met.

The conditions to preserve important characteristics of the reactor can be formulated through the following two equations [26]:

$$\int_{V_i} \overline{\Sigma_g^x}(r)\overline{\phi_g}(r)dr = \int_{V_i} \Sigma_g^x(r)\phi_g(r)dr \tag{3.33a}$$

$$-\int_{S_i^k} \overline{D_g}(r)\nabla\overline{\phi_g}(r)dS = \int_{S_i^k} J_g(r)dS \tag{3.33b}$$

where g=1,2,...,G is the energy group index, x = *tot, a, f,* is the cross section type index, r the spatial variable, ϕ denotes the neutron flux, D denotes the diffusion coefficient, J - the neutron current, S_{ik} is the k-th surface of the i-th region, and the variables of a homogenised cell are denoted by a bar.

Since all homogenised parameters are assumed to be spatially constant within each i-th region, the homogenised parameters can be rigorously defined:

$$\overline{\Sigma_{g,(i)}^x} = \frac{\int_{V_i} \Sigma_{g,i}^x(r)\phi_g(r)dr}{\int_V \overline{\phi_g(r)dr}}, \tag{3.34a}$$

$$\overline{D_g^{(i)}} = -\frac{\int_{S_i^k} J_g(r)dS}{\int_{S_i^k} \overline{\nabla\phi_g(r)dS}}. \tag{3.34b}$$

The difficulties are seen from the last two equations: an a priori knowledge of the integrated reaction rates and net currents for each cell is required. The flux shape

resulting from the use of the homogenised constants must also be known. Thus a nonlinearity is introduced into the process of evaluation of homogenised constants. Additionally Eq. (3.34b) must be valid for all surfaces, k, of the region i. If continuity conditions of scalar flux and net current are imposed on all surfaces, Eq. (3.34b) will define values of diffusion coefficients which are different for each surface. Hence, an effective procedure requires an approximation and the most commonly employed procedures for determining homogenised parameters relax the conditions for which the quantities of interest are preserved:

The numerators of Eqs. (3.34) are approximated by performing a cell lattice calculation for each distinct cell type in the reactor. The equality of integrals over detailed and averaged fluxes is assumed:

$$\int_{V_i} \overline{\phi}(r)dr = \int_{V_i} \phi(r)dr \tag{3.35}$$

This relationship is not automatically satisfied since none of the homogenised regions in realistic reactors satisfies the white boundary condition for which the heterogeneous flux shape is computed. Thus, Eq. (3.34) has to be understood as an approximation.

The homogenised diffusion coefficients can be defined such that:

$$\frac{1}{\overline{D_{g,i}}} = \frac{\int_{V_i} \frac{1}{D_g(r)} \phi_g(r)dr}{\int_{V_i} \phi_g(r)dr}, \tag{3.36}$$

while for all other types of cross sections the formula is assumed:

$$\overline{\Sigma^x_{g,i}} = \frac{\int_{V_i} \Sigma^x_g(r)\phi_g(r)dr}{\int_{V_i} \phi_g(r)dr}. \tag{3.37}$$

In practical calculations the cell/macrocell region is composed of several subregions for which the average flux is computed. The integrals in Eqs. (3.36, 3.37) are changed into sums over subregions $j \in i$

$$\frac{1}{\overline{D_{g,i}}} = \frac{\sum_{j \in i} \frac{1}{D_{g,j}} \phi_{g,j} V_j}{\sum_{j \in i} \phi_{g,j} V_j}, \tag{3.38}$$

$$\overline{\Sigma^x_{g,i}} = \frac{\sum_{j \in i} \Sigma^x_{g,j} \phi_{g,j} V_j}{\sum_{j \in i} \phi_{g,j} V_j}. \tag{3.39}$$

Homogenised parameters determined by making the approximation defined by Eqs. (3.36-3.39) are generally referred to as flux-weighted constants and have been used in standard lattice spectrum codes. The conventional diffusion theory, using this approximation cannot exactly reproduce all integral reaction rates, average fluxes in each cell and the averaged fluxes and currents at the interfaces. To adjust a diffusion theory solution to all these physical quantities additional degrees of freedom must be introduced [26]. The assumption given by Eq. (3.36) is the most inaccurate one and its improvements are dated even over 20 years ago. The modern homogenisation methods are based on the postulate that the integral reaction rates, average fluxes and average leakage are conserved. Various approaches have been proposed, some of them being already implemented into reactor code systems.

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