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13 March - 14 April 2000

Reactor Lattice Codes

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The

ABDUS SALAM
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1. What is a reactor lattice code?

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. 1.

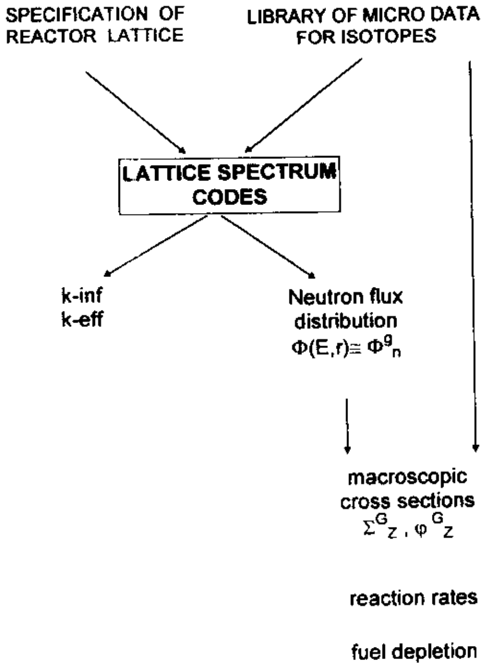

Figure 1: General diagram of the input and output of a reactor lattice code.

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.

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 [1,2], as shown in Fig. 2:

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.

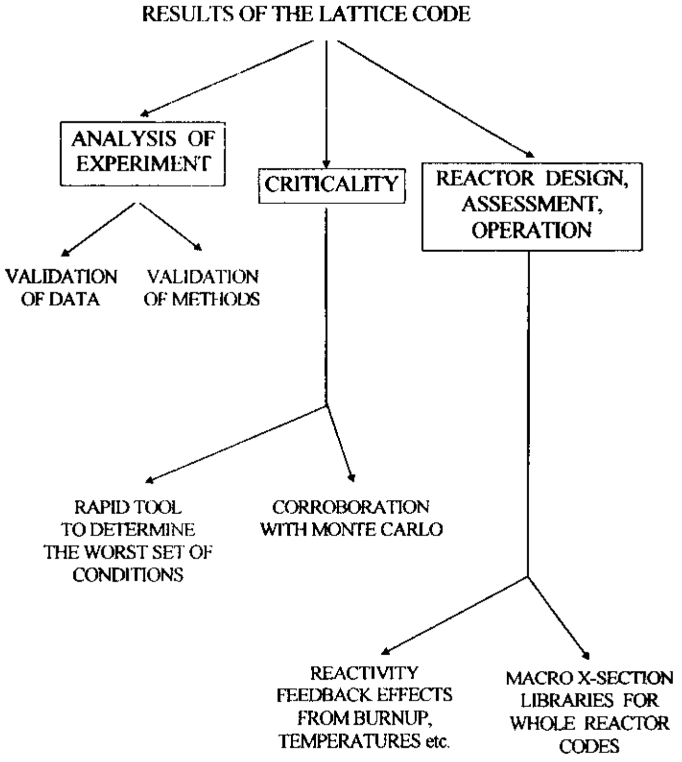

Figure 2: Areas of application of the lattice code results.

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.

2. The WIMSD lattice codes

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 [3] 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 [4] and WIMSD-5 [2]. Nevertheless the general approach to the solution of the transport equation over a reactor lattice is common for all the WIMS versions.

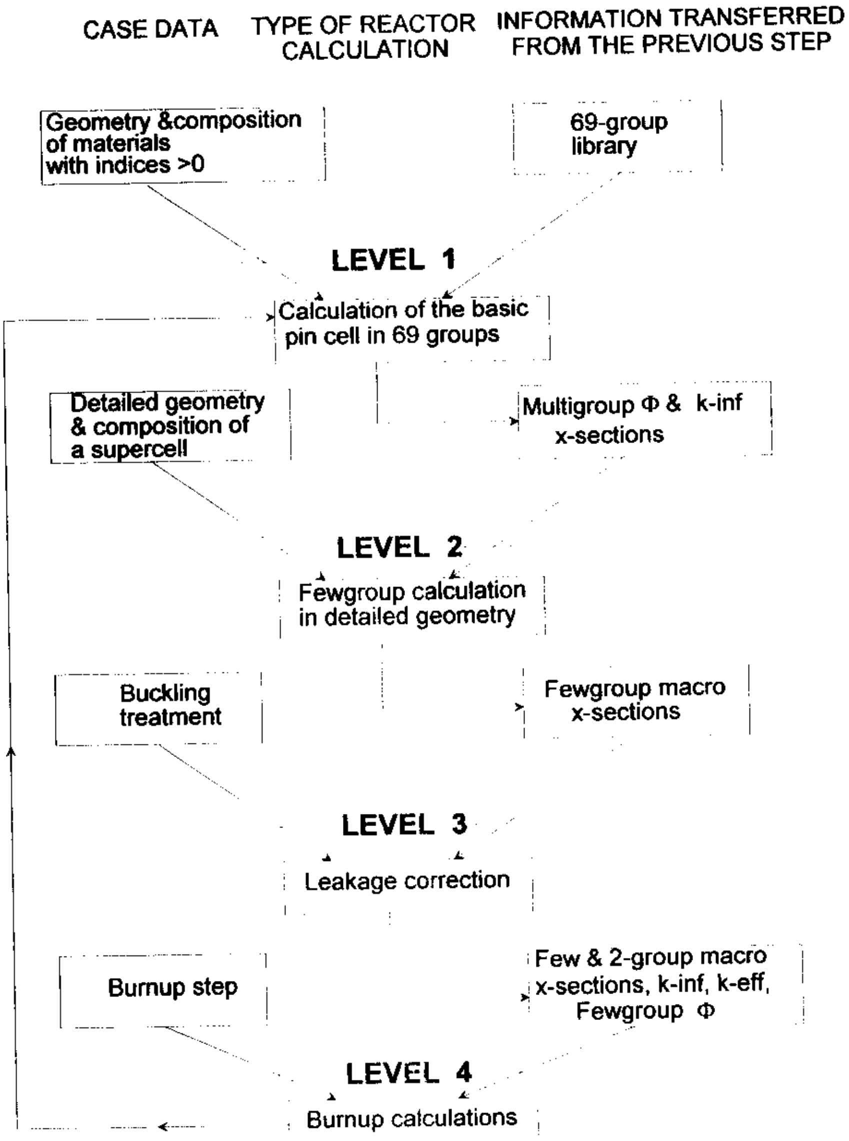

Figure 3: Simplified flowchart of WIMSD calculations.

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 [2,5]. The general scheme of the WIMS code is presented in Fig. 3 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.

2.2. *A unit cell definition in WIMSD*

In the first part of calculations (called 'level 1' in Fig. 3) 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 1.1 of "Reactor Lattice Transport Calculatiios", 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. 4).

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.

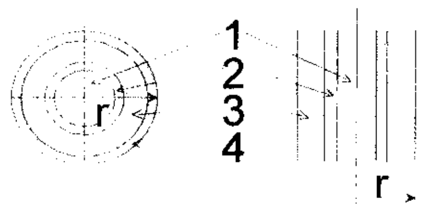

Figure 4: Spatial model of representative elementary cells:
fuel - index 1, can - index 2, coolant - index 3, moderator - index 4.

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 3 of "Reactor Lattice Transport Calculations" [6,7]. 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. 9 of "Reactor Lattice Transport Calculations". 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 [6,8]. 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:

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

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. 9 of section 3 of “Reactor Lattice Transport Calculations”, 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 [3,8]. 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 [8].

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.

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 [9]. 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 [10] 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 1.3 of of "Reactor Lattice Transport Calculations"). 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,

$$\alpha=\frac{1-\gamma}{a\gamma+(1-\gamma)}, \qquad \gamma=\frac{1-D_n}{\beta} \tag{3.9}$$

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.

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

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:

$$E_3(x)=\int_1^{\infty}\frac{\exp(-xu)}{u^3}du, \tag{3.11}$$

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 [5].

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

$$I_{out}^{cl} = I_{het}^{pin} + \frac{M}{N}(I_{het}^{cl} - I_{het}^{pin}), \tag{3.12}$$

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 [5] or by a subroutine due to Carlvik [11] 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 [12]:

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

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

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.

2.4. *Macrocell concept in WIMSD*

In the second part of the calculations ('level 2' in Fig. 3) 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 [13] or collision probability called PERSEUS [14], are possible here.

The simplest and the most frequently used is the 'cluster' model shown in Fig. 5, 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.

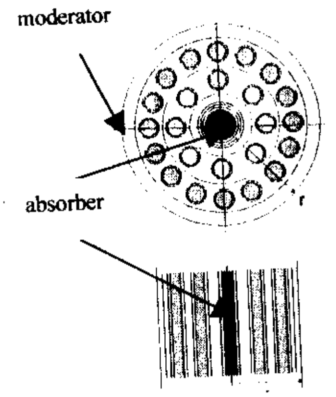

Figure 5: Model of a 'cluster' in cylindrical and plane geometry.

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:

$$\mathrm{f}_{G,K,M} = \frac{\varphi_{G,L,M}}{\overline{\varphi_{G,M}}} = \frac{\Phi_{G,L}}{\sum_{K} (V_K \Phi_{G,L})} \tag{3.15}$$

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 [15].

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 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. 5 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. 6, 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. 7,
- multicell calculations with cells or clusters coupled through input collision probabilities as shown in Fig. 8.

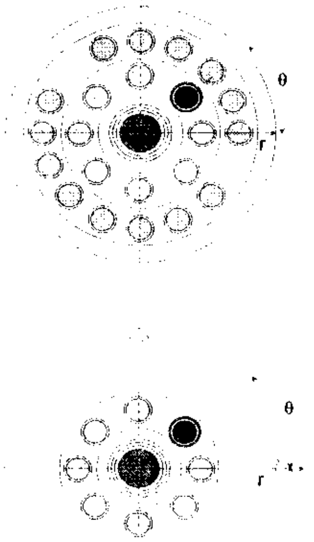

Figure 6. Examples of clusters treated by PIJ- PERSEUS.

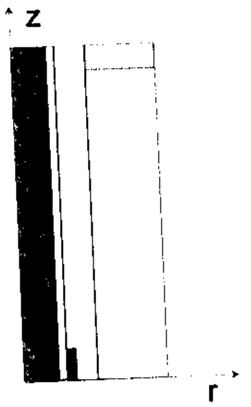

Figure 7. Example of a cell calculated in (r-z) geometry.

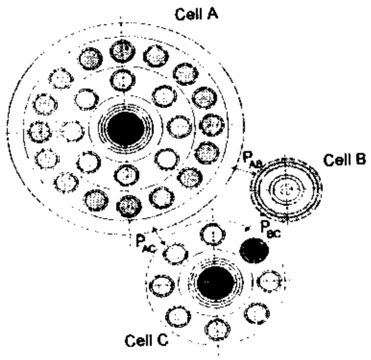

Figure 8. Example of a system calculated as 'multicell'.

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.

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.3) 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:

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

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_g^f includes the fission source and the multiplication factor of the system:

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

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 6.3 of "Introduction to the Neutron Transport Phenomena" 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.

2.6. *Burn-up calculations*

In the next step ('level' 4 in Fig.4) the time dependence is introduced, i.e., the fuel burn-up calculations are performed whose flowchart is given in Fig. 9. The main steps of calculations, namely, the lattice calculations, flux normalisation to the required power level (pt. (iv) in Fig. 9), solution of burn-up equations (pt. (v) in Fig. 9), can be easily distinguished. These points repeat the general diagram of burn-up calculations given in Fig. 7 of section 1.8 of of "Reactor Lattice Transport Calculations". 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 9). 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.

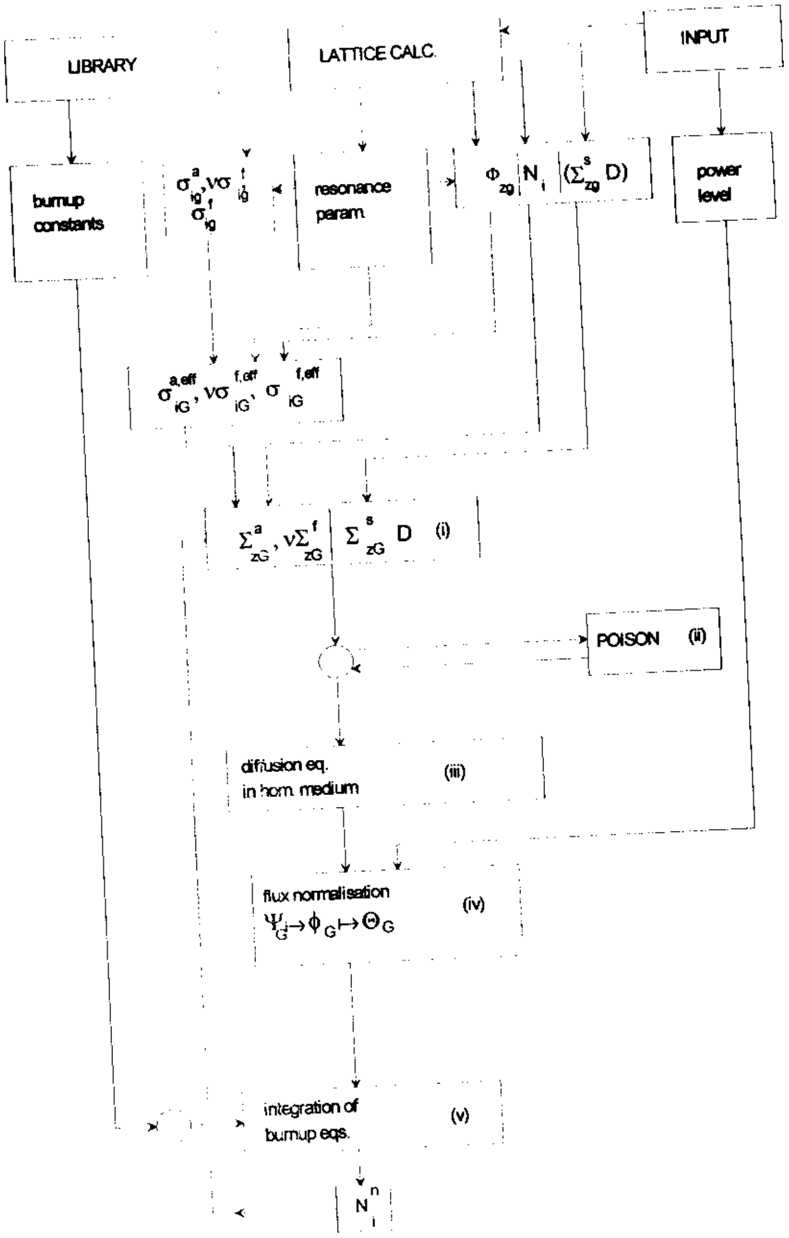

Figure 9: Diagram of WIMSD burn-up calculations.

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:

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

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. 9.

(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.

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

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.

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

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:

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

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. 9) 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' [4]. 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.

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

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):

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

(iv) Flux normalisation.

First the fission reaction rate is calculated:

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

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

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

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 [16,17] 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

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

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:

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

(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.

$$\frac{dN^i_m(t)}{dt} = -(\lambda^i + \{RR\}^{a,i}_m)N^i_m(t) + \sum_k q^{i,k'}_m(t)N^k_m(t) = \sum_k q^{i,k}_m(t)N^k_m(t), \quad (3.30)$$

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 [2,18].

3. Results of lattice calculations

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 *reaction 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:

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

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:

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

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

$$\{RR\}^{x,i}_{g} = \sum_z N_z^i V_z \sigma_g^{x,i} \varphi_{g,z}, \qquad (3.32)$$

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

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 [19]:

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

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

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:

$$\overline{\Sigma^x_{g,(i)}} = \frac{\int_{V_i} \Sigma^x_{g,i}(r)\phi_g(r)dr}{\int_{V} \overline{\phi_g(r)}dr}, \qquad (3.34a)$$

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

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:

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

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:

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

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

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

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 $j \in i$

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

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

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 [19]. 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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