REACTOR LATTICE TRANSPORT CALCULATIONS

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The present lecture is a continuation of the lecture on Introduction to the Neutron Transport Phenomena, where the basic ideas have been recalled necessary to understand lattice cell calculations. Reactor lattice calculations are carried out by reactor lattice codes. There are several such codes used currently for standard lattice calculations. The most popular of them is the WIMS code applied in several versions in various laboratories. Here the attention will be focused on the most recent version of WIMS, WIMSD-5B, distributed by NEA DATA BANK.

1   Goal of reactor lattice calculations

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 in an infinite reactor lattice. Thus, during the calculation the reactor lattice is assumed to be infinite and only corrections are applied to take care of specific phenomena characteristic for a finite medium with the actual reactor core structure.

The lattice codes include algorithms 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.

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.

2   Reactor lattice

2.1   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, hexagons or rings. The fuel plates are arranged in parallel bundles
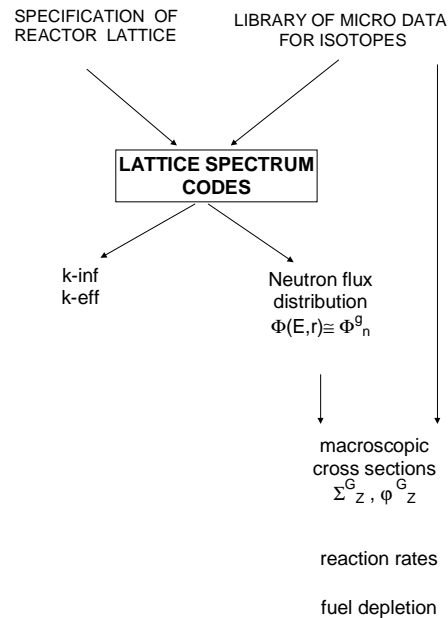
Figure 1. General diagram of the input and output of a reactor lattice code.

.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. 2.

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. 1). The unit cell for TRIGA is most often hexagonal with a cylindrical rod; the MTR unit cell is a fuel plate, claded on both sides and surrounded by water. Typical shapes of unit cells are shown in Fig. 2.

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.2.
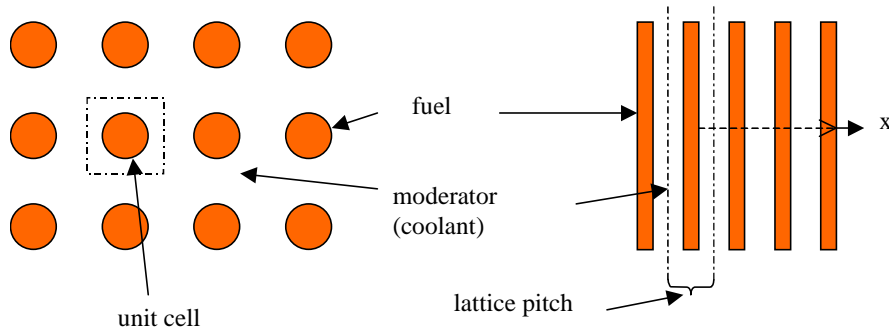
Figure 2. Fragment of a horizontal intersection of a square and plane lattice with a unit cell.

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 2.3 of "Introduction to the Neutron Transport Phenomena", 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.3), 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.
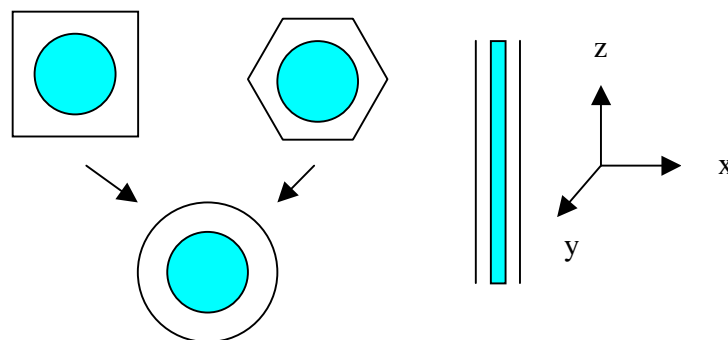

Figure 3. Typical shapes of unit cells.

The transport equation over the unit cell is 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.

A unit cell in the WIMS code has a limitation concerning its structure: Only 4 types of materials are allowed with material defined as fuel, occupying the central position of the unit cell (index 1), then cladding (index 2), coolant (index 3) and possibly moderator (index 4), as shown in Fig. 4.
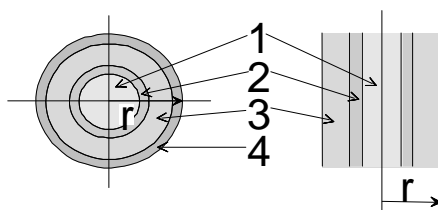
Figure 4. Spatial model of representative elementary cells in WIMS:
fuel - index 1, can - index 2, coolant - index 3, moderator - index 4.

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.

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 WIMS code.

For the unit cell the integral neutron transport equation is solved in WIMS by a collision probability method. 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. 4. 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. 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

2.2 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 heterogeneity 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 a macrocell are shown in Fig. 5.
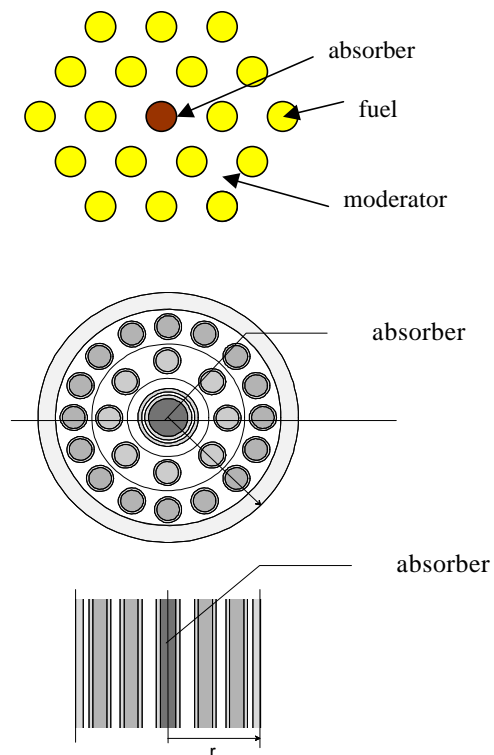

Figure 5. Possible macrocells with fuel rods and fuel plates with an absorber.

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.

In WIMS a typical two-step process is used for macrocells. After the infinite multiplication factor and neutron flux is obtained for the 4 (3) basic regions of a unit cell the macrocell can be treated with coefficients of the transport equations, i.e., the macroscopic cross sections obtained from that flux. A group condensation is possible before macrocell calculations. Several spatial models can be used depending on the user choice. The choice is an important step in lattice calculations and the reactor physicist is responsible for a correct representation of the analyzed system.

Five geometry models and two numerical methods: DSN or collision probability called PERSEUS, are possible here. The simplest and the most frequently used is the 'cluster' model shown in Fig.6, 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.
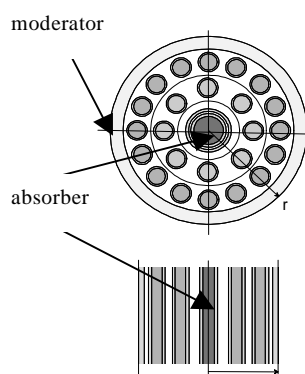
Figure 6. Model of a 'cluster' in cylindrical and plane geometry.

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:

1. Condensation of the multigroup flux obtained for each spectrum type L of the unit cell to the few-group structure:

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

2. Calculation of the average group flux for each annulus (plate) M from the few-group flux distribution calculated at for a macrocell in mesh points m:

$$\overline{\varphi_{G,M}} = \frac{\sum\limits_{m \in M} (\varphi_{G,m} V_m)}{\sum\limits_{m \in M} V_m},$$

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

$$\varphi_{G,L,M} = \frac{\Phi_{G,L}}{\sum\limits_{K} (V_K \Phi_{G,L})} \overline{\varphi_{G,M}},$$

Dividing both sides of the last equation 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:

$$f_{G,K,M} = \frac{\varphi_{G,L,M}}{\overline{\varphi_{G,M}}} = \frac{\Phi_{G,L}}{\sum\limits_{K} (V_K \Phi_{G,L})}$$

It is easy to see that the RHS of the last equation 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

Choosing the cluster option the user should remember that the neutron flux, calculated for a unit cell in its 4 basic regions, enters the final solution through the unsmearing process. For that reason 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. 6 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. 7, 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. 8,

☐ multicell calculations with cells or clusters coupled through input collision probabilities as shown in Fig. 9.
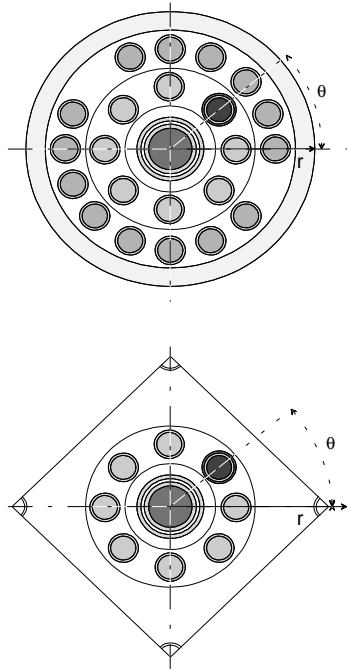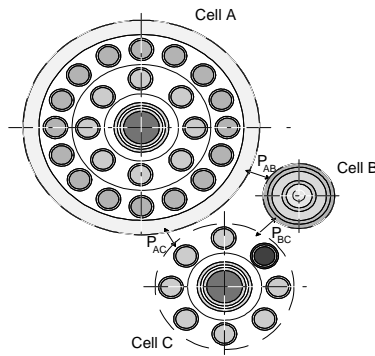

Figure 7. Examples of clusters treated by PIJ- PERSEUS.
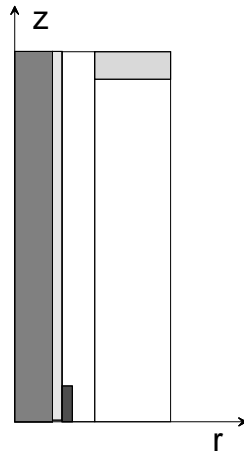
Figure 8. Example of a cell calculated in (r-z) geometry.

Figure 9. Example of a system calculated as 'multicell'.

It should be stressed that the WIMS 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   Energy dependence

The energy dependence in lattice calculations is treated through the multigroup approach. In WIMS the infinite lattice calculations are carried out always in the number of groups equal to that in which the library data are given. The macrocell calculations can be done in the same or a reduced number of groups. 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 majority of fission reactions takes place and both up- and down scattering of neutrons are possible.

The most complicated physical models have to be applied in the resonance energy region. To carry out the effective solution of the transport equation for a unit cell the coefficients of equations have to be known. Those are expressed through macroscopic cross sections for respective 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 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. 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 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 different resonance isotopes. The algorithms applied for all these corrections vary for various authors.

The actual reactor system is heterogeneous and to define properly resonance integrals for such a system the WIMS model uses the approach based on the equivalence principle. It consists in replacement of a heterogeneous problem by an equivalent homogeneous one. In WIMS, 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. These can be either calculated in the code or supplied by the user through the input cards.

In the WIMS model of a macrocell a ring of moderating material may surround the ring(s) of fuel pins. The Dancoff factor for a cluster model is calculated separately for the outermost layer of fuel pins. 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.

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:

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

where

σ_b - potential scattering cross section in the fuel region,

a - Bell factor,

l - mean chord length of the fuel region,

$$\alpha = \frac{1-\gamma}{a\gamma + (1-\gamma)},$$

$$\gamma = \frac{1-D_n}{\beta}$$

where D_n is the Dancoff factor given in WIMS 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.

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

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 the Dancoff factor is 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:

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

and taken with an argument corresponding to a sum of macroscopic total cross sections multiplied by can and coolant widths. A more complicated algorithm is used to calculate G_{ij} for other geometries.

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

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

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

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

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

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.

It is recommended to choose the more advanced algorithm of Dancoff factors calculations in case of square and hexagonal geometry.

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. In WIMS the first order correction of scattering cross sections is introduced for the thermal energy diapason. The P1 matrices exist in the code library, however, for several chosen nuclides only, for whom they are considered to be the most important. The code user should remember that the P1 matrices should be used only if such matrices exist in the code library for all principal nuclides in the material (e.g H_2O or pure graphite).

4   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. The change in isotopic composition caused by the fuel depletion can be described by a general equation:

$$\frac{dN^i}{dt} = -\lambda^i \cdot N^i - \{RR\}^i_{abs} \cdot N^i + \sum_k \{ \delta[i, j^i_1(k)] \cdot \alpha^{k,i} \cdot \{RR\}^k_c \cdot N^k \} +$$

$$+ \sum_k \{ \delta[i, j^i_2(k)] \cdot \beta^{k,i} \lambda^k \cdot N^k \} + \sum_k \{ Y^{k,i} \cdot \{RR\}^k_f \cdot N^k \}$$

where N^i denotes the number density of isotope i, λ^i is a decay constant, $\{RR\}^k_x$ is a microscopic reaction rate of type x and isotope k, $\alpha^{k,i}$ and $\beta^{k,i}$ are fractions of isotope i arising from, respectively, capture and decay of isotope k, $Y^{k,i}$ is a fission yield of isotope i from isotope k, $\delta[i, j^i_n(k)]$ are functions indicating existence or lack of possibility of a given reaction.

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:
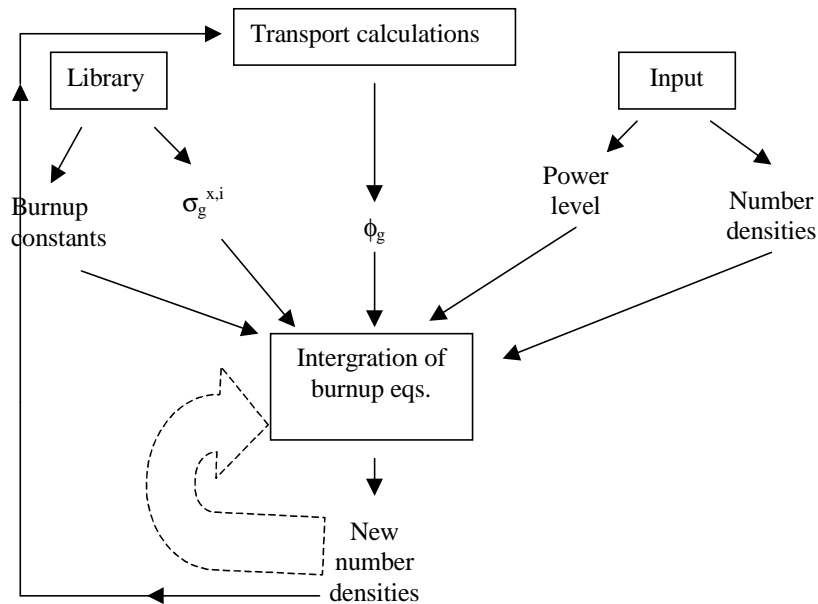

Figure 10. General scheme of depletion calculations.

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 crosses 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.

5   Results of lattice calculations

The direct results of the solution of the neutron transport equation in lattice calculations are *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. In case of burnup calculations the results include the compositions of all burnable materials..

These results can be then used in secondary calculations to deliver other needed quantities. WIMSD-5B has several possibilities of secondary homogenisation in energy and space. The homogenised diffusion coefficients can be defined such that:

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

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

$$\overline{\Sigma_{g,i}^x} = \frac{\int_{V_i} \Sigma_g^x(r)\phi_g(r)dr}{\int_{V_i} \phi_g(r)dr} \, .$$

 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 of lattice calculations, may be only a rough approximation of this quantity. It is obtained through a substitution of the streaming term in the diffusion equation by an expression DB^2 with B^2 calculated very often from the core dimensions. The theory underlying this approach assumes a regular lattice inside the reactor core and a regular shape of the core. Thus the *k-eff* result has to be used with caution.

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 have been already defined in 'The Introduction to Neutron Transport Phenomena'. However, here the attention is drawn to an ambiguity in their definition. The basic definition is usually that for a reaction of type *x*, where *x* can be absorption, fission or production, the reaction rate in group *g* is:

$$\{ RR \}_g^x = \frac{\sum\limits_{i,z} V_z \sigma_g^{x,i} \varphi_{g,z}}{\sum\limits_{z} V_z}$$

and is effectively calculated as a finite sum over materials and isotopes. 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.

The quantity based on macroscopic, instead of microscopic, cross sections is called the *number of reactions* of a given type x, in group g for isotope i, but it is also known as macroscopic reaction rate. Special caution is needed to avoid confusion of those two quantities. Both of them can be calculated in the WIMS code.

6 The recent version of WIMSD-5B

6.1 Subjects of modifications

Under the Co-ordinated Research Programme on WIMS Library Update Project new libraries have been developed. The new developed library has an increased number of isotopes and exists in two versions: with 69 and 172 library groups. The standard WIMS code in all its versions, including the last one WIMSD-5B, has been developed for a library with maximum number of 69 groups. Although the number of library groups used in WIMS calculations is read from that library, there exists a set of auxiliary variables in the code with dimensions adjusted to the requirements limited by the 69-group library. Those arrays had to be identified and modified if the extended 172-group library was to be used. The total number of library groups is connected to the number of fast, resonance and thermal groups and those 'partial' numbers of groups entered also the dimensions of particular arrays that required modifications. A similar situation existed with the number of isotopes in the library, i.e., the total number of isotopes, the number of fissionable isotopes and the number of fission products are also read from the library. All of them, although formally taking the library values, exist inside the particular subroutines with limitations imposed on their magnitudes in an indirect way.

Thus, the main goal of the WIMSD-5B code modification has been to enable the code to deal with the 172-group cross section library. Some minor changes had to be introduced to make the code work in all its options with an increased number of isotopes. Finally, the arrays with fixed dimensions have been included into the general scheme of dynamic memory organisation adapted in the WIMS code.

An additional possibility proposed by Guennadi Jerdev has been added. This introduces a possibility of multiple product nuclei in the burnup chains. In the

standard WIMS approach there is a limitation of a single capture and a single decay product. To introduce a possibility of branching a modification has been needed both in the code and in the library. The presently described WIMSD-5B version includes the modification allowing for branching if a special library FOND22 or ENDFB6EB is applied. In the extended libraries, several chosen isotopes received additional 'virtual' isotopes corresponding to their additional burnup channels. The convention has been adopted that an isotope with ID≥100000 is virtual. The virtual isotope is a copy of isotope with ID-$N\times100000$ (N=1...9), called 'base'. The approach is explained in Fig.11, prepared by the author of the method, with one base (Am) and two virtual isotopes with IDs 109241 and 209241.
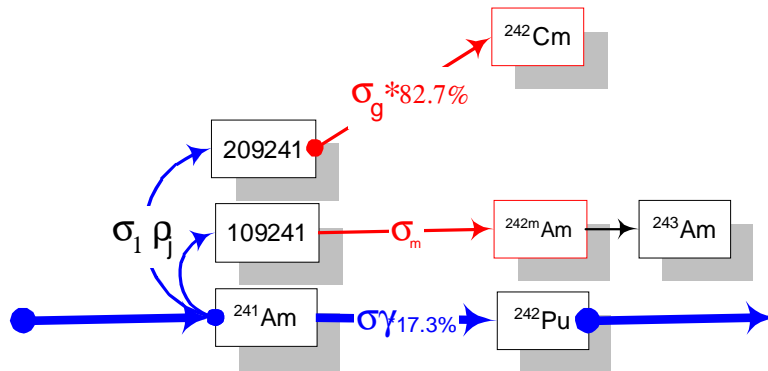

Fig. 11. Base isotope Am-241, virtual 109241 and 209241.

If during the burnup chain execution the isotope with ID≥100000 is identified the respective base isotope is searched and its number density is taken as the number density of a respective virtual isotope. A convention has been assumed to allow for using library cross sections of the base isotopes for the virtual isotope(s) in case the latter's data is missing in the library: if the library capture cross sections of the virtual isotope are not greater than zero the capture cross sections for the virtual isotope are copied from its base isotope, otherwise they are taken from the library. The virtual isotopes then enter the regular procedure for reaction rates calculation and burnup equation integration giving the respective contributions to the daughter isotopes not accounted for in the standard WIMS approach. The data for virtual isotopes have been prepared by the author for ENDFB-VI and FOND22 based libraries. This group of code modifications does not influence results obtained for standard libraries.

It should be stressed that the libraries with extended numbers of isotopes and groups cause a necessity of updating several standard test cases distributed by NEA DATA BANK with the code.

The extended code version has been tested on 16 standard WIMSD-5B test cases. The set of CRP benchmarks has been also calculated by the modified code. Several remarks needed for application of the new libraries are given below.

6.2   Technical remarks

The basic assumption underlying the work on the WIMSD-5B code extension has been to leave untouched its original version distributed by NEA DATA BANK. For that reason a code package has been prepared in the form of a so called UPDATE deck, composed of three files. The source deck is distributed with file identification **src** and comprises the program divided into decks, each of them preceded by the card ***ident namedeck** and with all cards in the deck named and numbered in columns 73 through 80. The division of the WIMSD-5B follows the original code modules, and hence the **namedeck**s have the respective names of those modules. Besides the source deck the code package includes a file with modifications named **upn**. Each modification in the **upn** file refers to the address in **src** given as **namedeck.xxxx**, with **xxxx** denoting the card number in the **namedeck**. The third member of the code package is the auxiliary program **upd**. This program has to be compiled and run. It takes the **upn** deck and introduces the modifications into the program deck **src**. The result of **upd** execution is a set of fortran programs divided into modules corresponding to **namedeck**s. Those create the modified WIMSD-5B code and have to be compiled in a standard way. The modifications introduced by the above-described procedure can be easily traced in the updated modules as they have the identifications of respective corrections in columns 73 through 80.

The list of modifications can be found in the materials of CRP on WLUP.

Every change from 69 to 172-group library (or back) requires modification of the input. The modification is necessary in the FEWGROUP card, THERMAL, ALPHA and PARTITION, if the last two are included in the input. To facilitate those changes the correspondence between the 172-group and 69-group scheme, based on the respective group boundaries, is given in Table 1.

Table 1
Correspondence between 172 and 69 energy groups

172-group	69-group	172-group	69-group	172-group	69-group
8	1	77	24	140	47
11	2	81	25	142	48
14	3	84	26	143	49
17	4	92	27	145	50
22	5	94	28	146	51

25	6	97	29	147	52
28	7	101	30	148	53
31	8	108	31	150	54
33	9	113	32	152	55
35	10	116	33	155	56
37	11	117	34	157	57
41	12	119	35	159	58
43	13	120	36	160	59
45	14	121	37	161	60
47	15	123	38	162	61
49	16	124	39	163	62
51	17	126	40	164	63
54	18	127	41	165	64
57	19	129	42	166	65
61	20	131	43	167	66
64	21	133	44	168	67
67	22	135	45	170	68
71	23	137	46	172	69

The pseudo-tape option cannot be used with the 172-group library unless the size of the memory needed for calculations, equal at present to 1000000, is substantially increased. A suitable information message has been inserted into the program.

With the new libraries the standard test cases distributed by NEA Data Bank will give different answers. The correct adaptation of WIMSD-5B cannot be verified any longer by comparison with results distributed with the code. The k-infinity values obtained with various libraries differ mostly by 0.1 - 0.2% but for some cases the differences are several times higher. Besides, several entries have to be changed in the standard test cases to run them. These changes are connected with the increased number of isotopes or with the nuclide IDs in the new libraries. They are listed in Table 2. The number of isotopes depends on the library applied. The value in Table 2 corresponds to the largest presently met requirement, i.e. ENDFB-VI with 69 groups and expanded burnup. The most severe problems are connected with options modifying the library: REPLACE, MULTIPLY, INCREASE. The actual positions of cross sections in the computer memory have to be given here. The values in Table 2 should be treated as an example since they are valid only for the ENDFB-VI based library with 69 groups and without the expanded burnup approach.

Table 2
Changes to be introduced to the standard WIMSD-5B test cases.

Test case	original text	correction for CRP library
test04	nisotopes 60	nisotopes 92

test06	store 200000 replace 1521 1521 multiply 1662 1662 increase 1523 1523 increase 1533 1533	store 600000 replace 1918 1918 multiply 2392 2392 increase 1920 1920 increase 1930 1930
test12	4157 (Gd-157)	2157
test13	9056 (SS)	follow composition of SS