CALCULATION OF ACCURATE ALBEDO BOUNDARY CONDITIONS FOR THREE-DIMENSIONAL NODAL DIFFUSION CODES BY THE METHOD OF CHARACTERISTICS

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ABSTRACT

Most of the few-group three-dimensional nodal diffusion codes used for neutronics calculations of the WWER reactors use albedo type boundary conditions on the core-reflector boundary. The conventional albedoes are group-to-group reflection probabilities, defined on each outer node face. The method of characteristics is used to calculate accurate albedoes by the following procedure. A many-group two-dimensional heterogeneous core-reflector problem, including a sufficient part of the core and detailed description of the adjacent reflector, is solved first. From this solution the angular flux on the core-reflector boundary is calculated in all groups for all traced neutron directions. In order to calculate the albedoes from macro-group g to all macro-groups, an inhomogeneous boundary value problem for the reflector only is solved with the incoming angular fluxes on the core-reflector boundary taken from the global solution for the transport groups within macro-group g and set to zero for all other transport groups. From this solution the partial in- and out-currents on all assembly faces on the core-reflector boundary and for all macro-groups are calculated, from which the albedo coefficients from macro-group g to all macro-groups for each assembly face are calculated. The method is exact as far as the two-dimensional heterogeneous solution by the method of characteristics is exact.

The group-to-group albedoes, however, depend strongly on the core loading, because a significant part of the neutrons entering a particular assembly face come from the neighbor faces. The above described procedure can be modified to calculate a new type of albedoes, the reflection probabilities of neutrons leaving the core through face j in macro-group h to return back through face i in group g. These new albedoes depend on the core loading more than 10 times less than the conventional ones and are practically invariant with respect to the core loading. If the assembly faces are too wide, they can be divided into segments.

Accurate boundary conditions can be calculated for the radial, top and bottom reflectors as well as for the absorber part of the WWER-440 control assemblies. The algorithm can be used to estimate also albedoes, coupling outer node faces on the radial reflector in the axial direction. Numerical results for the WWER-440 reactor are presented.

Introduction

In the old 1995-version of the two-group three-dimensional nodal diffusion code SPPS-1.6[1] the absorber part of the control assembly and the radial, top, and bottom reflectors are described by the conventional albedo boundary conditions, which can be stated in the following form:

$$j_f^- = \alpha_{f\leftarrow f} j_f^+ + \alpha_{f\leftarrow t} j_t^+,$$

$$j_t^- = \alpha_{t\leftarrow f} j_f^+ + \alpha_{t\leftarrow t} j_t^+,$$

where j_g^+ is the partial current in group g from the fuel assembly to the reflector, j_g^- is the partial current in group g from the reflector to the fuel assembly, and $\alpha_{h\leftarrow g}$ is the albedo from group g to group h, i.e. the probability that a neutron in group g passing from the fuel assembly to the reflector will return back as neutron of group h. Such boundary conditions are widely used in three-dimensional nodal codes. The coefficients $\alpha_{h\leftarrow g}$ are different on all outer assembly faces on the radial core boundary. Different $\alpha_{h\leftarrow g}$ are used for three axial zones of the absorber part of the control rod. Separate $\alpha_{h\leftarrow g}$ are used for the upper and lower reflector and for the top end of the fuel part of the control assembly. In fact the so-called γ-matrices are used in SPPS-1.6, but there is one-to-one correspondence between the α- and γ-matrices.

In principal these albedos are adequate provided they can be calculated exactly. The old procedure for generation of albedo boundary conditions was based on the WIMSD4 code[2, 3], used for calculation of macroscopic cross sections, and the one-dimensional S_N transport code ANISN[4], used to solve the neutron transport equation. Cylindrical geometry was used for the absorber and plane geometry for all other reflectors. A single calculation with ANISN yields a set of out-going and in-coming partial currents which form two equations, but the unknown coefficients are four. The missing two equations are obtained by solving another problem with different fuel assemblies (e.g., with different enrichment). Because the radial core boundary is quite different from one-dimensional plane geometry, manual fitting was applied for the outer assembly faces. This procedure for generation of boundary conditions was the best choice in 1995, when the code's library was generated.

From general considerations it follows that the boundary conditions on the radial reflector should depend on the fuel loading. If they do, however, the nodal code cannot be run independently and its application would be too complicated. Therefore, it is desirable that the boundary conditions will be invariant with respect to the core loading.

The method of characteristics is probably the only method which can be used for calculation of accurate albedo boundary conditions. In this method the neutron transport equation is solved for the generic angular neutron flux in selected directions of neutron motion and for each direction in equidistant parallel tracks, covering the domain of solution. The accuracy of the solution depends on the number and choice of the traced directions and on the track separation. The present day computers allow accurate solution of the neutron transport equation in two-dimensional real geometry.

The current work is based on the MARIKO code[5, 6, 7], which solves the multi-group neutron transport equation in general two-dimensional geometry by the method of characteristics. The domain of solution can be either a rectangle or a right hexagon with the most general periodic boundary conditions. Any mirror or rotational symmetry inside the domain is fully accounted for. There are three levels of geometric structures—regions, cells, and macro-cells. The domain of solution is divided into macro-cells, the macro-cells

are divided into cells, and the cells are divided into regions. The outer boundary of a macro-cell and cell can be any polygon. The outer boundary of a region can be practically any combination of straight line and circular arc segments. A fuel assembly should be described as a separate macro-cell.

The MARIKO code accounts for P1-scattering and the neutron source within a region can be represented as linear function of the spatial coordinates. The code has been verified by comparison with accurate Monte Carlo calculations for difficult transport problems.

In the following section the algorithm of calculating albedo boundary conditions is presented. Then in the next section some aspects of its implementation are discussed. Numerical results for the WWER-440 absorber and radial reflector are presented in the third section. The procedure of using the face-group to face group albedoes in SPPS-1.6 is outlined in the next section. Finally, some conclusions are drawn.

Method of calculation

Let us consider the problem of calculating albedo boundary conditions for radial faces of the absorber part of the WWER-440 control assembly. The neutron transport equation must be solved for a two-dimensional hexagonal domain with lattice pitch 3 times greater than the assembly lattice pitch and with periodic boundary conditions on its outer boundary. The absorber itself is at the centre of the domain. A 30-degree sector of the domain is presented on Fig. 1 in macro-cell level and on Fig. 2 in region level.

Let us assume that the transport equation has been solved for the whole domain in a number of transport groups and the transport solution is available. From this transport solution the angular neutron flux at all points, where the tracks enter the absorber, and in all traced directions and all transport groups can be calculated. In the method of characteristics the neutron travel is accounted for only along the tracks and neutrons may enter the absorber only along the tracks. Therefore, an inhomogeneous boundary value problem can be stated within the absorber only using the same tracks with the in-coming angular fluxes on the outer absorber boundary taken from the global solution. The solution of this problem must coincide with the global solution within the absorber. This fact does not help much except that it gives a clue for testing the algorithm for solving the inhomogeneous boundary value problem and its implementation.

Now let us consider another problem. The in-coming angular fluxes on the outer absorber boundary are kept the same as for the global solution in all transport groups corresponding to the fast diffusion group, but are set to zero for all thermal transport groups. For this problem the in-coming (to the absorber) partial currents in the fast transport groups are the same as for the global solution and those in the thermal groups are zero. Solving this new problem the out-going partial currents can be calculated and using the basic albedo equation the coefficients $\alpha_{f\leftarrow f}$ and $\alpha_{t\leftarrow f}$ can be calculated.

By analogy, setting to zero the in-coming angular fluxes in all fast groups and retaining the global incoming angular fluxes in all thermal groups, a new inhomogeneous boundary value problem can be stated. From its solution the remaining coefficients $\alpha_{f\leftarrow t}$ and $\alpha_{t\leftarrow t}$ can be calculated. It would be cheaper to use the partial currents from the global solution to form the two additional equations for the four albedo coefficients.

The above described method is applicable for any number of diffusion groups. Moreover, with a little modifications it can be used to calculate group to group and face to face albedoes. Considering the outer assembly faces on the radial boundary, the in-coming (to

the fuel assembly) partial current on face i in group g can be presented as

$$j_{ig}^{-} = \sum_{j,h} \alpha_{ig \leftarrow jh} j_{jh}^{+},$$

where j_{ig}^{-} and j_{ig}^{+} are the partial currents on face i in group g and $\alpha_{ig \leftarrow jh}$ is the probability that a neutron, which has left the core through face j in group h will return back to the core through face i in group g. In order to determine the coefficients $\alpha_{ig \leftarrow jh}$ from a particular pair of face j and group h to all i and g, the in-coming (to the reflector) angular fluxes must be set to zero on all faces and in all groups except on face j and in group h (in group h means all transport groups corresponding to macro-group h). In this case only one term will be none-zero on the right hand side of the above equation.

Implementation

The MARIKO code has been equipped with modules for automatic generation of the geometry structure of the WWER-440 fuel assemblies, reflector, and absorber. A fuel assembly may consist of any number of adjacent 30-degree sectors, thus covering practically all possible variants of a fuel assembly. The reflector region is described as a number of assembly like macro-cells, each one consisting of any number of adjacent 30-degree sectors. The reflector macro-cells are divided into cells like the cells in a fuel assembly, but without fuel pins. Given the standard rectangular coordinates of the macro-cell, the code automatically overlays the core shroud, basket, shaft, the stainless steel cylindrical bodies in the dummy assemblies, etc. Minimum number of human input data are supplied by the user. A separate subroutine models the absorber, because finer spatial discretization is required around the boron steel inserts.

A preliminary step in calculating boundary conditions is the solution of the global eigenvalue problem and recording the final results to a disk file. It is performed by the standard calculation path in MARIKO.

In order to calculate boundary conditions the 'reflector' region must be specified first. The implementation is very simple—the user specifies which macro-cells form the 'reflector'. A macro-cell in the 'reflector' must not contain fuel, but not all none-fuel macro-cells have to be included in the 'reflector'. Thus, boundary conditions can be calculated not only on the outer fuel assembly faces, but further in the reflector, which is necessary for the fine-mesh diffusion codes and some nodal diffusion codes. Since the reflector macro-cells can be constructed from any number of 30-degree sectors, the 'reflector' can be defines in a flexible way.

The next part of the algorithm identifies the points where the tracks enter and leave the 'reflector', together with additional information, such as which macro-cell side is intersected. In solving the inhomogeneous boundary value problem the ray tracing starts at the point where the track enters the 'reflector' with a known value of the angular flux at this point and continues until the track leaves the 'reflector'. Therefore, two new ray tracing procedures are required. The first one is almost the same as the standard ray tracing procedure in solving the eigenvalue problem. It passes all the tracks for the entire problem and does the usual integration to calculate the scalar flux, current, escape and transmission probabilities. In addition it saves the in-coming (to the 'reflector') angular fluxes. This procedure is performed once before the actual solution of the inhomogeneous boundary value problem or problems has started. It does not require user input.

In order to state the inhomogeneous boundary value problem the user must specify what kind of boundary conditions are to be calculated—a value of -2 of a control variable

means all group to group albedoes and a value of -1 means all face-group to face-group albedoes. If face-group to face-group albedoes from a particular face are required, then the user specifies the starting face number. This information is sufficient to organize the solution of the appropriate sequence of inhomogeneous boundary value problems, setting to zero the appropriate in-coming (to the 'reflector') angular fluxes.

The second additional ray tracing algorithm is used for solving the inhomogeneous boundary value problem for the 'reflector' only. It also passes all the tracks for the entire problem, but does nothing outside the 'reflector'. The integration starts at the point where the track enters the 'reflector' with a predefined value of the in-coming angular flux and continues until the track leaves the 'reflector'. This ray tracing procedure does not require user input.

In addition to the ray tracing procedure a number of algorithms are required in solving the neutron transport equation (for calculation of the neutron source, for acceleration of the self-scattering and up-scattering iterations, etc.). All these have been generalized to act properly in solving the eigenvalue and boundary value problems.

The most difficult and unexpected problems arose in solving the inhologeneous boundary value problem, which is not conventional in nuclear reactor analysis. It turned out that both the convergence criteria and the main iteration algorithms were not robust enough for the boundary value problems. The main problems were caused by the strong spatial variation of the fluxes in case of boundary sources in the thermal energy range only. Because the mean free path length of the thermal neutrons is small compared to the reflector size, the scalar fluxes die out by several orders of magnitude far from the surface source. This is quite different from the eigenvalue problem where the neutrons are transferred to the reflector in the fast energy range and the thermal flux is formed by slowing down. Moreover, the up-scattering produces strange-shaped sources above the thermal group energy range. In effect the deviations from the neutron balance happen to be so strong, that un-physical negative values for the angular fluxes, partial currents, and scalar fluxes were observed, thus violating the overall iteration process. All these problems have been overcome by applying more strict convergence criteria and negative fix-up procedures for the partial currents, scalar fluxes, etc. These problems occur during the first up-scattering iteration when the initial guess for the solution is with severe errors. The final algorithm is robust and no problems have been encountered in all cases of interest.

The new algorithm is implemented as a separate calculation path in the MARIKO code. Because the major part of the subroutines are common, the original calculation path of the code has been improved as well.

Numerical results

The group to group albedoes for the WWER-440 control rod benchmark (Ref. [8]) are presented in Table 1. The MARIKO calculation has been performed in 36 transport groups with macroscopic cross sections generated by WIMSD4, while the results in Ref. [8] have been obtained with other codes and cross section libraries. Moreover, the MARIKO calculation is in two-dimensional heterogeneous geometry with each fuel pin represented explicitly, while the results in Ref. [8] have been obtained in one-dimensional cylindrical geometry with the fuel pins smeared with the moderator. In these circumstances the agreement between both sets of results is surprisingly good.

It is observed that from the fast neutrons entering the absorber 65% return back as

Table 1: Albedoes for the WWER-440 control rod benchmark

	$\alpha_{f\leftarrow f}$	$\alpha_{f\leftarrow t}$	$\alpha_{t\leftarrow f}$	$\alpha_{t\leftarrow t}$
MARIKO	0.6527	0.0008	0.0165	0.3453
Ref. [8]	0.664	0.002	0.016	0.337
	$\alpha_{jf\leftarrow if}$	$\alpha_{jf\leftarrow it}$	$\alpha_{jt\leftarrow if}$	$\alpha_{jt\leftarrow it}$
2→2	.3159	.0007	.0109	.2933
2→3	.1261	.0001	.0022	.0259
2→4	.0310	.0	.0005	.0
2→5	.0219	.0	.0004	.0

fast neutrons and 1.6% return as thermal neutrons, about 33% being absorbed. From the thermal neutrons entering the absorber 34.5% return back as thermal neutrons and 0.08% as fast neutrons due to the up-scattering, 65.5% being absorbed. Since the fast partial current to the absorber is 8 times greater than the thermal one, the number of neutrons absorbed in the absorber, which enter as fast neutrons, is 4 times greater than those which enter as thermal.

The face-group to face-group albedoes for the same absorber problem are presented also in Table 1. The face numbering is shown on Figure 3. Face 2 is the one the neutrons enter through, face 3 is next to face 2 and there are two such faces, face 4 is the next one and there are two such faces as well, and face 5 is opposite to face 2. From the fast neutrons entering through a particular absorber face 32% return back through the same face, about 13% escape through each one of the nearest two faces, about 3% escape through each one of the next two faces, and about 2% escape through the opposite face. Therefore, more than half of the reflected fast neutrons do not return through the face they have entered through. Considering a typical situation with the absorber surrounded by assemblies with essentially different local multiplication factors, the partial currents to the absorber from the more powerful assemblies will be greater, but the returning neutrons will be redistributed inside the absorber. If the conventional group to group albedoes are used, this redistribution cannot be accounted for, while with the face-group to face-group albedoes the real neutron transfer is adequately described.

For the radial reflector an important question is how much the albedos depend on the core loading. In order to study this problem a core-reflector problem, presented on Figure 4 on macro-cell level and on Figure 5 on region level, has been used. Two cases are considered differing in the burnup of the fuel in macro-cells FA10 and FA19, both of them with initial enrichnent of 3.6%. In case A macro-cell FA10 is with burnup 30 MWD/kg and FA19 is with zero burnup, and in case B their burnups are interchanged. Face 1 is face 5 of FA10, faces 2, 3, and 4 are faces 5, 6, and 1 of FA19. The group to group albedoes are presented on Table 2. It is observed that $\alpha_{f\leftarrow f}$ for faces 1 and 2 differ by 0.04, which is an essential difference. The difference for $\alpha_{t\leftarrow f}$ is also significant. The out-going partial currents in the thermal group are 4 times smaller than in the fast group, therefore the remaining two albedoes are 4 times less important. The main conclusion is that the group to group albedoes depend strongly on the core loading.

The face-group to face-group albedoes for the same problem are presented on Table 3. It should be noted that $\alpha_{2g\leftarrow 2h}$ include the contribution from the face, which is opposite to face 2 with respect to the axis in angle 0°. Face 3 also has such symmetrical face, but it is at greater distance. Face 4 has a symmetrical face with respect to the axis in 30°.

Table 2: Radial group to group albedoes for different core loading

Face	$\alpha_{f\leftarrow f}$	$\alpha_{f\leftarrow t}$	$\alpha_{t\leftarrow f}$	$\alpha_{t\leftarrow t}$
1 A	.5035	.0017	.0960	.6058
1 B	.4642	.0017	.0882	.5880
2 A	.5579	.0016	.1218	.5800
2 B	.6002	.0016	.1298	.5959
3 A	.4596	.0015	.0798	.5163
3 B	.4669	.0015	.0822	.5175
4 A	.4895	.0016	.0993	.5718
4 B	.4899	.0016	.0999	.5720

It is observed that the difference between the values of $\alpha_{1f\leftarrow 1f}$ for the two cases is 0.004 against 0.04 for $\alpha_{f\leftarrow f}$. Therefore, the face-group to face-group albedoes depend 10 times less on the core loading than the group to group albedoes. From a practical point of view the new albedoes are invariant with respect to the core loading.

This is not the most important advantage of the new albedoes. Consider again fuel assemblies 10 and 19 (FA10 and FA19 on Figure 4) in the 60° sector of the WWER-440 full core. Assembly 10 is a control assembly and for a particular node in assembly 19 the neighbor node in assembly 10 can be either a fuel node or an absorber one. From the albedoes in Table 3 it can be estimated that at least 25% of the neutrons reflected trough face 5 of assembly 19 come from face 2 of assembly 10 (the out-going partial current from face 2 of assembly 10 is greater than the one from face 5 of assembly 19). If the next node in assembly 10 is occupied by absorber, these 25% will be missing. This had not been accounted for in the old version of SPPS-1.6, because the group to group albedoes in these two situations were the same. The new albedoes allow more accurate description of the neutron transport in this situation.

The new albedoes are less sensitive to the core loading, therefore they can be calculated using smaller core-reflector problems. They are practically insensitive to the fuel composition in the peripheral assemblies and they should depend on the moderator density and boron concentration in the reflector only.

Modifications in SPPS-1.6

In order to use the new face-group to face-group albedoes, modifications have been made in SPPS-1.6. By now the code requires both types of albedoes, but the group to group albedoes are used as initial guess only. The effective $\alpha_{h\leftarrow g}$ are calculated in a three step algorithm. The partial out-currents are calculated first at each outer node face using the latest estimate of the effective albedoes. Using these out-currents and $\alpha_{ig\leftarrow jh}$, the partial in-currents are calculated also at each node face, but the contribution from different groups is separated:

$$j^-_{i,g\leftarrow h} = \sum_j \alpha_{ig\leftarrow jh} j^+_{jh}.$$

Finally the effective albedoes are calculated:

$$\alpha_{i,g\leftarrow h} = j^-_{i,g\leftarrow h}/j^+_{ih}.$$

Table 3: Radial face-group to face-group albedoes for different core loading

Faces	$\alpha_{if \leftarrow jf}$	$\alpha_{if \leftarrow jt}$	$\alpha_{it \leftarrow jf}$	$\alpha_{it \leftarrow jt}$
1→1 A	.3158	.0013	.0526	.4842
1→1 B	.3122	.0014	.0522	.4844
1→2 A	.1291	.0002	.0278	.0637
1→2 B	.1299	.0002	.0277	.0633
1→3 A	.0066	.0	.0022	.0002
1→3 B	.0069	.0	.0023	.0002
1→4 A	.0005	.0	.0002	.0
1→4 B	.0005	.0	.0002	.0
2→1 A	.1322	.0002	.0287	.0727
2→1 B	.1320	.0002	.0292	.0765
2→2 A	.3518	.0013	.0713	.4920
2→2 B	.3545	.0013	.0716	.4915
2→3 A	.0300	.0	.0103	.0126
2→3 B	.0294	.0	.0101	.0118
2→4 A	.0015	.0	.0006	.0
2→4 B	.0015	.0	.0006	.0
3→1 A	.0041	.0	.0024	.0002
3→1 B	.0041	.0	.0024	.0002
3→2 A	.0292	.0	.0137	.0166
3→2 B	.0291	.0	.0137	.0174
3→3 A	.3675	.0014	.0509	.4827
3→3 B	.3684	.0013	.0511	.4827
3→4 A	.0334	.0	.0127	.0136
3→4 B	.0330	.0	.0126	.0132

This procedure is repeated in each iteration. It introduces another source of none-linear effects in the iteration process, which is too strong and divergence was observed in some cases. It was avoided by applying under-relaxation to the partial out-currents with an under-relaxation factor of 0.6.

Conclusions

An algorithm for calculation of both group to group and face-group to face-group albedo boundary conditions has been developed. Based on two-dimensional heterogeneous solution of the neutron transport equation by the method of characteristics, it ensures adequate representation of the absorber and radial reflector and accurate albedoes. The albedo matrix is calculated by a single code by two different calculation paths. It has been demonstrated that the new face-group to face-group albedoes are practically invariant with respect to the core loading and describe adequately the neutron transport in the absorber and reflector. The SPPS-1.6 code has been modified in order to use the new albedo type boundary conditions.

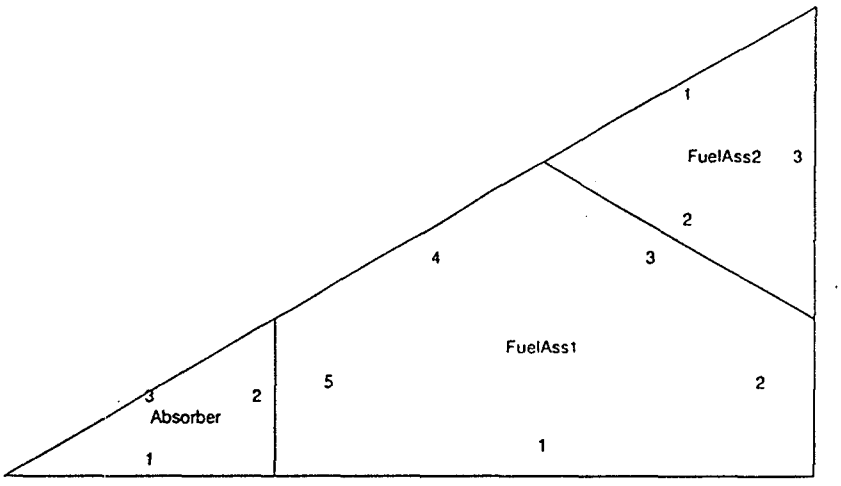

Figure 1: 30-degree sector of the absorber benchmark in macro-cell level

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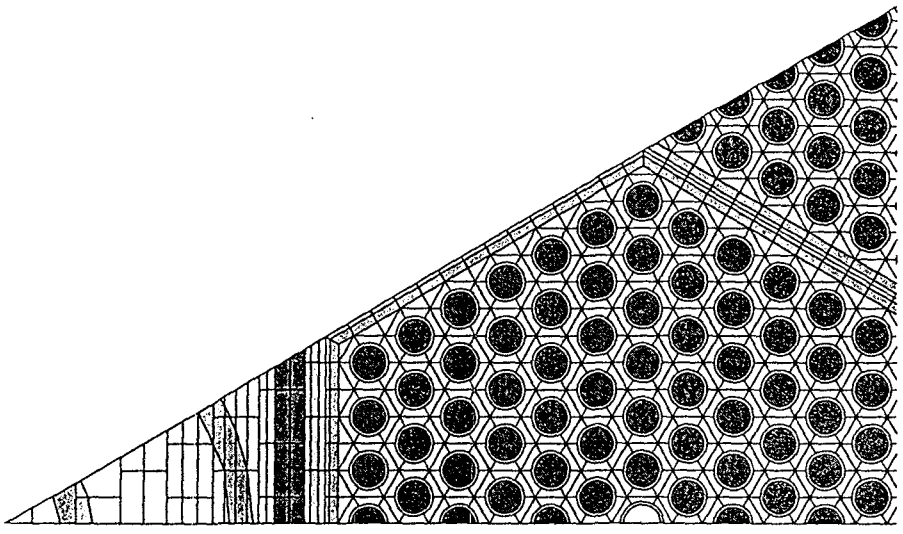

Figure 2: 30-degree sector of the absorber benchmark in region level

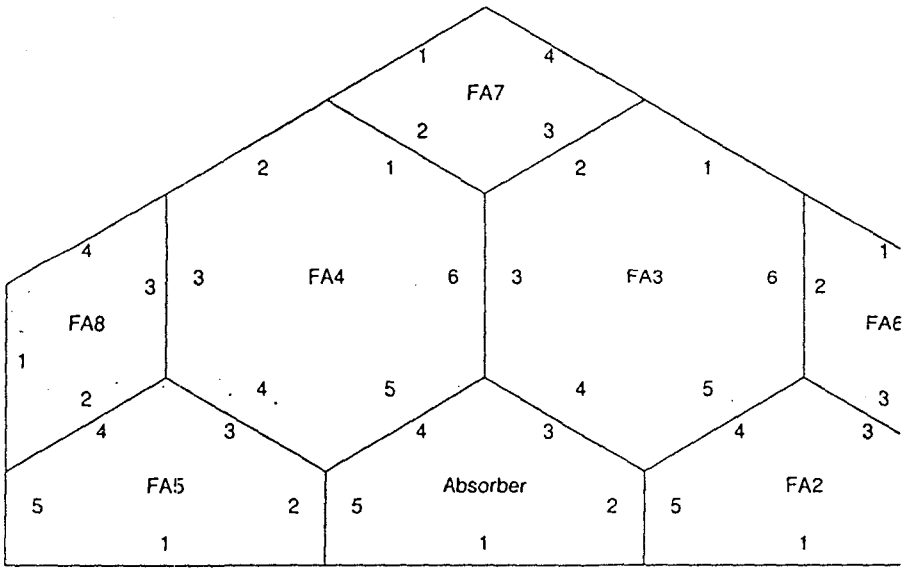

Figure 3: 180-degree sector of the absorber benchmark in macro-cell level

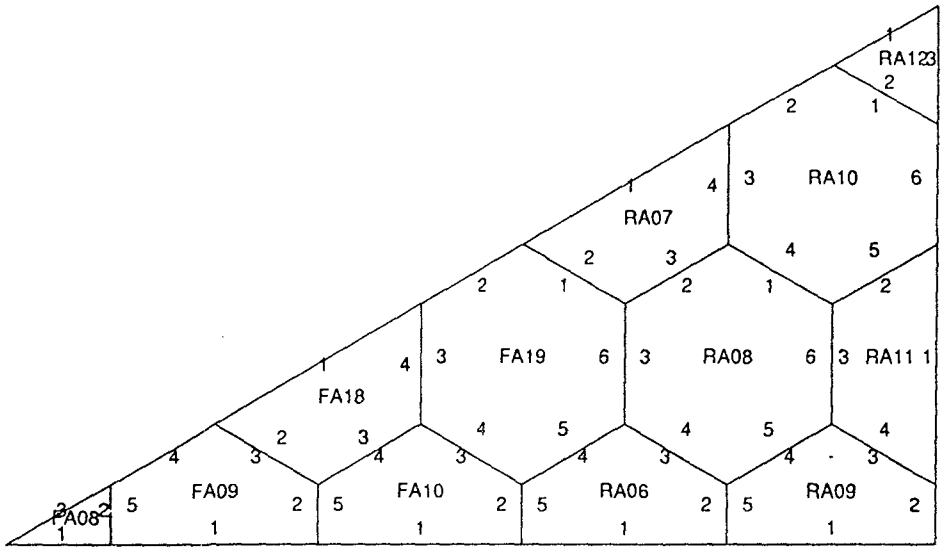

Figure 4: 30-degree sector of the core-reflector problem in macro-cell level

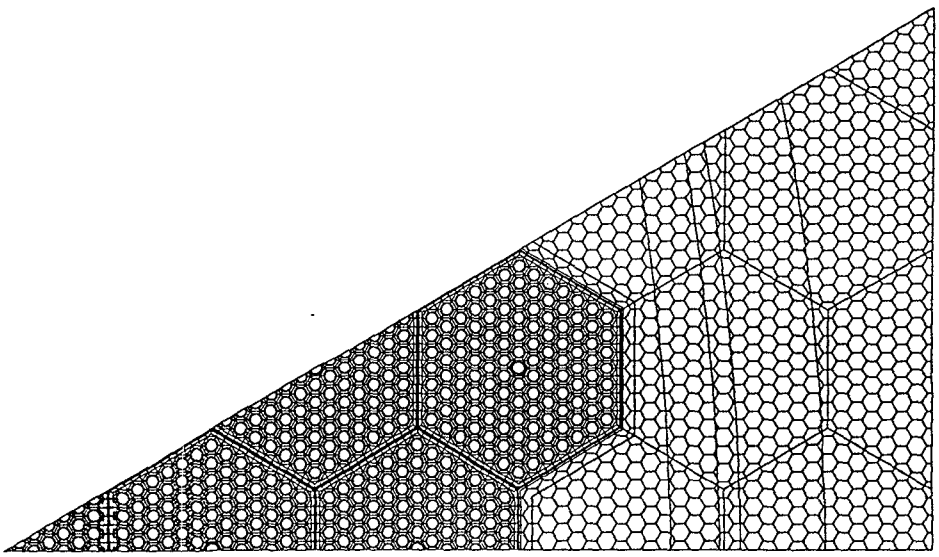

Figure 5: 30-degree sector of the core-reflector problem in macro-cell level