PELLET BY PELLET NEUTRON FLUX CALCULATIONS COUPLED WITH NODAL EXPANSION METHOD

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Abstract

We present a technique whose aim is to replace 2D pin by pin de-homogenisation, currently done in core reactor calculations with the nodal expansion method (NEM), by a 3D finite difference diffusion calculation. This fine calculation is performed as a zoom in each node taking as boundary conditions the results of the NEM calculations. The size of fine mesh is of the order of a fuel pellet. The coupling between fine and NEM calculations is realised by an albedo like boundary condition. Some examples are presented showing fine neutron flux shape near control rods or assembly grids. Other fine flux behaviour as the thermal flux rise in the fuel near the reflector is emphasised. In general the results show the interest of the method in conditions where the separability of radial and axial directions is not granted.

Introduction

Pin by pin information within nodal expansion method calculations for reactor analysis are currently obtained by a de-homogenisation technique. The core diffusion calculation permits to get node average flux and surface average flux and current that are used as constraints in pin by pin calculations. The power density of each pin is obtained by a superposition of a coarse mesh distribution taking into account the current node conditions and a fine distribution computed in infinite medium conditions. This technique gives good results in situations where the spatial flux behaviour is not too far from the fundamental mode. As the fine calculation is done in 2D no further axial information is available from it. To fill this lack of information an axial de-homogenisation technique has been developed several years ago at Framatome ANP. This technique permits to reconstitute the behaviour of the power distribution near the grids, but it adds to the fundamental mode approximation the axial-radial separability approximation.

To reduce the impact of these approximations a study has been done to evaluate the feasibility of a fine neutron diffusion calculation. The technique consists in performing a diffusion calculation inside the nodes using the nodal results as boundary conditions. This calculation is done in 3D with mesh having the size of a fuel pellet.

The study has been done for the steady state critical calculations only but the method can be extended to kinetic situations.

Method

Nodal flux calculations are based on data obtained by homogenisation of the results of a 2D pin by pin transport calculation. As stated by the equivalence theory (see [1] for a discussion on this subject) the use of the discontinuity factors permits to obtain average surface fluxes and currents very close to the ones that could be obtained from a fine pin by pin calculation. This information can hence be used as boundary condition for a fine flux calculation inside the node. The method described here takes this information to compute a flux distribution inside the node by solving the two-group diffusion equation. For this purpose the node is divided in fine mesh, one mesh point per pin cell in the x y directions and of the size of a pellet in the z direction. The calculation is done separately and independently in one or more nodes.

Although the flux and the current are known at the node surfaces, we have avoided performing a source like calculation. Indeed the problem could be posed in an inhomogeneous form and the flux could be computed as a response to an external neutron source applied to the boundary of the domain. This approach would be correct if the fine cross section distribution was rigorously equivalent to the homogeneous cross sections used by the nodal calculation. This condition is difficult to be obtained. This means that, if the medium multiplication properties were under estimated, the fine solution would have a depression in the centre. In the opposite case we would not have a physical meaningful solution.

The approach used is that of a critical calculation with the evaluation of a k_{eff} that could differ from the one of the nodal calculation. The solved equations, coming from the finite difference discretization of the two-group diffusion equation in mesh point n, are the following, for the fast group:

$$\sum_{f=1}^{6} \alpha_{f,n,1}(\Phi_{n,1} - \Phi_{f,1}) + (\Sigma_{a,n,1} + \Sigma_{r,n})\Phi_{n,1} = \sum_{g=1}^{2} \frac{1}{k_{\text{eff}}} \nu\Sigma_{f,n,g}\Phi_{n,g} \qquad (1)$$

and for the thermal group:

$$\sum_{f=1}^{6} \alpha_{f,n,2}(\Phi_{n,2} - \Phi_{f,2}) + \Sigma_{a,n,2}\Phi_{n,2} = \Sigma_{r,n}\Phi_{n,1} \tag{2}$$

where $\Phi_{n,g}$ is the group g neutron flux, $\nu\Sigma_{f,n,g}$ is the fission neutron production cross section, $\Sigma_{a,n,g}$ is the absorption cross section, Σ_r is the removal from fast to thermal cross section, $\alpha_{f,n,g}$ are the coupling coefficients between mesh point n and the mesh point beyond face f, $\Phi_{f,g}$ is the average flux in mesh point beyond face f. The boundary conditions are taken from the nodal calculation. The details are done in the following sections.

To avoid confusion between the nodal and fine spatial elementary calculation domains we will use the term node to refer to the nodal calculation and mesh to refer to the fine calculation. For simplicity we will neglect the neutron group index in the following discussion.

Evaluation of the boundary conditions from the nodal calculation

With the following definitions:

$\Phi(r_{surf})$: neutron flux at the point r_{surf} of the node surface,
$J(r_{surf})$: projection of the net neutron current at point r_{surf} of the node surface on the unit vector perpendicular to the surface,

the boundary condition is expressed as an albedo condition by the following equation:

$$\frac{J(r_{surf})}{\Phi(r_{surf})} = a(r_{surf}) \tag{3}$$

where the function $a(r_{surf})$ is determined from the surface nodal results. Two different approaches have been analysed (and implemented).

The first approach is to consider a flat function a on the surface:

$$a(r_{surf}) = \frac{J_{surf,NEM}}{\Phi_{surf,NEM}} \tag{4}$$

where:
$\Phi_{surf,NEM}$: nodal neutron flux at the node surface,
$J_{surf,NEM}$: projection of the nodal net neutron current at node surface on the unit vector perpendicular to the surface.

The second approach is to use a second order polynomial expansion:

$$a(r_{surf}) = \frac{b_{J,0,0} + \sum_{i=1}^{2}[b_{J,1,i}P_i(u) + b_{J,2,i}P_i(v)]}{b_{F,0,0} + \sum_{i=1}^{2}[b_{F,1,i}P_i(u) + b_{F,2,i}P_i(v)]} \tag{5}$$

where the polynomials P_i are the same of the nodal calculation:

$$P_1(u) = u$$
$$P_2(u) = u^2 - \frac{1}{12} \tag{6}$$

and u v are the reduced coordinates on the surface. For example, for a surface perpendicular to the z axis, denoting with x and y the coordinates with the origin in the lower surface corner, with Δx and Δy the corresponding mesh width, the reduced coordinates are:

$$u = \frac{x}{\Delta x} - \frac{1}{2}$$
$$v = \frac{y}{\Delta y} - \frac{1}{2} \tag{7}$$

The coefficients $b_{J,k,i}$ and $b_{F,k,i}$ (k=1,2; i=1,2) are determined in a way similar to the one used to evaluate the transverse leakage behaviour in the transverse integrated 1D nodal equations. Consider the surface S_0 and its four neighbour surfaces S_k as depicted in Fig. 1.

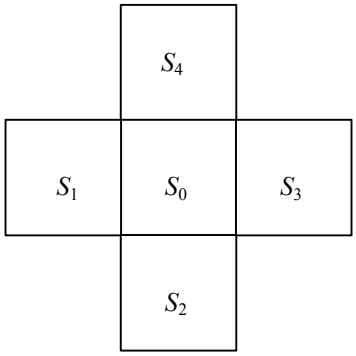

Fig. 1. Scheme of a node surface and its neighbours.

The constraint on the coefficients is that the average value of the current expansion on each one of the five surfaces must be equal to the nodal value of the current in that surface. The system solved is:

$$b_{J,0,0} + \sum_{i=1}^{2} \iint_S [b_{J,1,i} P_i(u) + b_{J,2,i} P_i(v)] du dv = J_{k,\mathrm{NEM}} \tag{8}$$

where index k denotes the five surfaces (k=0,…,4). Similarly for the flux we have:

$$b_{F,0,0} + \sum_{i=1}^{2} \iint_S [b_{F,1,i} P_i(u) + b_{F,2,i} P_i(v)] du dv = \Phi_{k,\mathrm{NEM}} \tag{9}$$

In reality these systems are not true systems of 5 equations with 5 unknowns, because, thanks to the polynomial hortogonality, one of the equations becomes, for the current:

$$b_{J,0,0} = J_{0,\mathrm{NEM}} \tag{8bis}$$

and for the flux:

$$b_{F,0,0} = \Phi_{0,\mathrm{NEM}} \tag{9bis}$$

The remaining equations are decoupled 2 by 2. Hence we must solve 4 systems of 2 equations each (for each neutron group).

Fine discretization and numerical solution

The fine flux calculation is done applying the finite difference method.

With the following definitions:

Φ_i: average neutron flux inside mesh point i,
Φ_{ix+}: average neutron flux inside the neighbour in $x+$ direction of mesh point i,
$J_{x+,i}$: projection on the unit vector perpendicular to the surface in the positive x direction, of the net neutron current from mesh point i to the neighbour $ix+$,
Δx_i: width of mesh point i in the x direction,

the contribution relative to the x plus surface, to the leakage term of the diffusion equation is:

$$\frac{J_{x+,i}}{\Delta x_i} = -\alpha_{x+,i}(\Phi_{ix+} - \Phi_i) \tag{10}$$

where $a_{x+,i}$ denotes the coupling coefficient between mesh point i and mesh point $ix+$ defined as:

$$\alpha_{x+,i} = 2\frac{\Delta x_i D_i + \Delta x_{ix+} D_{ix+}}{\Delta x_i (\Delta x_i + \Delta x_{ix+})^2} \tag{11}$$

and D_i is the diffusion coefficient.

To define the coupling coefficients corresponding to the mesh surfaces laying on the node surface let us start from the Fick's law. With the following definition:

$\Phi_{x+,i}$: average neutron flux on the mesh i surface in the positive x direction,

the net current component in the x direction is expressed by:

$$J_{x+,i} = -D_i \frac{\Phi_{x+,i} - \Phi_i}{\Delta x_i / 2} \tag{12}$$

Taking into account the boundary condition expressed by Eq. (3) we also have:

$$J_{x+,i} = a_i \Phi_{x+,i} \tag{13}$$

where the coefficients a_i are either taken from Eq. (4) or interpolated using Eq. (5).

Eliminating $\Phi_{x+,i}$ from Eq. (13) and Eq. (12) we can deduce the relation between the average flux and the surface current:

$$J_{x+,i} = \frac{a_i}{1 + a_i \frac{\Delta x_i}{2D_i}} \Phi_i \tag{14}$$

Taking into account the definition of the coupling coefficient at the boundary as the factor multiplying the average flux to obtain the net neutron flow through the surface per unit volume:

$$\frac{J_{x+,i}}{\Delta x_i} = \alpha_{x+,i}\Phi_i \tag{15}$$

we have:

$$\alpha_{x+,i} = \frac{a_i}{\Delta x_i(1 + a_i \frac{\Delta x_i}{2D_i})} \tag{16}$$

Similarly for the boundary in the negative *x* direction we have:

$$\alpha_{x-,i} = \frac{a_i}{\Delta x_i(1 - a_i \frac{\Delta x_i}{2D_i})} \tag{16bis}$$

The same is done for the *y* and *z* directions.

The solution of the two-group discretized diffusion equation is done by application of the power method. The inner iteration is performed by a Jacobi scheme with Chebyshev acceleration.

Cross sections evaluation

The fine cross sections are evaluated by a simple de-homogenisation procedure. The homogeneous cross sections used in the nodal calculation are taken as a base shape on which are superposed deltas. The delta cross sections are estimated on the basis of the 2D pin by pin distribution corresponding to the transport infinite medium calculation that produced the cross section library for the nodal calculation. The general de-homogenisation function for a reaction *X* cross section (*X* is either absorption, fission or scattering) is the following:

$$\Sigma_{X,i} = \Sigma_{X,\mathrm{H}}(Bu, \rho_{\mathrm{H2O}}, T_{\mathrm{fuel}}, C_{\mathrm{B}}, N_{\mathrm{Xe}}, h) + \Delta\Sigma_{X,\mathrm{H}} \tag{17}$$

where:

$\Sigma_{X,i}$: fine cross section in mesh point *i*,
$\Sigma_{X,\mathrm{H}}$: homogeneous cross section, interpolated at the current conditions in the node, characterised by burnup (Bu), water density (r_{H2O}), fuel temperature (T_{fuel}), boron concentration (C_{B}), xenon density (N_{Xe}), spectral history parameter (h),
$\Delta\Sigma_{X,\mathrm{H}}$: difference between the homogenised cross section in the fuel pins and the homogenised cross section in the whole 2D infinite medium configuration.

For the study purpose some simplification has been introduced:

- no intranodal shape of $\Sigma_{X,\mathrm{H}}$ has been evaluated and a flat base distribution has been taken,
- no interpolation is done for $\Delta\Sigma_{X,\mathrm{H}}$ (it is considered a second order correction with respect to $\Sigma_{X,\mathrm{H}}$),
- no pin by pin thermal feedback is computed (only nodal feedback has been considered).

The first and second simplification limits the usage of the procedure to assemblies with low burnup gradient and with only one fuel type.

For the water holes the cross sections used are the corresponding homogenised values of the 2D infinite medium configuration interpolated at the actual node conditions.

A delta absorption cross section $\Delta\Sigma_a$ is added in the mesh points containing a control rod. For mesh points containing the tip of the rod a volume weighting is done. This $\Delta\Sigma_a$ is taken from the 2D infinite medium configuration.

A delta absorption cross section $\Delta\Sigma_a$ and a delta removal (from group 1 to group 2) cross section $\Delta\Sigma_r$ is added to the mesh points containing the grids. These are constant values for each grid type.

Results

The 3D fine flux diffusion calculation method has been implemented in the SMART system [2]. Eq. (5) has been used to evaluate the boundary conditions.

Some calculations have been done and we report here two of the most interesting. As one of the major points of interest in our study is the modelisation of phenomena not following the radial-axial separability, a flux calculation along a fuel assembly with a control rod inserted is presented. In order to separate the influence of the grids from that of the control rod, this calculation is done without their explicit representation. A calculation with explicit grid representation is presented separately. The calculations have been performed on a 368 cm reactor model at the beginning of an equilibrium fuel cycle.

A comparison with deterministic reference solutions is not possible for this kind of calculations, because a pellet by pellet code is not available. Nevertheless, the flux behaviour along an assembly obtained with our method is consistent with incore measurements in similar configurations. An accuracy analysis of the method could be performed on simpler 3D benchmark configurations or on realistic configurations with Montecarlo codes.

Fine flux calculation in an assembly containing a control rod without grid representation

For this calculation the core has been axially modelled by 16 equally spaced nodes. The upper and lower reflectors have been modelled by 1 node each. Radially, each assembly has been modelled by 2×2 nodes. Nodes chosen for fine calculation have been divided in 2000 mesh points: 20 in the axial direction z and 10×10 in the radial directions x y, in order to have a mesh point per pin and a mesh point for the water gap separating one assembly from the other ones.

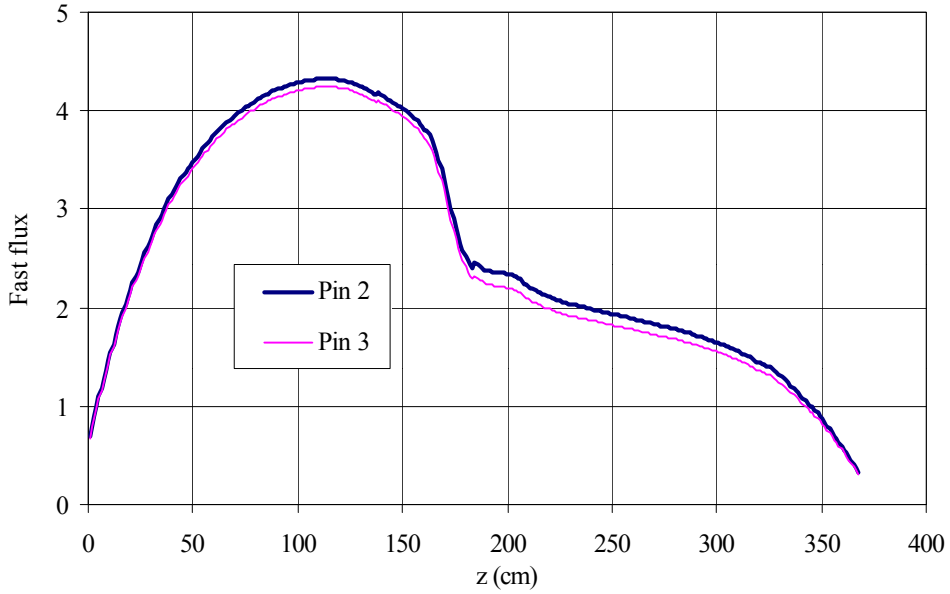

Fig. 2. Axial fast flux distribution in two pins of an assembly containing a control rod.

Control bank N2 (a black control bank) has been inserted by 53% in order to fill the 9th node (starting from the bottom) by 50%. This permits to analyse rod cusping induced effects. Just one assembly has been chosen for the fine calculation: a fresh fuel assembly controlled by bank N2.

The results are shown in Fig. 2 and 3 for two pins: one near an absorber pin (pin 3) and the other far from it. We can see that the curves have a smooth behaviour. Discontinuities across the node's boundaries are less than 1%. This result has been obtained by using a special homogenisation procedure for the control rods in the nodal calculation [3]. This procedure minimises rod cusping effect. With a simple volume weighting procedure, discontinuities can reach 80%. It is interesting to notice that the reflector induced thermal flux rise in the fuel extremities is well represented even without an explicit representation of it in the fine calculation. The reflector is represented implicitly by the albedo boundary conditions. A mesh effect appears in the node above the one containing the rod tip. It is probably due to the limitation of the second order transverse leakage fit used in the nodal calculation and in the boundary condition setting of the fine calculation.

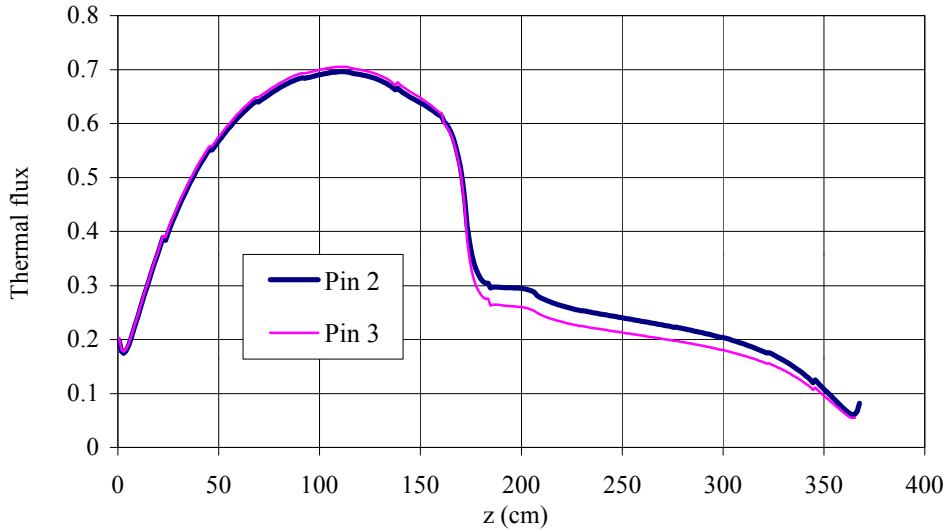

Fig. 3. Axial thermal flux distribution in two pins of an assembly containing a control rod.

Fine flux calculation in an assembly with grid representation

For this calculation the core has been axially modelled by 14 equally spaced nodes. The upper and lower reflectors have been modelled by 1 node each. Radially, each assembly has been modelled by 2 × 2 nodes. Nodes chosen for fine calculation have been divided in 2000 mesh points: 20 in the axial direction z and 10 × 10 in the radial directions x y, in order to have a mesh point per pin and a mesh point for the water gap separating one assembly from the other ones. The grids have been explicitly represented.

The results are shown in Fig. 4 and 5 for two pins: one near a water hole (pin 6) and the other far from it. We can see that the curves have a smooth behaviour. Discontinuities across the node's boundaries are less than 0.5%. This result has been obtained by using a special homogenisation procedure for the grids in the nodal calculation. This procedure is similar to the one proposed by K.S. Smith [4] and is based on a flux weighting of the grid cross sections and on the use of grid axial discontinuity factors. With a simple volume weighting procedure, discontinuities of about 2% appear on all of the node boundaries. This discrepancy is due to the big excursion of the neutron spectrum in a node containing a grid. Such a variation can not be represented by the nodal expansion without discontinuity factors.

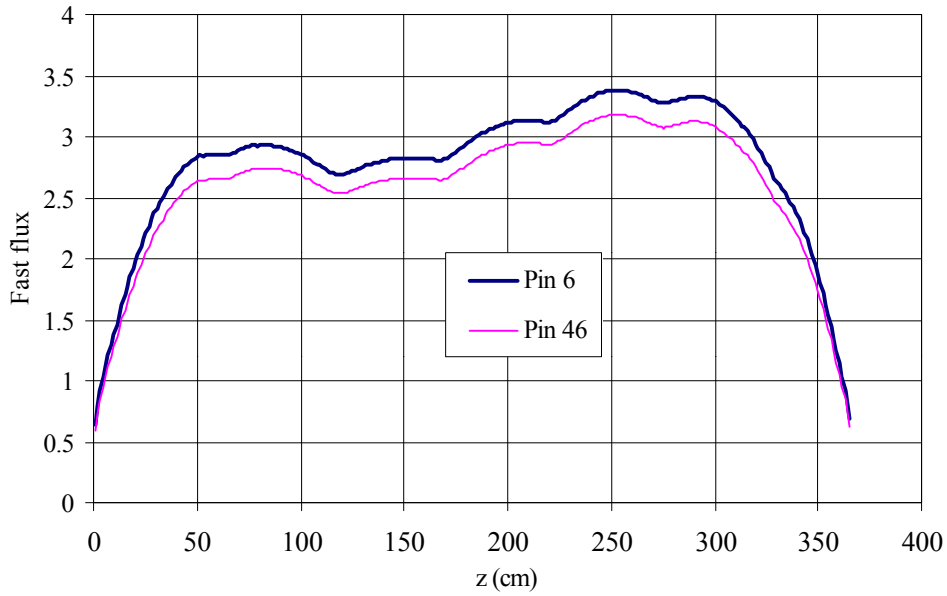

Fig. 4. Axial fast flux distribution in two pins of an assembly with explicit representation of the grids.

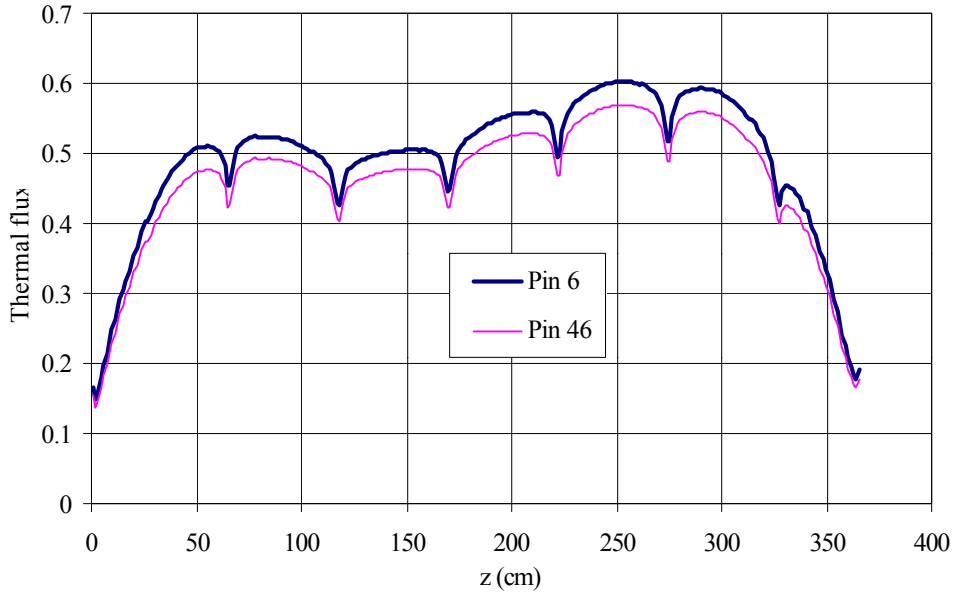

Fig. 5. Axial thermal flux distribution in two pins of an assembly with explicit representation of the grids.

Possible evolutions

Some evolutions are necessary to implement our approach for design purposes. We can summarise them in the following list:

- the use of intranodal cross section shapes to determine the base pellet by pellet distribution inside the node,
- the introduction of simple parametrized tables of delta cross sections,

- the numerical compression of the information constituted by the pellet by pellet burnup distribution and the use of interpolation functions to determine pellet by pellet nuclide densities from nodal values,
- the use of physical models more accurate than diffusion theory,
- the use of a method faster than Jacobi Chebyshev in solving the diffusion equation,
- the application of parallel processors (fine calculation in nodes can be performed independently).

A major evolution would be to modify the global calculation scheme by introducing the fine calculation in the iterative nodal calculation algorithm. This could be done, as suggested by K.S. Smith [1], in homogenising the fine cross sections on the fine flux computed between nodal iterations. In this case the second order transverse leakage fit must be abandoned both in the nodal calculation and in the boundary condition setting expressed by Eq. (5). Instead a 3D evaluation must be introduced as done in [5]. Framatome ANP has tested recently an alternative approach that eliminates this approximation.

Conclusions

The smooth behaviour of the axial flux curves presented confirms the consistency between the nodal and fine flux calculations. Indeed the boundary conditions guarantee the continuity of the ratio between the current and the flux only, not each of them. This continuity can be achieved only if consistent homogenisation procedures are used in the nodal calculation for heterogeneities like control rods or grids.

Due to the difficulty of performing reference full-core pellet by pellet calculations, a validation of this method could be performed on simple benchmark calculations.

The approach presented here can be considered as a good compromise between a full core 3D pin by pin calculation and a de-homogenisation calculation. It can be used in replacement of the latter for a limited choice of nodes for the following purposes.

- analyse assemblies containing replaced pins,
- modelise explicitly history effects for long time inserted control rods,
- modelise explicitly grids,
- modelise explicitly deformations of assembly water gaps.

In kinetic calculations a pin by pin approach can be irreplaceable in situations where the fundamental mode hypothesis, on which the de-homogenisation method is based, fails.

Acknowledgements

I would like to dedicate this paper to the memory of Michel Grosshans, who suggested this study in 1996.

This study has been possible thanks to the collaboration of Ludovic Bergé and Rachid Chaddi. The former has implemented the solving module in the SMART system. The second has performed a series of test cases including those presented in this paper.

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