Tomáš Berka; Marek Brandner; Milan Hanuš; Roman Kužel; Aleš Matas

Numerical modeling of neutron flux in hexagonal geometry

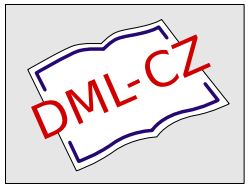
In: Jan Chleboun and Petr Přikryl and Karel Segeth and Tomáš Vejchodský (eds.): Programs and Algorithms of Numerical Mathematics, Proceedings of Seminar. Dolní Maxov, June 1-6, 2008. Institute of Mathematics AS CR, Prague, 2008. pp. 15–22.

Persistent URL: http://dml.cz/dmlcz/702852

Terms of use:

© Institute of Mathematics AS CR, 2008

Institute of Mathematics of the Czech Academy of Sciences provides access to digitized documents strictly for personal use. Each copy of any part of this document must contain these *Terms of use*.



This document has been digitized, optimized for electronic delivery and stamped with digital signature within the project *DML-CZ: The Czech Digital Mathematics Library* http://dml.cz

NUMERICAL MODELING OF NEUTRON FLUX IN HEXAGONAL GEOMETRY*

Tomáš Berka, Marek Brandner, Milan Hanuš, Roman Kužel, Aleš Matas

1. Introduction

Our concern in this paper is the *neutron flux* in the *VVER type nuclear reactors*. A nuclear reactor is composed of the fuel assemblies. An important feature of the VVER type nuclear reactors is that their fuel assemblies have *hexagonal shape*.

The *transport theory* and the *diffusion theory* are the two general ways how to model the neutron flux. In this paper we particularly study the *two-dimensional two-group neutron diffusion model*. We formulate the mathematical model in Section 2.

In the key Section 3 we present a modern variant of the *CMFD-nodal methods* suited particularly for solving the neutron diffusion equation on a hexagonal mesh. The method is build upon the *conformal mapping*. CMFD-nodal methods employ the technique called *transverse integration*. When applied to a hexagonal mesh, certain singular terms arise. Wagner's approach ([5] and [3]) is to simply ignore these terms. The approach involving conformal mapping gives more accurate results.

In Section 5 we introduce the integral part of nodal methods, the technique of *homogenization*. It determines how to transform the general equations with variable coefficients to the equations with node-wise constant coefficients. Such a procedure is based on conditions of preserving certain physical quantities.

2. Mathematical model

In the active zone of a nuclear reactor we consider the two-group neutron diffusion model. It is a *generalized eigenvalue problem* and can be written in the following way

$$\begin{aligned} \nabla \cdot \mathbf{j}^1(\mathbf{x}) + \Sigma_r^1(\mathbf{x})\phi^1(\mathbf{x}) &= \frac{1}{k_{\text{eff}}}\left[\nu\Sigma_f^1(\mathbf{x})\phi^1(\mathbf{x}) + \nu\Sigma_f^2(\mathbf{x})\phi^2(\mathbf{x})\right] \stackrel{\text{def.}}{=} s_1(\mathbf{x}), \\ \nabla \cdot \mathbf{j}^2(\mathbf{x}) + \Sigma_r^2(\mathbf{x})\phi^2(\mathbf{x}) &= \Sigma_s^{1\to 2}(\mathbf{x})\phi^1(\mathbf{x}) \stackrel{\text{def.}}{=} s_2(\mathbf{x}). \end{aligned} \tag{1}$$

The unknown quantities in (1) are the *neutron flux* ϕ^g (eigenfunction, $g = 1, 2$) and the *reactor critical number* k_{eff} (inverse of the largest eigenvalue). The superscript g corresponds to the energy group. The term $\mathbf{j}^g$ is the *neutron current* and we link it

*This work has been supported by the projects MSM4977751301 and 1M0545.

to the neutron flux ϕ^g through the following constitutive relation, which is called the *Fick's law*

$$\mathbf{j}^g(\mathbf{x}) = -D^g(\mathbf{x})\nabla\phi^g(\mathbf{x}). \tag{2}$$

The other terms present in (1) are given. They characterize certain material properties of the fuel assemblies.

At the boundary of the active zone of a nuclear reactor it is usual to consider the *albedo boundary conditions* of the form

$$\gamma\phi^1(\mathbf{x}) - \mathbf{j}^1(\mathbf{x})\cdot\mathbf{n}(\mathbf{x}) = 0, \quad \gamma\phi^2(\mathbf{x}) - \mathbf{j}^2(\mathbf{x})\cdot\mathbf{n}(\mathbf{x}) = 0, \tag{3}$$

where γ is a given albedo coefficient.

3. Conformal mapping method

For numerical solution of the problem (1)–(3), we use the *conformal mapping method*. This method is a variant of the *CMFD-nodal methods* which are a combination of the CMFD (Coarse Mesh Finite Differences) and the *two-node problems* (see [5], [3]). CMFD is just a finite volume method applied to the physical node-wise discretization mesh of an active zone. It gives us the neutron fluxes averaged over particular nodes, six values of neutron currents averaged over the nodal faces and the critical number. Two-node problems are solved semianalytically and give us more accurate surface currents, which we use to correct the iteration matrix of the CMFD. These two general steps are repeated until convergence is achieved. The CMFD is a nonlinear procedure in this context and is intended to accelerate convergence of the whole process.

Conformal mapping method is designed specifically for hexagonal meshes, where it is more accurate then classical CMFD-nodal methods. The CMFD part is identical to another CMFD-nodal methods. Solution of the two-node problems is based on use of the conformal mapping, particularly the Schwarz-Christoffel transformation, which maps a complex half-plane onto the interior of a polygon. We utilize this transformation to map the interior of a hexagon in a complex plane $z = x + \mathrm{i}y$ onto the interior of a *rectangle* in a complex plane $w = u + \mathrm{i}v$ (see Fig. 1). Construction of the mentioned mapping is described in detail in [2].

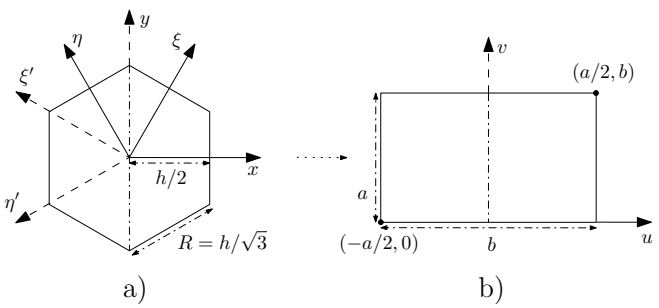


Fig. 1: *Conformally mapped hexagon onto a rectangle.*

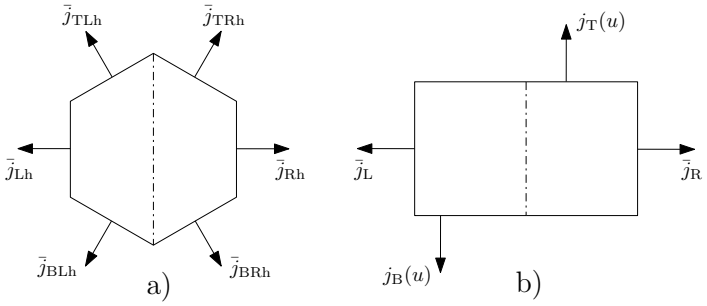


Fig. 2: *The notation of averaged currents.*

Below, we use the following notation; the quantities with the subscript "h" correspond to a hexagon, the other correspond to a rectangle. The subscripts "R", "L", "T", "B" stand for "right", "left", "top", "bottom" halves of a hexagon or a rectangle respectively; see Fig. 2 for the notation of averaged currents on the boundary of a hexagon and a rectangle. The over-bar denotes surface averaged quantities. The tilde denotes transverse integrated quantities (see Section 3.1).

3.1. Two-node problems

We solve three two-node problems corresponding to the directions x, ξ and η (see Fig. 1a) for the pairs of currents $(\bar{j}_{\mathrm{Lh}}, \bar{j}_{\mathrm{Rh}})$, $(\bar{j}_{\mathrm{TRh}}, \bar{j}_{\mathrm{BLh}})$ and $(\bar{j}_{\mathrm{TLh}}, \bar{j}_{\mathrm{BRh}})$ respectively. These steps are performed successively. We present the x-step. The other steps are analogous.

In the following, we omit the group index. If we transform the first equation in (1) valid over the interior of a hexagonal node $\mathcal{H}_i$ from the coordinate system xy to the coordinate system uv we obtain

$$-D\Delta\phi(u,v) + \Sigma_r g^2(u,v)\phi(u,v) = g^2(u,v)s(u,v) \tag{4}$$

valid over a rectangle $\mathcal{R}_i$. The second equation in (1) can be proceeded in the same way. The function $g(u,v)$ is defined on a hexagonal node as

$$g(u,v) = \left|\frac{\mathrm{d}z}{\mathrm{d}w}\right|. \tag{5}$$

The term $1/g^2(u,v)$ appears in the image of the Laplace operator as a weighting factor.

Now we apply the *transverse integration* on (4) and obtain

$$-D\frac{\mathrm{d}^2\tilde{\phi}(u)}{\mathrm{d}u^2} + \Sigma_r\tilde{g^2}(u)\tilde{\phi}(u) = \tilde{g^2}(u)\tilde{s}(u) - l_v(u), \tag{6}$$

where

$$\tilde{\phi}(u) = \frac{1}{b}\int_0^b \phi(u,v)\,\mathrm{d}v, \quad \tilde{g^2}(u) = \frac{\frac{1}{b}\int_0^b g^2(u,v)\phi(u,v)\,\mathrm{d}v}{\tilde{\phi}(u)} \sim \frac{1}{b}\int_0^b g^2(u,v)\,\mathrm{d}v. \tag{7}$$

The approximation of the term $\tilde{g^2}(u)$ is discussed in [2].

The *transverse leakage* $l_v(u)$ on a rectangle in the direction v at a point u is defined as follows

$$l_v(u) = \frac{1}{b}\big(j_{\mathrm{T}}(u) - j_{\mathrm{B}}(u)\big). \tag{8}$$

There are several ways how to approximate this term. The simplest method is to consider *constant leakage on the hexagon half-nodes*. It can be expressed on a rectangle as

$$l_{v\mathrm{L}}(u) = \frac{1}{b}g(u,0)(\bar{j}_{\mathrm{TLh}} - \bar{j}_{\mathrm{BLh}}), \quad l_{v\mathrm{R}}(u) = \frac{1}{b}g(u,0)(\bar{j}_{\mathrm{TRh}} - \bar{j}_{\mathrm{BRh}}). \tag{9}$$

The other possibility is to assume the transverse leakage *linear on the boundary half-nodes* and *constant on the inner half-nodes*, which is more complicated. We need to determine two unknowns for a linear function. We acquire them from the global boundary condition information and from the condition of preservation of the total leakage on the boundary half-nodes (see [6]).

3.2. Semi-analytic solution

We seek for a solution of (6) in the following form

$$\tilde{\phi}(u) = \underbrace{a_0 p_0(u) + a_1 p_1(u) + a_2 p_2(u)}_{\text{particular}} + \underbrace{a_3 \sinh(ku) + a_4 \cosh(ku)}_{\text{homogeneous}}, \tag{10}$$

where

$$k = \sqrt{\frac{\tilde{g^2}(a/2)\Sigma_r}{D}}. \tag{11}$$

The solution (10) has two parts. The homogeneous part is the approximation of the analytical solution to the homogeneous part of the equation. The particular part is sought in the space of quadratic polynomials (p_0, p_1, p_2) in the weighted residue sense and solves approximately the complete inhomogeneous equation.

The solution has five unknown coefficients. One of them is determined from the condition of preserving the CMFD's node averaged flux. Another three are given by matching the zeroth, first, and second moment conditions of the weighted residue. The last one arises from the continuity of the flux and current at the interface of two adjacent nodes. On the boundary, we employ the boundary condition instead (see e.g. [3]).

The surface averaged currents at the points $u = \pm a/2$ can be derived from (10) and (2) as follows

$$\bar{j}_{\mathrm{L}} = \tilde{j}(u = -a/2) = -D\frac{\mathrm{d}\tilde{\phi}(u)}{\mathrm{d}u}\bigg|_{u=-a/2}, \tag{12}$$

$$\bar{j}_{\mathrm{R}} = \tilde{j}(u = +a/2) = -D\frac{\mathrm{d}\tilde{\phi}(u)}{\mathrm{d}u}\bigg|_{u=+a/2}. \tag{13}$$

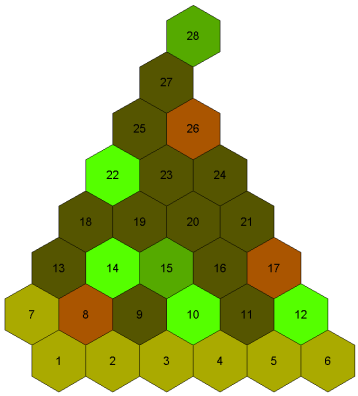
It can be proved (after proper normalization of $g(u, v)$) that the following relations between the currents on a hexagon and the currents on a rectangle hold true

$$\bar{j}_{\mathrm{Lh}} = \frac{b}{R}\bar{j}_{\mathrm{L}}, \quad \bar{j}_{\mathrm{Rh}} = \frac{b}{R}\bar{j}_{\mathrm{R}}. \tag{14}$$

The quantities $\bar{j}_{\mathrm{Lh}}$ and $\bar{j}_{\mathrm{Rh}}$ are used to correct the CMFD iteration matrix.

4. Benchmark

We undertook a numerical test on a sample configuration of a VVER-440 reactor, the experiment parameters are detailed in Benchmark no. 6 in [1]. On the picture below we see the scheme of the configuration of one sixth of the core, which is one sixth rotationally symmetric. The reactor critical number k_{eff} and the *node averaged power distributions* (PD, derived from the neutron fluxes) were computed using the approach described in previous sections with constant leakage (code of Roman Kužel). Then we compared the results with accurate result of the FVM on a fine mesh (code of Milan Hanuš).



- $k_{\mathrm{eff}} = 1.01447$
- k_{eff} error $= -7.89 \times 10^{-5}$
- PD avg. error $= 1.48\%$
- PD max. error $= 1.93\%$

5. Homogenization

As soon as analytical approach is to be used for solving neutron diffusion equation, it is necessary to transform the general diffusion equation with variable coefficients to an equation with node-wise constant coefficients. We call the original problem heterogeneous and the latter homogeneous. Such a transformation is possible through the technique of *homogenization*. Generally, it means that we require certain physical quantities from the heterogeneous problem to be preserved in the solution of the homogeneous problem. In this way, we acquire the constant coefficients. Let us consider only one energy group. The other groups can be proceeded in a similar way (see [4]).

We denote quantities corresponding to the homogeneous problem with a hat over a quantity. The other correspond to the heterogeneous problem. The symbol i stands for the index of a node.

5.1. Principle

Our main goal is to preserve the reactor critical number. We proceed with the one-group (for more groups, see [4]) integral formulation of the system (1) in a node $\mathcal{H}_i$

$$\sum_{k=1}^{6} \int_{\Gamma_{i,k}} \mathbf{j}(\mathbf{x}) \cdot \mathbf{n}_{i,k} \, \mathrm{d}S + \int_{\mathcal{H}_i} \Sigma_r(\mathbf{x}) \phi(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \frac{1}{k_{\mathrm{eff}}} \nu \int_{\mathcal{H}_i} \Sigma_f(\mathbf{x}) \phi(\mathbf{x}) \, \mathrm{d}\mathbf{x}, \qquad (15)$$

where $\Gamma_{i,k}$ is a k-th surface ($k = 1, \ldots, 6$) of a hexagonal node $\mathcal{H}_i$. Preservation of the reactor critical number can be directly fulfilled by (15) if we define the constant coefficients, such that the *reaction rates* and the *surface averaged currents* are preserved

$$\int_{\mathcal{H}_i} \hat{\Sigma}^i_{(.)} \hat{\phi}(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \int_{\mathcal{H}_i} \Sigma_{(.)}(\mathbf{x}) \phi(\mathbf{x}) \, \mathrm{d}\mathbf{x} \quad \Rightarrow \quad \hat{\Sigma}^i_{(.)} = \frac{\int_{\mathcal{H}_i} \Sigma_{(.)}(\mathbf{x}) \phi(\mathbf{x}) \, \mathrm{d}\mathbf{x}}{\int_{\mathcal{H}_i} \hat{\phi}(\mathbf{x}) \, \mathrm{d}\mathbf{x}},$$

$$\int_{\Gamma_{i,k}} \hat{\mathbf{j}}(\mathbf{x}) \cdot \mathbf{n}_{i,k} \, \mathrm{d}S = \int_{\Gamma_{i,k}} \mathbf{j}(\mathbf{x}) \cdot \mathbf{n}_{i,k} \, \mathrm{d}S \quad \Rightarrow \quad \hat{D}^i = \frac{\int_{\Gamma_{i,k}} \mathbf{j}(\mathbf{x}) \cdot \mathbf{n}_{i,k} \, \mathrm{d}S}{-\int_{\Gamma_{i,k}} \nabla \hat{\phi}(\mathbf{x}) \cdot \mathbf{n}_{i,k} \, \mathrm{d}S}.$$

5.2. Approximate theories

In the principle described above, we assume that the heterogeneous and the homogeneous solutions of the problem are known. They provide the homogenized parameters. In practice, we do not know the heterogeneous solution. At the beginning of the calculation, we also do not know the homogeneous solution. Therefore, we have to define the homogenized coefficients in a different way using *approximate homogenization theories* based on the flux-weighted constants (FWC) and on the general equivalence theory (GET), see [4], described in the following sections.

Instead of computing the heterogeneous solution of the global problem, we calculate the solution of the *one-node problems* for different types of assemblies. It means that we do not take into account the geometry of the active zone and we have to choose some suitable boundary conditions. Usually we impose zero net current at the boundary of an assembly. Then, we consider such solution as heterogeneous (exact) and use it to determine the homogenized parameters.

Another possibility is to consider the *seven-node problem*. To determine the homogenized parameters of some node $\mathcal{H}_i$ we solve the heterogeneous problem on the domain composed of $\mathcal{H}_i$ and its six neighbors. The zero net current BCs are prescribed on the surfaces of the neighbors. This approach leads to higher accuracy of the computed homogenized parameters of the considered node. It is necessary to take into account position of $\mathcal{H}_i$ in the active zone and to solve the seven-node problem for each node in the reactor.

5.3. Flux-weighted constants (FWC)

This is the simplest method for computing the homogenized coefficients. We consider two general approximations. The first is the following

$$\int_{\mathcal{H}_i} \phi(\mathbf{x})\,\mathrm{d}\mathbf{x} \approx \int_{\mathcal{H}_i} \hat{\phi}(\mathbf{x})\,\mathrm{d}\mathbf{x}. \tag{16}$$

The other approximation is the definition of the homogenized diffusion coefficient arising from the transport theory as follows

$$\frac{1}{\hat{D}^i} = \frac{\int_{\mathcal{H}_i} \phi(\mathbf{x})/D^g(\mathbf{x})\,\mathrm{d}\mathbf{x}}{\int_{\mathcal{H}_i} \phi(\mathbf{x})\,\mathrm{d}\mathbf{x}}. \tag{17}$$

The crucial problem of FWC is that we cannot determine one diffusion coefficient for one node, such that *surface averaged fluxes are continuous on each nodal surface.* For a thourough analysis of the problem, see [4].

5.4. General equivalence theory (GET)

This theory withdraws the problem of FWC by relaxing the continuity of the fluxes on the interfaces of the nodes. For this purpose, we introduce the new homogenization parameters called the *factors of discontinuity* corresponding to a node $\mathcal{H}_i$ on the surfaces $(\mathcal{H}_i, \mathcal{H}_{i+1})$ and $(\mathcal{H}_i, \mathcal{H}_{i-1})$ (considering direction x) as follows

$$f_i^{x+} = \frac{\int_{\Gamma_{i,x+}} \phi(\mathbf{x})\,\mathrm{d}S}{\int_{\Gamma_{i,x+}} \hat{\phi}(\mathbf{x})\,\mathrm{d}S}, \quad f_i^{x-} = \frac{\int_{\Gamma_{i,x-}} \phi(\mathbf{x})\,\mathrm{d}S}{\int_{\Gamma_{i,x-}} \hat{\phi}(\mathbf{x})\,\mathrm{d}S}. \tag{18}$$

To eliminate the unknown homogeneous solution from the definition of f_i^{x+} (analogically for f_i^{x-}) the following equalities must hold

$$\int_{\Gamma_{i,k}} \hat{\phi}(\mathbf{x})\,\mathrm{d}S = \int_{\mathcal{H}_i} \hat{\phi}(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_{\mathcal{H}_i} \phi(\mathbf{x})\,\mathrm{d}\mathbf{x}. \tag{19}$$

The first equality follows from the fact that the homogeneous solution of the one-node problems is constant. We can rewrite (18) for f_i^{x+} (analogically for f_i^{x-}) in the following way

$$f_i^{x+} = \frac{\int_{\Gamma_{i,x+}} \phi(\mathbf{x})\,\mathrm{d}S}{\int_{\Gamma_{i,x+}} \hat{\phi}(\mathbf{x})\,\mathrm{d}S} = \frac{\int_{\Gamma_{i,x+}} \phi(\mathbf{x})\,\mathrm{d}S}{\int_{\mathcal{H}_i} \phi(\mathbf{x})\,\mathrm{d}\mathbf{x}}. \tag{20}$$

At this point we substitute continuity of the flux on an interface with the *discontinuity condition*

$$f_i^{x+} \int_{\Gamma_{i,x+}} \hat{\phi}(\mathbf{x})\,\mathrm{d}S = f_{i+1}^{x-} \int_{\Gamma_{i+1,x-}} \hat{\phi}(\mathbf{x})\,\mathrm{d}S. \tag{21}$$

As we relaxed continuity of the flux, we can choose the diffusion coefficient entirely arbitrarily in so far it has a physical meaning. It is reasonable to use the FWC choice (17).

5.5. Algorithm

Solution procedure of the whole reactor problem together with homogenization can be summarized in the following steps:

1. Calculate the homogenized parameters from the one-node problems for different types of assemblies or from seven-node problems for the whole reactor.
2. Calculate the homogeneous solution of the whole reactor problem.
3. Calculate the homogenized parameters from the one-node or seven-node problems for the whole reactor. Use the surface currents calculated in the step 2 or 4 as a new boundary condition for these problems.
4. Calculate the homogeneous solution of the whole reactor problem.
5. Check the convergence of the homogenized parameters by inspection of two successive approximations. If the difference is too large continue from step 3.

Usually two iterations of the whole algorithm are sufficient to achieve required accuracy.

References

[1] Y.A. Chao, Y.A. Shatilla: *Conformal mapping and hexagonal nodal methods – II: Implementation in the ANC-H code.* Nuclear Science and Engineering, **121**, 1995, 210–225.

[2] Y.A. Chao, N. Tsoulfanidis: *Conformal mapping and hexagonal nodal methods – I: Mathematical foundation.* Nuclear Science and Engineering, **121**, 1995, 202–209.

[3] M. Hanuš: *Numerical modelling of neutron flux in nuclear reactors.* Bachelor's thesis, Univ. of West Bohemia, Pilsen, 2007.

[4] K.S. Smith: *Spatial homogenization methods for light water reactor analysis.* PhD Thesis, Nuclear Engineering, Massachusetts Institute of Technology, 1980.

[5] M.R. Wagner: *Three-dimensional nodal diffusion and transport theory methods for hexagonal-z geometry.* Nuclear Science and Engineering, **103**, 1989, 377–391.

[6] V.G. Zimin, D.M. Baturin: *Polynomial nodal method for solving neutron diffusion equations in hexagonal-z geometry.* Annals of Nuclear Energy, **29**, 2002, 303–335.