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# Polynomial nodal method for solving neutron diffusion equations in hexagonal-z geometry

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## Abstract

A polynomial nodal method is developed to solve few-group neutron diffusion equations in hexagonal-z geometry. The method is based on conformal mapping of a hexagon into a rectangle. The resulting equations are solved using a fourth-order expansion of the transverse-integrated neutron flux into orthogonal polynomials. The transverse leakage is represented using constant neutron currents at the faces of the internal reactor nodes and a linear approximation of the current at the faces of the nodes at the reactor boundary. A nonlinear iteration procedure is used for solving the nodal equations. The neutron flux expansion coefficients are found by considering a two-node problem for each node interface. Due to orthogonality of the polynomials,  $8G$  nodal equations for the two-node problem are reduced to two systems of  $G$  and  $2G$  equations. The method is implemented into the nodal neutron kinetics code SKETCH-N. The results of steady-state benchmark problems have demonstrated excellent accuracy of the method. © 2002 Elsevier Science Ltd. All rights reserved.

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## 1. Introduction

In the Russian pressurized water reactors VVER-440 and VVER-1000, fuel assemblies form a hexagonal lattice. The hexagonal geometry is also used in liquid-metal fast breeder reactors and designs of heavy water reactors and high-temperature gas cooled reactors. For analysis of these reactor types, a neutron diffusion code should be able to treat a hexagonal spatial mesh. Since the middle of the 1970s, various methods to solve the neutron diffusion equations in this geometry have been

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developed. In this introduction, we briefly discuss only the papers directly related to our work, the reviews by Kulikowska (1981), by Lawrence (1986) and by Gadó and Schmidt (1987) provide further references to the literature on the subject.

Presently, the most popular methods are of a nodal type, where the primary unknowns are node-averaged and face-averaged quantities. In the case of Cartesian geometry, the transverse-integrated nodal methods become practically standard tools, due to their high accuracy and low computing time. The recent papers by Chao and coworkers (Chao and Shatilla, 1995; Chao and Tsolfanidis, 1995, 1995) provide a sound mathematical basis for an extension of these methods to hexagonal geometry using conformal mapping of the hexagon into a rectangle. A transverse-integrated procedure is applied in the new coordinate system and the methods developed for Cartesian geometry can be used. However, some differences arise because the rectangle in the new coordinate system is heterogeneous, with heterogeneity imposed by the conformal mapping scale function.

In the ANC-H code (Chao and Shatilla, 1995), a semi-analytic nodal method is applied for a solution of the transformed neutron diffusion equations. The basic functions of the method include hyperbolic sine and cosine, which are introduced by an analogy with Cartesian geometry. The transverse leakage is constructed assuming a linear shape of the neutron current at the faces of the hexagon. A slope of the linear function is estimated from the flux values on the adjacent surfaces. The presented numerical results of the benchmark problems demonstrate the excellent accuracy of the method (Chao and Shatilla, 1995). Following the work of Chao, conformal mapping has been also applied in the PANTHER code (Knight et al., 1995), where an analytic nodal method is used. Analytic basic functions for heterogeneous node are precalculated and presented in the code using a rational approximation. This approach minimizes the errors of the neutron flux expansion, but requires an additional work to precompute and to approximate the analytic basic functions. Moreover, a selection of the order of the rational approximation, which provides the desired accuracy and minimizes the computing time, is a problem dependent. The transverse leakage in the PANTHER code is constructed from a step function assuming constant neutron currents at the faces of the hexagon.

In this paper, the conformal mapping is also used to transform the hexagon into a rectangle. The differences from the methods cited above are in the transverse leakage approximation and in the method of solving the resulting one-dimensional equation. The transverse leakage for internal reactor nodes is approximated assuming constant currents at the faces of the hexagon as in the PANTHER code (Knight et al., 1995), while for the boundary nodes a linear shape of the transverse leakage is assumed at the half of the node adjacent to the boundary. A slope of the linear function is estimated from the boundary conditions. This linear approximation significantly improves the method accuracy especially in the cases when a radial reflector is not considered explicitly but treated as boundary conditions, and involves only a quite limited amount of additional computations. Resulting one-dimensional equations are solved by a polynomial nodal method. The polynomials are chosen to form an orthogonal system. The transverse-integrated neutron flux is expanded into the polynomials up to the fourth order. The solution of the nodal equations is similar to

that of the polynomial nodal method developed for Cartesian geometry (Zimin et al., 1998). A nonlinear iteration procedure is used. The solution of the neutron diffusion equations is decoupled into global iterations of a coarse-mesh finite-difference method and a recalculation of the coupling coefficients by solving the nodal equations for local two-node problems. For each two-node problem, the nodal equations consist of nodal balance equations, first- and second-order moment-weighting equations and conditions of the flux and current continuity at the face between two nodes. Due to orthogonality of the polynomials a system of  $8G$  nodal equations is reduced to two systems of  $G$  and  $4G$  equations.

The paper is organized as follows. In Section 2, we give a brief description of the conformal mapping of the hexagon into a rectangle and present the neutron diffusion equations in the new coordinate system. A transverse leakage approximation is discussed in Section 3. A polynomial nodal method for a solution of the resulting one-dimensional equations is given in Section 4. Section 5 demonstrates accuracy of the method presenting results of steady-state benchmark problems. Section 6 gives a summary and concludes the paper.

## 2. Neutron diffusion equations under conformal mapping

Let us consider a reactor domain consisting of a union of hexagonal-z nodes. In terms of the local coordinates, the node  $k$  is defined as

$$V^k(x, y, z): \quad \begin{aligned} x &\in [-h/2, h/2]: \\ y &\in [-y_s(x), y_s(x)], \quad y_s(x) = (h - |x|)/\sqrt{3}; \\ z &\in [-\Delta z^k/2, \Delta z^k/2]; \end{aligned}$$

where  $h$  is the assembly lattice pitch and the  $x$ -axis is taken perpendicular to a one pair of the opposite faces of the hexagon.

Few-group steady-state neutron diffusion equations are written in the matrix form as follows

$$\begin{aligned} -D^k \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \varphi^k(x, y, z) + \\ \left[ \Sigma_r^k - \Sigma_s^k - \frac{1}{k_{\text{eff}}} \chi \left( v \Sigma_f^k \right)^T \right] \varphi^k(x, y, z) = 0, \end{aligned} \quad (1)$$

where  $\varphi(x, y, z) = \text{col}\{\varphi_1(x, y, z), \dots, \varphi_G(x, y, z)\}$  is the neutron flux;  $\Sigma_r$  is the diagonal matrix of the removal cross-sections;  $\Sigma_s$  is the matrix of the macroscopic scattering cross-sections;  $k_{\text{eff}}$  is the reactor multiplication factor;  $\chi = \text{col}\{\chi_1, \dots, \chi_G\}$  is the prompt fission spectrum;  $v \Sigma_f = \text{col}\{v \Sigma_{f1}, \dots, v \Sigma_{fG}\}$  is the production cross-sections;  $D$  is the diagonal matrix of the diffusion coefficients;  $T$  is the index of the transpose operation.

Integrating Eq. (1) over the node in  $z$ -direction results in

$$-D^k \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \varphi_z^k(x, y) + \left[ \Sigma_r^k - \Sigma_s^k - \frac{1}{k_{\text{eff}}} \chi \left( v \Sigma_f^k \right)^T \right] \varphi_z^k(x, y) = -L_z^k(x, y), \quad (2)$$

where  $\varphi_z^k(x, y) = \frac{1}{\Delta z_k} \int_{-\Delta z_k/2}^{\Delta z_k/2} \varphi^k(x, y, z) dz$  is the  $z$ -integrated neutron flux;  $L_z^k(x, y) = \frac{1}{\Delta z_k} \{ J_z^k(x, y, \Delta z_k/2) - J_z^k(x, y, -\Delta z_k/2) \}$  is the leakage in  $z$ -direction;  $J_z^k(x, y, \pm \Delta z_k/2)$  is the  $z$ -component of the neutron current at the top (+) and bottom (−) faces of the node.

To solve Eq. (2), we apply a conformal mapping of the hexagon into a rectangle following the work of Chao and co-workers (Chao and Shatilla, 1995; Chao and Tsolfanidis, 1995). The conformal mapping is a coordinate transformation of the original complex plane  $\mathbb{Z} = x + iy$  into the complex plane  $\mathbb{W} = u + iv$ . The domain of the mapping is an interior of the hexagon, which is mapped into the interior of the rectangle of the  $\mathbb{W}$ -plane. The mapping is constructed using three successive conformal transformations: the rectangle into a half plane, the half plane into a circle and the circle into a hexagon. The explicit formulas are given in (Chao and Tsolfanidis, 1995). In the  $\mathbb{W}$ -plane, the rectangle is defined as

$$V^k(u, v) : u \in [-a/2, a/2] \text{ and } v \in [0, b].$$

The ratio of the rectangle sides  $a/b$  is defined by the conformal mapping. The values  $a$  and  $b$  are found from the requirement that the area of the rectangle is equal to the area of the hexagon and they are expressed in terms of the hexagonal assembly lattice pitch  $h$  as

$$a/h \approx 1.052557 \text{ and } b/h \approx 0.822872.$$

Laplacian operator is invariant under the conformal mapping in the following sense

$$\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) = \frac{1}{g^2(u, v)} \left( \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right),$$

where  $g(u, v) = |d\mathbb{Z}/d\mathbb{W}|$  is the mapping linear scale function.

In the following, we assume that the transverse leakage in the axial direction  $L_z^k(x, y)$  does not depend on the coordinates  $(x, y)$  and is equal to an average value as

$$L_z^k(x, y) = \bar{L}_z^k = \frac{1}{\Delta z^k} \left\{ \bar{J}_z^k(\Delta z^k/2) - \bar{J}_z^k(-\Delta z^k/2) \right\},$$

where  $\bar{J}_z^k(\pm \Delta z^k/2)$  are the face-averaged neutron currents in  $z$ -direction at the top (+) and bottom (−) faces of the node.

Integrating Eq. (2) over the node in  $v$ -direction results in the one-dimensional transverse-integrated equation as

$$-\frac{d^2\Phi^k(u)}{du^2} + (B^2)^k \bar{g}^2(u) \Phi^k(u) = -(D^k)^{-1} \left\{ L_v^k(u) + \bar{g}^2(u) \bar{L}_z^k \right\}, \quad (3)$$

where  $\Phi^k(u) = \frac{1}{b} \int_0^b \varphi_z^k(u, v) dv$  is the transverse-integrated neutron flux;  $(B^2)^k = (D^k)^{-1} [\Sigma_r^k - \Sigma_s^k - \frac{1}{k_{eff}} \chi(v \Sigma_f^k)^T]$  is the buckling matrix;  $\bar{g}^2(u) = \frac{1}{b} \frac{1}{\Phi^k(u)} \int_0^b g^2(u, v) \varphi_z^k(u, v) dv \approx \frac{1}{b} \int_0^b g^2(u, v) dv$ , the approximation discussed in (Chao and Tsolfanidis, 1995);  $L_v^k(u) = \frac{1}{b} \{J_v(u, b) - J_v(u, 0)\}$  is the transverse leakage in  $v$ -direction.

Note that the transverse integration on the  $\mathbb{W}$ -plane corresponds to integrating along the vertical curvilinear lines  $u = \text{constant}$  with the weighting factor  $1/g(u, v)$  on the  $\mathbb{Z}$ -plane.

Introducing the nondimensional coordinates  $\xi = 2u/a$ , the transverse-integrated neutron diffusion Eq. (3) is written as follows:

$$-\frac{d^2\Phi^k(\xi)}{d\xi^2} + (\hat{B}^2)^k \bar{g}^2(\xi) \Phi^k(\xi) = -s_v^k(\xi) - s_z^k(\xi), \quad (4)$$

where  $s_v^k(\xi) = (a^2/4)(D^k)^{-1} L_v^k(\xi)$ ;  $s_z^k(\xi) = (a^2/4)(D^k)^{-1} \bar{g}^2(\xi) \bar{L}_z^k$ ;  $(\hat{B}^2)^k = \frac{a^2}{4} (B^2)^k$ .

### 3. Transverse leakage approximation

Normal components of the neutron current at the faces of the rectangle  $J_v(u, b)$  can be expressed in terms of the normal components of the neutron current at the faces of hexagon as

$$J_v(u, b) = g(u, b) J_T(x, y_s(x)) \quad \text{and} \quad J_v(u, 0) = g(u, 0) J_B(x, -y_s(x)),$$

where  $J_T(x, y_s(x))$ ,  $J_B(x, -y_s(x))$  are the normal components of the neutron current at the top and bottom faces of the hexagon, respectively; and  $g(u, b) = g(u, 0)$ .

The transverse leakage  $L_v^k(u)$  can be divided into two parts corresponding to the left and right halves of the node as follows

$$L_v^k(u) = L_{vL}^k(u) \mu(-u) + L_{vR}^k(u) \mu(u),$$

where  $L_{vL}^k(u)$ ,  $L_{vR}^k(u)$  are the transverse leakages for the left and right halves of the node;

$$\mu(u) = \begin{cases} 0 & \text{if } u < 0, \\ 1 & \text{if } u > 0 \end{cases} \text{ is the unit step function.}$$

Assuming that the normal components of the neutron current are constant at the faces of the hexagon we obtain

$$L_{vL}^k(u) = \frac{3h}{2b} g(u, 0) \bar{L}_{vL}^k \quad \text{and} \quad L_{vR}^k(u) = \frac{3h}{2b} g(u, 0) \bar{L}_{vR}^k,$$

where  $\bar{L}_{vL}^k = (2/3h)\{\bar{J}_{TL}^k - \bar{J}_{BL}^k\}$  is the average transverse leakage in the left half of the hexagon;  $\bar{L}_{vR}^k = (2/3h)\{\bar{J}_{TR}^k - \bar{J}_{BR}^k\}$  is the average transverse leakage in the right half of the hexagon.

The definition of the normal components of the neutron current is illustrated in Fig. 1. The approximation of the face-averaged neutron current by a constant gives a step function representation of the transverse leakage shape, which is similar to the case of the “flat” leakage approximation in Cartesian geometry. First results of the benchmark problem calculations have shown that this approximation yields relatively large errors in the cases when a radial reflector is replaced by boundary conditions. To improve accuracy the neutron currents at the top and at the bottom faces of the half of the nodes adjacent to the boundary are approximated by linear functions. For example, considering a node with the boundary at the right, the neutron current at the top right face is approximated as

$$J_{TR}^k(x') = \bar{J}_{TR}^k + I_{TR}^k(x' - x'_0).$$

The local coordinate line  $x'$  is defined at the top right face of the hexagon as shown in Fig. 2. On the  $\mathbb{W}$ -plane, the neutron current is expressed as

$$J_{TR}^k(u) = g(u, 0) \left( \bar{J}_{TR}^k + I_{TR}^k \left[ \int_0^u g(u', 0) du' - x'_0 \right] \right).$$

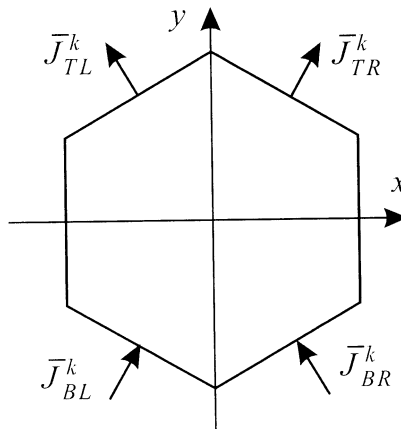


Fig. 1. Local coordinate system of a hexagon and the definition of the face-averaged neutron currents.

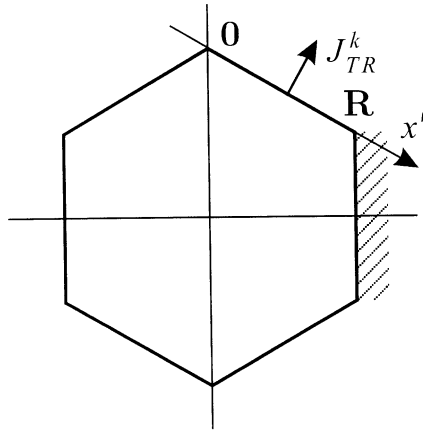


Fig. 2. Local coordinate system for linear approximation of the neutron current  $J_{TR}^k(x')$ .

Using a similar representation for the neutron current at the bottom right face of the node, the transverse leakage of the right half of the node is expressed as

$$L_{vR}^k(u) = \frac{3h}{2b} g(u, 0) \left( \bar{L}_{vR}^k + l_R^k \left[ \int_0^u g(u', 0) du' - x'_0 \right] \right),$$

where  $l_R^k = l_{TR}^k - l_{BR}^k$ .

Introducing the nondimensional coordinate  $\xi = 2u/a$  we obtain

$$L_{vR}^k(\xi) = \frac{3h}{2b} g(\xi, 0) \left( \bar{L}_{vR}^k + \hat{l}_R^k [f(\xi) - \xi_0] \right),$$

where  $f(\xi) = \int_0^\xi g(\tau, 0) d\tau$ ;  $\hat{l}_R^k = R l_R^k$ ;  $\xi_0 = x'_0/R$ .

The constant  $\xi_0$  is defined from the condition of preserving the average transverse leakage over the right half of the node, i.e.

$$\xi_0 = \int_0^1 g(\xi, 0) f(\xi) d\xi / \int_0^1 g(\xi, 0) d\xi.$$

The constant  $\hat{l}_R^k$  is determined by the requirement that the transverse leakage of the right half of the hexagon satisfies the boundary condition.

#### 4. Solution of the nodal equations

A nonlinear iteration procedure (Smith, 1984) is used as a global solution technique. In this procedure, the face-averaged neutron current is expressed as

$$J_{x+}^k = -\tilde{D}^k(\text{fd})\left(\bar{\Phi}^{k+1} - \bar{\Phi}^k\right) - \tilde{D}^k(\text{nod})\left(\bar{\Phi}^{k+1} + \bar{\Phi}^k\right),$$

where  $k+1$  is the index of the neighboring node in the positive  $x$ -direction;  $\tilde{D}^k(\text{fd})$  is the diagonal matrix of the known coupling coefficients of the mesh-centered finite-difference method;  $\tilde{D}^k(\text{nod})$  is the diagonal matrix of the unknown coupling coefficients of the nodal method.

Substituting this expression for the neutron current into a neutron balance equation we obtain a coarse-mesh finite-difference (CMFD) form of the neutron diffusion equations. Nonlinear iterations start with the nodal coupling coefficients  $\tilde{D}^k(\text{nod})$  set to zero. After several iterations solving CMFD equations, a new approximation for the node-averaged neutron fluxes and the eigenvalue is obtained. Using the equations of the nodal method, the values of the face-averaged neutron current are computed. Requiring that the CMFD method reproduces these values of the neutron current, the diagonal elements of the matrix of the nodal coupling coefficients are determined as

$$\left(\tilde{D}^k(\text{nod})\right)_{gg} = \frac{-J_{gx+}^k - \tilde{D}_g^k(\text{fd})\left(\bar{\Phi}_g^{k+1} - \bar{\Phi}_g^k\right)}{\bar{\Phi}_g^{k+1} + \bar{\Phi}_g^k}. \quad (5)$$

The nonlinear iterations are performed till convergence, when the nodal coupling coefficients do not change anymore. As a result, the global solution procedure is decoupled into the two processes: an iterative solution of the CMFD equations, where the node-averaged neutron fluxes and the eigenvalue are computed and a solution of the nodal equations to calculate the face-averaged neutron currents and the nodal coupling coefficients.

To solve Eq. (4), a polynomial nodal method developed for Cartesian geometry (Zimin et al., 1998) is adapted. Polynomials are chosen to be orthogonal with the weight  $\bar{g}^2(\xi)$  on the interval  $[-1, 1]$  and they are normalized to unity at the end of the interval as

$$\int_{-1}^1 P_i(\xi)\bar{g}^2(\xi)P_j(\xi)d\xi = \begin{cases} 0 & \text{if } i \neq j \\ N_i & \text{if } i = j \end{cases} \quad \text{and} \quad P_i(1) = 1.$$

Explicit formulas for polynomials are computed using a Gram–Schmidt orthogonalization procedure. The transverse-integrated neutron flux is expanded into the polynomials up to a fourth order as follows

$$\Phi^k(\xi) = \sum_{i=0}^4 a_{ui}^k P_i(\xi) = \bar{\Phi}^k + \sum_{i=1}^4 a_{ui}^k P_i(\xi), \quad (6)$$

where  $a_{u0}^k = \int_{-1}^1 \Phi^k(\xi)\bar{g}^2(\xi)d\xi = \bar{\Phi}^k$  is the node-averaged neutron flux.



The transverse leakage is expanded into the polynomials up to the second order as

$$s_{vz}^k = \sum_{i=0}^2 s_{vzi}^k P_i(\xi),$$

where  $s_{vzi}^k = \frac{1}{N_i} \int_{-1}^1 \{s_v^k(\xi) + s_z^k(\xi)\} P_i(\xi) d\xi$ .

Using the flux polynomial expansion (6) the face-averaged current is expressed in terms of the flux expansion coefficients as

$$\bar{J}_{x+}^k = \frac{b}{R} \bar{J}_{u+}^k = -\frac{b}{R} \hat{D}^k \left\{ \sum_{i=1}^4 c_i^J a_{ui}^k \right\}, \quad (7)$$

where  $\bar{J}_{x+}^k$  is the average neutron current at the right face of the hexagonal node;  $\bar{J}_{u+}^k$  is the average neutron current at the right face of the rectangular node;  $R = h/\sqrt{3}$  is the length of the hexagon side;  $\hat{D}^k = 2D^k/a$  is the nondimensional diffusion coefficient;  $c_i^J = \frac{dP_i(\xi)}{d\xi} \big|_{\xi=1}$ ,  $i = 1, \dots, 4$ .

The unknown flux expansion coefficients are computed considering a two-node problem for each node face, which contains the nodes  $k$  and  $k+1$ . For the two-node problem we have four unknown expansion coefficients per node per energy group or eight expansion coefficients per group per two-node problem. Thus, eight equations are required to compute them. The equations are

- nodal balance equations for the nodes  $k$  and  $k+1$  ( $2G$  equations);
- two moment-weighting equations for the nodes  $k$  and  $k+1$  ( $4G$  equations);
- continuity of the face-averaged flux at the internal face of the two-node problem ( $G$  equations);
- continuity of the face-averaged current at the internal face of the two-node problem ( $G$  equations).

In the case of the face at the boundary, we define a one-node problem for the boundary node. The flux and current continuity equations are replaced by boundary conditions and we have  $4G$  nodal equations for  $4G$  unknowns.

The solution procedure is practically identical to the case of Cartesian geometry (Zimin et al., 1998). Using the moment-weighting equations the higher-order expansion coefficients are expressed in terms of the low-order expansion coefficients as

$$a_{u3}^k = c_{31} \left\{ \left( \hat{B}^2 \right)^k a_{u1}^k + s_{vz1}^k \right\}, \quad (8)$$

and

$$a_{u4}^k = c_{42} \left\{ \left[ \left( \hat{B}^2 \right)^k - c_{22} \right] a_{u2}^k + s_{vz2}^k \right\}, \quad (9)$$

where

$$c_{31} = \frac{N_1}{\int_{-1}^1 P_1(\xi) \frac{d^2 P_3(\xi)}{d\xi^2} d\xi}; \quad c_{42} = \frac{N_2}{\int_{-1}^1 P_2(\xi) \frac{d^2 P_4(\xi)}{d\xi^2} d\xi};$$

and

$$c_{22} = \frac{1}{N_2} \int_{-1}^1 P_2(\xi) \frac{d^2 P_2(\xi)}{d\xi^2} d\xi.$$

Substituting the fourth expansion coefficient (9) into the neutron balance we obtain a system of  $G$  equations for the second expansion coefficients

$$\left\{ I_2^J + c_2 \left[ \left( \hat{B}^2 \right)^k - c_{22} \right] \right\} a_{u2}^k = \left( \hat{B}^2 \right)^k \bar{\Phi}^k + \{ s_{vz0}^k - c_2 s_{vz2}^k \}, \quad (10)$$

where  $c_2 = c_{42} c_4^J$ .

Substituting the third expansion coefficient (8) into the neutron flux and current continuity equations we obtain  $2G$  equations for the first expansion coefficients:  
*flux continuity*

$$\begin{aligned} & \left\{ I + c_{31} \left( \hat{B}^2 \right)^{k+1} \right\} a_{u1}^{k+1} + \left\{ I + c_{31} \left( \hat{B}^2 \right)^k \right\} a_{u1}^k \\ & = \left\{ \bar{\Phi}^{k+1} + a_{u2}^{k+1} + a_{u4}^{k+1} \right\} - \left\{ \bar{\Phi}^k + a_{u2}^k + a_{u4}^k \right\} - c_{31} \{ s_{vz1}^k + s_{vz1}^{k+1} \}, \end{aligned} \quad (11)$$

*current continuity*

$$\begin{aligned} & \hat{D}^{k+1} \left\{ I + c_1 \left( \hat{B}^2 \right)^{k+1} \right\} a_{u1}^{k+1} - \hat{D}^k \left\{ I + c_1 \left( \hat{B}^2 \right)^k \right\} a_{u1}^k \\ & = \hat{D}^{k+1} \{ c_2^J a_{u2}^{k+1} + c_4^J a_{u4}^{k+1} - c_1 s_{vz1}^{k+1} \} + \hat{D}^k \{ c_2^J a_{u2}^k + c_4^J a_{u4}^k - c_1 s_{vz1}^k \}, \end{aligned} \quad (12)$$

where  $c_1 = c_{31} c_3^J$ .

As a result, the initial system of  $8G$  nodal equations is reduced to  $G$  Eqs. (10) with respect to the second expansion coefficients of the node  $k+1$  and  $2G$  Eqs. (11) and (12) with respect to the first expansion coefficients of the nodes  $k+1$  and  $k$ . The even expansion coefficients of the node  $k$  are known from the solution of the previous two-node problem ( $k-1, k$ ). When the neutron flux expansion coefficients are computed, the face-averaged nodal current  $\bar{J}_{x+}^k$  is calculated using Eq. (7) and the nodal coupling coefficients are updated by Eq. (5).

## 5. Numerical results

The hexagonal polynomial nodal method has been incorporated into the neutron diffusion code SKETCH-N (Zimin et al., 2001). The solution procedure and applied iterative techniques are the same as that for Cartesian geometry. The hexagonal

nodal method is used in the solution of the two-node problems for radial node faces. The two-node problems for axial faces of the nodes are treated in the same way as in Cartesian geometry using the polynomial nodal method based on Legendre polynomials (Zimin et al., 1998). Accuracy of the method has been estimated using several 2D and 3D steady-state benchmark problems, which are mostly taken from (Chao and Shatilla, 1995), except of 2D VVER-1000 four group benchmark developed by Makai (1984) and 3D VVER-1000 Schultz benchmark (Kolev et al., 1999). Two methods of the transverse leakage approximation are examined for 2D problems: the “flat” transverse leakage approximation for all nodes and a combination of the “flat” leakage approximation for internal nodes with a linear approximation for the nodes at the reactor boundary. Table 1 summarizes the errors of the SKETCH-N solutions for 2D benchmark problems, where the following notations are used:  $\Delta P_{\max}(\Delta P_{\text{av}})$  is the maximum (average) error of the assembly power;  $\Delta k_{\text{eff}}$  is the error in the reactor eigenvalue. The results show that for the cases where a radial reflector is included into the reactor model, even the “flat” leakage approximation provides acceptable accuracy. The errors of the “flat” leakage approximation are relatively large only for the problems VVER-1000 and IAEA without reflector, when the vacuum boundary conditions ( $\alpha = 0.5$ ) are imposed at the reactor core boundary. In these cases, the linear transverse leakage approximation applied to the boundary nodes significantly improves the code accuracy.

3D benchmark problems VVER-440 (Chao and Shatilla, 1995) and VVER-1000 (Kolev et al., 1999) have been also computed. The axial mesh size is 25 cm for VVER-440 problem and 35.5 cm for VVER-1000 problem. The linear approximation of the radial transverse leakage is applied for the boundary nodes. The errors in the power distribution and in the reactor multiplication factor are summarized in Table 2. The following notations are used:  $\Delta P_{\max}^{3D}(\Delta P_{\text{av}}^{3D})$  is the maximum (average) error of the three-dimensional nodal power distribution;  $\Delta P_{\max}^{2D}$  is the maximum error of the axially-averaged assembly power;  $\Delta P_{\max}^{1D}$  is the maximum error of the radially-averaged axial power distribution. The presented results show the excellent accuracy of the developed polynomial method. For all the computed problems

Table 1  
SKETCH-N numerical results of the steady-state 2D benchmark problems

Problem	$\Delta P_{\max}$ (%)	$\Delta P_{\text{av}}$ (%)	$\Delta k_{\text{eff}}$ (pcm)
VVER 440 <sup>a</sup>	0.5 (0.8) <sup>b</sup>	0.2 (0.4)	24 (35)
VVER 1000 <sup>a</sup> ( $\alpha = 0.125$ )	0.8 (2.8)	0.3 (1.4)	7 (60)
VVER 1000 <sup>a</sup> ( $\alpha = 0.5$ )	2.1 (5.9)	0.6 (2.3)	0 (62)
VVER 1000 <sup>c</sup> (four groups)	0.5 (0.4)	0.2 (0.1)	−2 (6)
IAEA <sup>a</sup> w/o reflector ( $\alpha = 0.125$ )	0.6 (1.5)	0.2 (0.7)	4 (71)
IAEA <sup>a</sup> w/o reflector ( $\alpha = 0.5$ )	1.3 (4.8)	0.5 (1.9)	−6 (121)
HWR <sup>a</sup>	0.5 (0.5)	0.1 (0.1)	8 (8)

<sup>a</sup> Reference solution: DIF3D-FD results from Chao and Shatilla (1995).

<sup>b</sup> Values in the parenthesis are computed using the “flat” transverse leakage approximation for all nodes.

<sup>c</sup> Reference solution: VENTURE results from (Noh and Cho, 1996).

Table 2

SKETCH-N numerical results of the steady-state 3D benchmark problems

Problem	$\Delta P_{\max}^{3D}$ (%)	$\Delta P_{\text{av}}^{3D}$ (%)	$\Delta P_{\max}^{2D}$ (%)	$\Delta P_{\max}^{1D}$ (%)	$\Delta k_{\text{eff}}$ (pcm)
VVER-440 <sup>a</sup>	1.4	0.4	0.7	0.6	25
VVER-1000 <sup>b</sup>	1.9	0.7	0.8	1.2	26

<sup>a</sup> Reference solution: DIF3D-FD results from Chao and Shatilla (1995).<sup>b</sup> Reference solution: CRONOS results from Kolev et al. (1999).

maximum errors in the power distribution are below 2.1% and errors in the reactor multiplication factor do not exceed 26 pcm.

## 6. Conclusions

A polynomial nodal method has been developed for the solution of the neutron diffusion equations in hexagonal-z geometry. The method uses conformal mapping of a hexagon into a rectangle. The neutron diffusion equations in the new coordinate system are solved using a fourth order expansion of the transverse-integrated neutron flux into orthogonal polynomials. A transverse leakage is approximated using constant average values of the neutron currents at the faces of the internal reactor nodes and a linear shape of the currents at the faces of the nodes at the reactor boundary. Due to the application of the conformal mapping and orthogonality of the applied polynomials, the solution of the nodal equations is similar to that in Cartesian geometry. A nonlinear iteration procedure is used as a global solution technique. Considering a two-node problem ( $k, k+1$ ) for each node face,  $8G$  nodal equations are formed, where  $G$  is a number of neutron energy groups. The system is sparse and decoupled and after a simple algebra it is reduced to  $G$  equations for the second flux expansion coefficients of the node  $k+1$  and  $2G$  equations for the first expansion coefficients of the nodes  $k$  and  $k+1$ .

The method is implemented into the neutron diffusion code SKETCH-N. A set of 2D and 3D steady-state benchmark problems have been computed. A comparison with the reference solutions demonstrated excellent accuracy of the method: for all the computed benchmarks maximum errors in power distribution do not exceed 2.1% and the errors in the reactor eigenvalue are below 30 pcm.

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