Proceedings of the Reactor Physics Asia 2015 (RPHA15) Conference
Jeju, Korea, Sept. 16-18, 2015

Development of Hexagonal Nodal Diffusion Codes at National Tsing-Hua University

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1. Introduction

Among the six types of the Gen-IV [1] reactors, the VHTR (Very High Temperature Reactor) is a good candidate for the next generation power reactor, high-temperature applications and the production of hydrogen. The authority agencies in Taiwan support NTHU a long-term and on-going research project in this area starting from 2010. It includes three major sub-projects in reactor physics, thermal hydraulics, and material researches. The first subproject focusing on reactor physics aims at establishing a complete platform for VTHR core analyses and design, starting from cross-section processing, lattice and whole core calculations, to the coupling between neutronics and thermal hydraulic calculations. The development of an in-house nodal diffusion code that can handle hexagonal geometry is a key ingredient toward this goal.

In 2010, through a cooperation with Idaho National Laboratory (INL), a master student, Chih-Wei Chang, went to INL learning the Hybrid Nodal Green's Function Method (HNGFM) [2] used in full-core calculations under the supervision of Dr. Ougouag. He successfully developed a rectangular nodal diffusion code and used it to evaluate the Doppler effect of heat spots in a reactor core [3]. Another master student, Jui-Yu Wang, also went to INL in 2012 for interim study supported by the VHTR project. Based on Chih-Wei Chang's work, he developed another 2D nodal diffusion code that can be used in both rectangular and hexagonal geometries [4]. To further improve the accuracy of nodal calculation in hexagonal geometry, Tzung-Yi Lin recently developed a new code by integrating the conformal mapping technique together with HNGFM. This paper presents an overview of these code developments regarding research progress and future plan.

2. Hybrid Nodal Green's Function Method in Direct Coarse Mesh Finite Difference Formulation

The HNGFM was first proposed by Ougouag in 1981 [2]. The method solves the transverse-integrated 1D differential diffusion equation by transforming the equation into an integral form. The resulting flux can be directly related to an effective source term, flux derivative terms and Neumann type Green's Functions [2], i.e.

$$\begin{aligned}\phi_{gu}^{k}(u) = {} & \int_{-a_u^k}^{+a_u^k} du_0 S_{gu}^{k}(u_0) G_{gu}^{k}(u|u_0) \\ & + D_g^k G_{gu}^{k}(u|+a_u^k)\left[\frac{\partial}{\partial u_0}\phi_{gu}^{k}(+a_u^k)\right] \\ & - D_g^k G_{gu}^{k}(u|-a_u^k)\left[\frac{\partial}{\partial u_0}\phi_{gu}^{k}(-a_u^k)\right] \end{aligned} \quad (1)$$

where

$\phi_{gu}^{k}(u)$ = transverse-integrated flux,
$S_{gu}^{k}(u_0)$ = effective source term,
D_g^k = diffusion coefficient,
$G_{gu}^{k}(u|u_0)$ = Green's Function with Neumann-type boundary conditions,
k, g = node and group indexes.

Note that Eq. (1) is a general expression of the HNGFM, the detail formulation of each term depend on the geometry and dimension of the problem.

2.1 Rectangular case

In rectangular geometry, the derivative of the flux in Eq. (1) can be directly related to surface net currents through Fick's Law:

$$\mathrm{J}_{\mathrm{gu}}^{\mathrm{k}}(\pm\mathrm{a}_{\mathrm{u}}^{\mathrm{k}}) = -D_g^k \frac{\partial}{\partial u_0}\phi_{gu}^{k}(\pm a_u^k) \quad (2)$$

By substituting Eq. (2) into Eq. (1), the flux distribution inside the k[th]-node can be expressed in terms of surface net currents and within-node source distribution.

2.2 Hexagonal case with Fitzpatrick's approach

In hexagonal geometry as shown in Fig. 1, the expression of the transverse-averaged flux and transverse-averaged current can be written as

$$\phi_{gu}^{k}(x) = \frac{1}{2y_s(x)}\int_{-y_s(x)}^{y_s(x)} dy \phi_g^k(x,y) \quad (3)$$

$$J_{gu}^{k}(x) = -\frac{1}{2y_s(x)}\int_{-y_s(x)}^{y_s(x)} dy D_g^k \frac{\partial}{\partial x}\phi_g^k(x,y) \quad (4)$$

where

$\mathrm{y_s}(x) = \frac{2h-|x|}{\sqrt{3}}$,

x, y = coordinate variables.

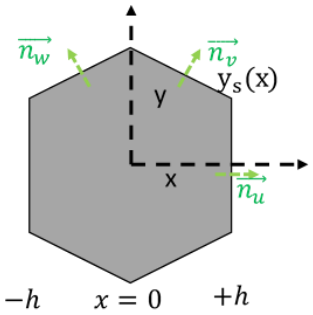

Fig. 1. A hexagonal node and its coordinate system

Unlike in rectangular geometry, non-physical terms arise from the transverse integration process (TIP) in hexagonal geometry.

$$-\mathrm{D}_{\mathrm{g}}^{\mathrm{k}}\frac{\partial}{\partial \mathrm{x}}\phi_{\mathrm{gx}}^{\mathrm{k}}(\mathrm{x}) = \mathrm{J}_{\mathrm{gx}}^{\mathrm{k}}(\mathrm{x}) + \mathrm{D}_{\mathrm{g}}^{\mathrm{k}}\frac{\mathrm{sgn}(\mathrm{x})}{2\mathrm{y_s(x)}\sqrt{3}}\cdot \left[\phi_{\mathrm{g}}^{\mathrm{k}}(\mathrm{x}, \mathrm{y_s(x)}) + \phi_{\mathrm{g}}^{\mathrm{k}}(\mathrm{x}, -\mathrm{y_s(x)}) - 2\phi_{\mathrm{gx}}^{\mathrm{k}}(\mathrm{x})\right] \quad (5)$$

To deal with non-physical terms, Fitzpatrick (1995) chose to neglect these terms first in solving the equation and then include their contribution later by enforcing a rigorous nodal balance relationship [5].

$$\frac{1}{\mathrm{V_k}}\sum_{\mathrm{i}\in\mathrm{S}}\int_{\mathrm{r_s}\in\mathrm{S_i}}\hat{\mathrm{n}}_{\mathrm{i}}\cdot \mathrm{J}_{\mathrm{g}}^{\mathrm{k}}(\mathrm{r_s})\mathrm{d}^2\mathrm{r_s} + \Sigma_{\mathrm{g}}^{\mathrm{r,k}}\overline{\phi_{\mathrm{g}}^{\mathrm{k}}} = \overline{\mathrm{Q_g^k}} \quad (6)$$

2.3 Direct coarse mesh finite difference formulation

By using Eq. (1), i.e. the flux distribution inside a node, the continuity of interface net currents, the discontinuity of interface fluxes, and the neutron balance equation, one can couple a node-average flux in one node with those of the neighboring nodes. These equations were thus re-cast in the form dubbed the Direct Coarse Mesh Finite Difference (D-CMFD) for convenience of solution.

The D-CMFD method was first proposed by Chao in 1999 [6]. The main idea of this method is to use relatively sophisticated diffusion coefficients, which still can be analytically derived, to simplify the equations to improve the overall calculation efficiency. The effectiveness of this method can be found in Ref. [13]. By using D-CMFD, these equations can be expressed in a matrix form as follows:

$$\boldsymbol{B}_{gu}\overline{\phi}_g = R_{gu} \quad (7)$$

where

$\boldsymbol{B}_{gu}$ = coefficient matrix,

$\overline{\phi}_g$ = nodal-average flux in vector form,

R_{gu} = right-hand-side terms in vector form.

3. Implementation of Conformal Mapping Technique

Applying the conformal mapping technique to hexagonal nodal methods was first proposed by Chao [7]. He transformed the hexagonal plane into a rectangle plane by using the conformal mapping technique as shown in Fig. 2.

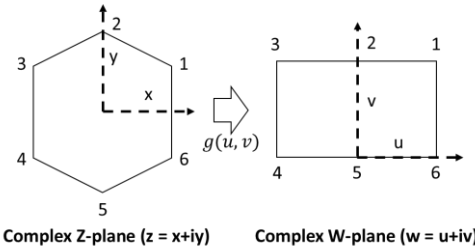

Fig. 2. Conformal mapping of a hexagon to a rectangle

The transformed diffusion equation can be written as

$$-D_g^k\left(\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial v^2}\right)\phi_g^k(u,v) + \Sigma_g^{r,k}g^2(u,v)\phi_g^k(u,v) = g^2(u,v)\left[Q_g^k(u,v)\right] \quad (8)$$

where

$g^2(u,v)$ = mapping area scale function, and

$Q_g^k(u,v)$ = Fission and scattering source term.

Since the TIP is applied after transformation, it avoids the nonphysical terms arising in hexagonal cases. Therefore, higher accuracy can be achieved. After applying the HNGFM to the resulting transverse-integrated 1D ODE, the solution is similar to Eq. (1). Then those equations are also re-cast into the D-CMFD form.

4. Benchmark Results

Benchmark problems were performed to verify the accuracy of the codes.

4.1 Rectangular cases

The codes developed in NTHU are benchmarked against the results of Ougouag [2] and Rajic [8]. Ougouag and Rajic used the HNGFM formulation, but used surface net currents to couple the nodes rather than the more recent D-CMFD.

4.1.1 The 2-D test problem

The 1st problem is a simplified model of the IAEA 2-D PWR benchmark problem [2]. The core contains 177 fuel assemblies and 9 inserted control rod clusters. Each fuel assembly and control rod cluster is 20 cm wide. The core is 1/4th symmetric and surrounded by a water reflector. The results are summarized in Table I, showing good agreement in k_{eff}. The mesh size is 20x20cm^2 in all cases.

Table I. Results of 2-D Test Problem

	NTHU Jui-Yu [4]	NTHU Chih-Wei [3]	Ougouag[2]
k_{eff}	1.02994	1.02994	1.02997
Iterations	194	194	196

4.1.2 The 2-D 4-group LMFBR problem

The 2nd problem is a 4-group Liquid Metal Fast Breeder Reactor (LMFBR) with 1000MWe [8]. There are two-core zones surrounded by a radial blanket and reflected with a 30cm wide reflector. The results are summarized in Table II. The deviations in k_{eff} from in the reference solution are ~20pcm.

Table II. Results of 2-D 4-Group LMFBR Problem

	NTHU Jui-Yu [4]	NTHU Chih-Wei [3]	Rajic[8]
k_{eff}	1.05680	1.05702	1.05694
Δk_{eff} (pcm)	-15	-23	0

4.2 Hexagonal cases

For hexagonal problems, the codes developed at NTHU were benchmarked against HEXPEDITE [5], DIF3D-N [10], ANC-H [9] and SKETCH-N [11]. DIF3D-N uses the Nodal Expansion Method and functions to approximate the discontinuous terms that arise from the TIP. HEXPEDITE uses the HNGFM to solve the equation and Fitzpatrick's Approach (an augmented version of Wagner's approach [12]) to deal with the discontinuous terms. The ANC-H code has two different modules, ANC-HW, which uses Wagner's approach and ANC-HM, which uses the conformal mapping method. SKETCH-N uses the polynomial nodal method together with the conformal mapping technique.

The calculation results performed by Jui-Yu Wang are denoted as NTHU-JY, and the results obtained by Tzung-Yi Lin are denoted as NTHU-TY. Both are based on the HNGFM in D-CMFD formulation. However, the former one use Fizpatrick's Approach while the latter uses the conformal mapping technique to avoid the non-physical terms arising from the TIP. The methodologies of these codes are summarized in Table III.

Table III. Comparison of the Methodologies of Hexagonal Codes

Codes	Hexagonal Treatment	Nodal Method	Coupling Strategy
DIF3D-N[10]	Functions to approximate nonphysical terms	NEM	$J_{\pm}$
ANC-HW[9]	Wagner's Approach	NEM	J_{net}
HEXPEDITE[5]	Augment Wagner's Approach	HNGFM	
NTHU-JY[4]		HNGFM	$\overline{\phi}$
ANC-HM[9]	Conformal Mapping Approach	NEM	J_{net}
SKETCH-N[11]		PNM	J_{net}
NTHU-TY		HNGFM	$\overline{\phi}$

4.2.1 The 2-D IAEA benchmark problem

This problem [9] is a modified IAEA benchmark problem for hexagonal geometry. The core is 1/12th reflected symmetric with 13 fuel assemblies across the core diameter and 13 control rod cluster units. The pitch of the assemblies is 20 cm. There are two variant problems of this geometry – IAEA-WR, surrounded by a water reflector and IAEA-WOR, without the water reflector.

Two different albedos were used, corresponding to realistic (albedo equals to 0.125) and vacuum boundary conditions (albedo equals to 0.5). The definition of albedo here is the ratio of the total surface-averaged net current to the surface-averaged flux. Table IV summarizes the results.

Table IV. Comparison of Results of Different Hexagonal Nodal Codes to the Reference Solution for the IAEA-WOR and IAEA-WR Problems

Code Option	0.125 Albedo		0.5Albedo	
	ΔP_{max} (%)	Δk_{eff} (pcm)	ΔP_{max} (%)	Δk_{eff} (pcm)
IAEA-WOR				
Reference Value [9]	**k_{eff} = 0.991378**		**k_{eff} = 0.978077**	
DIF3D-N [9]	4.0	173.6	4.3	208.2
ANC-HW [9]	2.2	169.1	6.4	233.3
ANC-HM [9]	0.5	6.0	0.8	-7.3
SKETCH-N [11]	0.6	4.0	1.3	-6
HEXPEDITE [5]	-	-	5.24	166
NTHU-JY [4]	1.75	136.6	1.44	217.0
NTHU-TY	0.31	3.9	0.35	-0.3
IAEA-WR				
Reference Value [9]	**k_{eff} = 1.006630**		**k_{eff} = 1.005507**	
DIF3D-N [9]	20.2	-409.5	18.1	-338.8
ANC-HW [9]	6.8	-87.0	7.2	-111.7
ANC-HM [9]	0.5	7.0	0.7	-1.7
HEXPEDITE [5]	-	-	6.48	100.5
NTHU-JY [4]	4.9	-95.3	1.66	11.6
NTHU-TY	0.3	7.4	0.41	11.3

The accuracy of the results of NTHU-JY is similar to that of ANC-HW and HEXPEDITE, since Wagner's approximation [12] is used in these codes. On the other hand, the accuracy of the results of NTHU-TY is similar to those of ANC-HM and SKETCH-N, since conformal mapping technique is imbedded in these codes. Better agreement was achieved when conformal mapping technique was used, because this technique avoids the approximations of the nonphysical terms arisen during TIP in hexagonal geometry. The computation time of NTHU-JY was ~0.19s on Intel i7-3820 platform and NTHU-TY took ~0.5s on Intel i7-930 platform.

4.2.2 The 2-D VVER-1000 benchmark problem

The 2D VVER-1000 benchmark problem is a 1/6th

cyclic symmetry core with 15 fuel assemblies across the core diameter and 25 control units inside the reactor [9]. The assembly pitch is 23.6 cm. Again, the same albedo values were applied in this problem. The results are summarized in Table V.

The outcome is similar to the previous cases. The results of NTHU-JY are close to those of ANC-HW, while the results of NTHU-TY are close to those of ANC-HM and SKETCH-N. The agreement was better for the group using the conformal mapping technique. In this case, the computation time of NTHU-JY was 0.21s on Intel i7-3820 platform, and NTHU-TY took ~0.75s on Intel i7-930 platform.

Table V. Comparison of Results from Different Hexagonal Nodal Codes to Reference Solutions for the 2-D VVER-1000 Problem

Code Option	0.125 Albedo		0.5Albedo	
	ΔP_{max} (%)	Δk_{eff} (pcm)	ΔP_{max} (%)	Δk_{eff} (pcm)
Reference Value [9]	**k_{eff} = 1.014407**		**k_{eff} = 1.006485**	
DIF3D-N [9]	4.7	32.9	5.0	23.7
ANC-HW [9]	9.2	192.3	19.7	161.5
ANC-HM [9]	0.7	16.0	0.7	7.2
SKETCH-N [11]	0.8	7.0	2.1	0.0
NTHU-JY [4]	9.1	153.0	19.2	146.8
NTHU-TY	0.71	13.6	0.79	14.5

5. Summary

Hexagonal nodal diffusion codes for VHTR core analyses were developed at NTHU during the past years. The methodologies behind the code development mainly consist of the HNGFM, D-CMFD, and conformal mapping technique. Preliminary results for the benchmark problems show reasonably good agreement with those published data in the literature. Continued efforts to improve the code accuracy and efficiency are still on-going.

Acknowledgements

The authors would like to thank Yung-An Chao for helpful discussions on the conformal mapping technique. The Taiwan members of the team were supported by the Ministry of Science and Technology (former National Science Council) and Atomic Energy Council in Taiwan, under contract number NSC99-3113-Y-042-001. Chih-Wei Chang and Jui-Yu Wang thank the INL for its hospitality during their respective stays there for extended visits. The work of one of us (Abderrafi M. Ougouag) was supported by the U.S. Department of Energy, under DOE Idaho Operations Office Contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes. All sources of support are gratefully acknowledged.

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