# Application of the SP3 TPEN Method for Hexagonal Core Transient Analysis

Cheon Bo Shim<sup>a</sup>, Jin Young Cho<sup>a</sup>, and Han Gyu Joo<sup>b\*</sup>

<sup>a</sup>Korea Atomic Energy Research Institute, 111, Daedeok-daero 989beon-gil, Yuseong-gu, Daejeon, 34057, Korea <sup>b</sup>Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul, 08826, Korea <sup>\*</sup>Corresponding author: joohan@snu.ac.kr

### 1. Introduction

Due to the increase of various demands and purposes that cannot be fulfilled by conventional PWRs, plenty of FBRs and SMRs have been widely studied and being developed. Since these reactor types have large mean free path and small system size compared to commercial PWRs, the conventional diffusion approximation is not valid anymore for FBR and SMR neutronics analysis. Direct transport approach based on Monte Carlo (MC), Method of Characteristics (MOC), or other sophisticated transport methods can be used to achieve fidelity core analysis, but unacceptable computational burden is needed especially for core transient simulations under various accident situations. In order to accomplish accurate and efficient core simulation for these reactor types, improved core analysis procedure is necessary.

The simplified Pn (SPn) method [1,2] is one of the best solutions. This method expands the neutron angular flux using the  $n^{\text{th}}$  order Legendre polynomial on the cosine of the neutron flight angle in computational reactor physics. The SPn solution is quite accurate compare to the conventional diffusion solution that can be obtained by the P1 method. Also, the formulation of the SPn equations is similar to that of the diffusion equation, so the SPn method is easy to adopt nodal methods for efficient core analysis. With this background, there have been various studies to apply SPn nodal methods with the order of 3 (SP3) [3-6] and it has been proved that the SP3 application takes significant enhancement on core analysis accuracy especially in SMR, FBR, and some cores where large spatial flux variation is formed such as MOX loaded cores or cores under the ARI condition.

Most SP3 researches are, however, limited on the steady-state analysis. Although there are a few studies for SP3 application to core transient analysis [7-9], they are available only in rectangular core problems. Since a number of SMRs and FBRs use hexagonal fuel assemblies, it is worth evaluating the effect of the SP3 application in hexagonal core transient analysis.

Triangle-based polynomial expansion nodal (TPEN) method [10] is one of the nodal methods applied in hexagonal geometry. In this method, each hexagon node is split to 6 triangles and the intra-nodal spatial flux distribution is expressed as a third order polynomial on 2-D space in each triangle. This method is implemented in the PARCS [11] and MASTER [12]

core analysis codes and its effectiveness has been already proved.

In this study, the SP3 method is applied to hexagonal core transient simulation with applying the TPEN method. In the next section, time-dependent SP3 TPEN equations are introduced briefly. The effectiveness of the SP3 TPEN method in core transient simulation is then evaluated in the simplified VVER440 rod ejection benchmark problem [13]. And the significant of this work is discussed in the last section.

#### 2. Time-Dependent SP3 TPEN Equations

The governing equations for SP3 core transient simulation consist of the time-dependent SP3 equations [14] and the precursor balance equation represented as follow:

$$\vec{\nabla} \cdot \vec{\phi}_{1,g}(\vec{r},t) + \left( \sum_{rg}(\vec{r},t) + \frac{1}{v_g} \frac{\partial}{\partial t} \right) \phi_{0,g}(\vec{r},t) \\ = (1-\beta) \chi_{pg} \psi(\vec{r},t) + \sum_{k=1}^{6} \chi_{dgk} \lambda_k C_k(\vec{r},t) + \sum_{g'=1}^{G} \Sigma_{0,g'g}(\vec{r},t) \phi_{0,g'}(\vec{r},t) \\ \frac{1}{3} \vec{\nabla} \phi_{0,g}(\vec{r},t) + \frac{2}{3} \vec{\nabla} \phi_{2,g}(\vec{r},t) + \left( \sum_{trg}(\vec{r},t) + \frac{1}{v_g} \frac{\partial}{\partial t} \right) \vec{\phi}_{1,g}(\vec{r},t) = 0 \quad (1) \\ \frac{2}{5} \vec{\nabla} \cdot \vec{\phi}_{1,g}(\vec{r},t) + \frac{3}{5} \vec{\nabla} \cdot \vec{\phi}_{3,g}(\vec{r},t) + \left( \sum_{tg}(\vec{r},t) + \frac{1}{v_g} \frac{\partial}{\partial t} \right) \phi_{2,g}(\vec{r},t) = 0 \\ \frac{3}{7} \vec{\nabla} \phi_{2,g}(\vec{r},t) + \left( \sum_{tg}(\vec{r},t) + \frac{1}{v_g} \frac{\partial}{\partial t} \right) \vec{\phi}_{3,g}(\vec{r},t) = 0 \\ \frac{\partial C_k(\vec{r},t)}{\partial t} = \beta_k \psi(\vec{r},t) - \lambda_k C_k(\vec{r},t) \quad (2)$$

where  $\phi_{m,g}(\vec{r},t)$  and  $\vec{\phi}_{m,g}(\vec{r},t)$  are respective even and odd moment of angular flux and *m* is the order of moment.

Eq. (1) can be replaced to radial 2-D and axial 1-D SP3 equations by the transverse integration on respective z-direction and x-y plane. The TPEN method is applied to the 2-D equation for hexagonal geometry and the 1-D equation is solved by any nodal methods applied in rectangular core analysis. Also, any temporal discretization techniques are required to solve the time-dependent equations numerically. Temporal discretized transverse integrated radial 2-D SP3 equations are expressed as follow:

$$\begin{split} \sum_{u=x,y} \frac{\partial \phi_{lu,g}^{i}(\vec{r}_{2})}{\partial u} + \Sigma_{rg}^{i} \phi_{0,g}^{i}(\vec{r}_{2}) &= q_{g}^{ss,i}(\vec{r}_{2}) - q_{0,g}^{t,i}(\vec{r}_{2}) + q_{0,g}^{ts,i}(\vec{r}_{2}) \\ \frac{1}{3} \frac{\partial}{\partial u} \Big( \phi_{0,g}^{i}(\vec{r}_{2}) + 2\phi_{2,g}^{i}(\vec{r}_{2}) \Big) + \Sigma_{trg}^{i} \phi_{lu,g}^{i}(\vec{r}_{2}) \\ &= -\frac{1}{v_{g}} \frac{\partial}{\partial t} \phi_{lu,g}(\vec{r}_{2},t) \bigg|_{t=t_{i}} \quad (u = x, y) \\ \frac{1}{5} \frac{\partial}{\partial u} \sum_{u=x,y} \Big( 2\phi_{lu,g}^{i}(\vec{r}_{2}) + 3\phi_{3u,g}^{i}(\vec{r}_{2}) \Big) + \Sigma_{tg}^{i} \phi_{2,g}^{i}(\vec{r}_{2}) \\ &= -\frac{2}{5} q_{0,g}^{t,i}(\vec{r}_{2}) - \frac{3}{5} q_{2,g}^{t,i}(\vec{r}_{2}) + q_{2,g}^{ts,i}(\vec{r}_{2}) \\ \frac{3}{7} \frac{\partial \phi_{2,g}^{i}(\vec{r}_{2})}{\partial u} + \Sigma_{tg}^{i} \phi_{3u,g}^{i}(\vec{r}_{2}) = -\frac{1}{v_{g}} \frac{\partial}{\partial t} \phi_{3u,g}(\vec{r}_{2},t) \bigg|_{t=t_{i}} \quad (u = x, y) \end{split}$$

where  $\vec{r}_2 = (x, y)$  and *i* is time index for  $t = t_i$ . The steady-state source  $q_g^{ss,i}$ , transverse leakage source  $q_{m,g}^{tl,i}$ , and transient specific source  $q_{m,g}^{ts,i}$  are defined as follow:

$$\begin{aligned} q_{g}^{ss,i}(\vec{r}_{2}) &= \chi_{g} \psi^{i}(\vec{r}_{2}) + \sum_{g'=1}^{G} \Sigma_{0,g'g}^{i} \phi_{0,g'}^{i}(\vec{r}_{2}), \\ q_{m,g}^{tl,i}(\vec{r}_{2}) &= \frac{\phi_{(m+1)zr,g}^{i}(\vec{r}_{2}) - \phi_{(m+1)zl,g}^{i}(\vec{r}_{2})}{h_{z}}, \\ q_{m,g}^{ts,i}(\vec{r}_{2}) &= \delta_{0m} \bigg( \Big( -\chi_{g} + (1-\beta)\chi_{pg} \Big) \psi^{i}(\vec{r}_{2}) + \sum_{k=1}^{6} \chi_{dgk} \lambda_{k} C_{k}^{i}(\vec{r}_{2}) \bigg) \\ &- \frac{1}{v_{g}} \frac{\partial}{\partial t} \phi_{m,g}(\vec{r}_{2}, t) \bigg|_{t=t_{i}}. \\ (m = 0, 2) \end{aligned}$$

The time-derivative of odd moments in the second and fourth equations of Eq. (3) is generally neglected by assuming that they are much smaller than spatial variation of even moments [8,9].

$$\frac{1}{v_{g}}\frac{\partial}{\partial t}\vec{\phi}_{1,g}(\vec{r}_{2},t) \ll \frac{1}{3}\vec{\nabla}\left(\phi_{0,g}(\vec{r}_{2},t) + 2\phi_{2,g}(\vec{r}_{2},t)\right)$$

$$\frac{1}{v_{g}}\frac{\partial}{\partial t}\vec{\phi}_{3,g}(\vec{r}_{2},t) \ll \frac{3}{7}\vec{\nabla}\phi_{2,g}(\vec{r}_{2},t).$$
(4)

Then Eq. (3) can be expressed to diffusion-like equations as follow:

$$\begin{bmatrix} -D_{0,g}^{i} \sum_{u=x,y} \frac{\partial^{2}}{\partial u^{2}} + \Sigma_{rg}^{i} & -2\Sigma_{rg}^{i} \\ -\frac{2}{3} \Sigma_{rg}^{i} & -D_{2,g}^{i} \sum_{u=x,y} \frac{\partial^{2}}{\partial u^{2}} + \tilde{\Sigma}_{irg}^{i} \end{bmatrix} \begin{bmatrix} \hat{\phi}_{g}^{i}(x,y) \\ \phi_{g}^{i}(x,y) \end{bmatrix}$$

$$= \begin{bmatrix} q_{g}^{ss,i}(x,y) - q_{0,g}^{d,i}(x,y) + q_{0,g}^{ts,i}(x,y) \\ -\frac{2}{3} q_{g}^{ss,i}(x,y) - q_{2,g}^{d,i}(x,y) - \frac{2}{3} q_{0,g}^{ts,i}(x,y) + \frac{5}{3} q_{2,g}^{ts,i}(x,y) \end{bmatrix}$$

$$(5)$$

where

$$D_{0,g}^{i} = \frac{1}{3\Sigma_{trg}^{i}}, \quad D_{2,g}^{i} = \frac{3}{7\Sigma_{tg}^{i}}, \quad \tilde{\Sigma}_{trg}^{i} = \frac{4}{3}\Sigma_{rg}^{i} + \frac{5}{3}\Sigma_{tg}^{i}$$
$$\hat{\phi}_{g}^{i}(x, y) = \phi_{0,g}^{i}(x, y) + 2\phi_{2,g}^{i}(x, y).$$

The two-dimensional intra-nodal SP3 TPEN solutions in each triangle node are defined as follow:

$$\phi_{m,g}^{i}(x, y) = c_{m0,g}^{i} + a_{mx,g}^{i} x + a_{my,g}^{i} y$$
  
+  $b_{mx,g}^{i} x^{2} + b_{mv,g}^{i} w^{2} + b_{mp,g}^{i} p^{2}$   
+  $c_{mx,g}^{i} x^{3} + c_{mv,g}^{i} w^{3} + c_{mp,g}^{i} p^{3}$   
(m = 0, 2) (6)

where p and w are coordinates defined in each node as noted in Fig. 1.



Fig. 1. Coordinates in a triangle node

The 9 coefficients for each moment in Eq. (6) are determined by the following 9 constraints.

- Node-average moment (1)
- x- and y-weighted node-average moments (2)
- Corner moments (3)
- Surface-average moments (3)

Intra-nodal solutions in 6 triangle nodes contained in a hexagon node are determined simultaneously by solving coupled equations constructed by above 9 constraints. Detail description of the TPEN method in SP3 formulation can be found in elsewhere [6].

### 3. Numerical Result

The time-dependent SP3 TPEN methods are implemented in the RENUS core simulator [15] developed in Seoul National University. Its effectiveness is evaluated in the VVER440 rod ejection benchmark problem whose ID is AER-DYN-003. Detail benchmark specification can be found in elsewhere [13] and the zero-incoming boundary condition is assumed in this work for simplicity.

Fig. 2 represents the core power behaviors of this problem. The diffusion (P1) TPEN solutions obtained by the PARCS and RENUS codes are also provided to confirm the effectiveness of the SP3 application. All computing options in RENUS and PARCS calculations are same except the temporal discretization method that the RENUS solution is obtained by the fifth BDF method [16] whereas the PARCS uses Crank-Nicholson with exponential transformation [11]. 1 ms small time step size is used to remove the effect come from the use of different temporal discretization methods.



Fig. 2. Core power behavior in the VVER440 rod ejection benchmark

As shown in Fig. 2, different power behaviors are observed in the P1 and SP3 applications. In general, core power behavior in rod ejection accidents is determined by the ejected rod worth. Table I represents the effective multiplication factors in rod-in and rod-out states and estimated ejected rod worth. Estimated rod worth is calculated as follow:

$$\rho_{rod} = \frac{1}{k_{rod\_in}} - \frac{1}{k_{rod\_out}}$$
(7)

and about 130 pcm reactivity difference is observed in the P1 and SP3 applications.

Table I: k-eff in rod-in and rod-out states and estimated rod worth in the VVER440 benchmark problem

	k-eff	k-eff	Rod Worth <sup>1)</sup>
	(Rod-in)	(Rod-out)	(pcm)
P1 (PARCS)	0.98931	1.00072	1152.5
P1 (RENUS)	0.98926	1.00075	1160.6
SP3 (RENUS)	0.98092	0.99092	1028.8

In order to verify that SP3 solution is accurate than P1 solution, P1, SP3, and Monte Carlos (MC) steadystate solutions are compared in a simplified 2-D VVER440 problem whose core configuration is the middle plane of the original 3-D problem. Two cases are simulated that total 6 periphery control rods are out in 'Case 1' whereas 'Case 2' simulates that 1 center control rod is out in the rod-out state. The MC solution is obtained by the McCARD transport code [17] using 100,000 particles per cycle with 50 inactive and 450 active cycles. Table II shows k-eff in the rod-in and rod-out states and estimated rod worth. Values in parenthesis are reactivity error and they are given as the pcm unit.

Гable II: k-е	ff in the	rod-in and	rod-out stat	es and estimated	l
rod wor	th in the	simplified	2-D VVER4	440 problem	

Tod worth in the simplified 2-D V VER440 problem						
		k-eff	k-eff	Rod Worth		
		(Rod-in)	(Rod-out)	(pcm)		
Case 1	MC	0.98787	1.01451	2658.1		
	P1	0.98491	1.01309	2824.5		
		(-304.6)	(-138.3)	(166.3)		
	SP3	0.98711	1.01385	2672.0		
		(-77.7)	(-63.9)	(13.8)		
Case 2	MC	0.98787	0.99922	1149.8		
	P1	0.98491	0.99782	1314.4		
		(-304.6)	(-140.0)	(164.6)		
	SP3	0.98711	0.99887	1102.0 (42.1)		
		(-77.7)	(-34.6)	1193.0 (43.1)		

In the VVER440 benchmark, the control rod has quite large thermal absorption XS, so huge spatial flux variation is formulated by control rod insertion. Thus it leads to significant inaccuracy on the P1 solution in the rod-in state. On the other hand, error of P1 solution decreases in the rod-out state because spatial flux becomes smooth. The rod worth is estimated by the difference of reactivity in rod-in and rod-out states, so large rod worth error occurs in the P1 method. On the other hands, SP3 produces reliable solutions in not only the rod-out state but the difficult rod-in state. Thus accurate rod worth can be estimated by the SP3 application.

## 4. Conclusion

In this work, the time-dependent SP3 TPEN method was developed to attain accurate hexagonal core transient solutions. In the SP3 TPEN approach, each hexagon node was split to 6 triangle nodes and the intra-nodal 2-D SP3 solutions were expressed as a third order polynomial in each triangle node.

The effectiveness of the SP3 TPEN method in hexagonal core transient analysis was verified in the VVER440 rod ejection benchmark problem. Considerable difference was observed in core power behaviors and estimated rod worth obtained by the P1 and SP3 methods. The superiority of the SP3 method was proved by comparing P1, SP3, and MC solutions that k-eff and estimated rod worth obtained by SP3 was much closer to the MC reference solutions.

Until now, core simulations have been conventionally performed by the P1 method. However, it renders inaccurate solutions especially for SMRs and FBRs whose geometry is generally hexagonal. Thus the SP3 TPEN method developed here can be used as the alternative methods that replace the conventional P1 solvers for accurate hexagonal core simulation.

### REFERENCES

[1] E. M. Gelbard, "Applications of the Simplified Spherical Harmonics Equations in Spherical Geometry," Tech. Rep. WAPD-TM-294, Bettis Atomic Power Laboratory, 1962 [2] E. W. Larsen, "Asymptotic Derivation of the Multigroup P1 and Simplified PN Equations with Anisotropic Scattering," Nucl. Sci. Eng., Vol.123, p. 328, 1996

[3] C. H. Lee and T. J. Downar, "A Hybrid Nodal Diffusion/SP3 Method Using One-Node Coarse-Mesh Finite Difference Formulation," Nucl. Sci. Eng., Vol.146, p. 176, 2004

[4] C. Beckert and U. Grundmann. "Development and Verification of a Nodal Approach for Solving the Multigroup SP3 Equations," Ann. Nucl. Energy, Vol.35, p. 75, 2008

[5] H. J. Jeong et al, "SP3 Nodal Core Calculation with Alternating Direction One-Dimensional Semi-Analytic Nodal Solutions," Trans. Am. Nucl. Soc., Nov.11-15, 2012, San Diego, California, USA

[6] M. H. Bae, "Development of Triangle-based Polynomial Expansion Nodal SP3 Method for Hexagonal Core Transport Calculation," Thesis, Seoul National University, 2010

[7] C. H. Lee, Tomasz Kozlowski, and Thomas J. Downar, "Analysis of Control Rod Ejection Accident in MOX and MOX/UOX Cores with Time-Dependent Multigroup Pin-by-Pin SP3 Methods," Proc. PHYSOR 2002, Oct.7-10, 2002, Seoul, Korea

[8] D. J. Lee, Tomasz Kozlowski, and Thomas J. Downar, "Multi-Group SP3 Approximation for Simulation of a Three-Dimensional PWR Rod Ejection Accident," Ann. Nucl. Energy, Vol.77, p. 94, 2015

[9] C. B. Shim, J. Y. Cho, and H. G. Joo, "Application of Source Expansion Nodal Method to SP3 Core Transient Analysis," Proc. RPHA15, Sep.16-18, 2015, Jeju, Korea

[10] J. Y. Cho et al., "Hexagonal CMFD Formulation Employing Triangle-based Polynomial Expansion Nodal Kernel," Proc. M&C 2011, Sep.9-13, 2001, Salt Lake City, Utah, USA

[11] H. G. Joo et al., "PARCS: A Multi-Dimensional Two-Group Reactor Kinetics Code Based on the Nonlinear Analytic Nodal Method," PUNE-98-26, Purdue University, 1998

[12] J. Y. Cho et al., "MASTER 3.0 User's Manual. Korea Atomic Energy Research Institute," KAERI/UM-8/2004, 2004

[13] Mihály Makai, "AER Benchmark Site," Proc. PHYSOR 2002, Oct.7-10, 2002, Seoul, Korea

[14] E. Olbrant, E. W. Larsen, M. Frank, and B. Seibold, "Asymptotic derivation and numerical investigation of timedependent simplified PN equations," J. Comput. Phys., V.238, p. 315, 2013

[15] J. I. Yoon and H. G. Joo, "Two-Level Coarse Mesh Finite Difference Formulation with Multigroup Source Expansion Nodal Kernels," J. Nucl. Sci. Technol., V.45, p. 668, 2008

[16] C. B. Shim et al., "Application of Backward Differentiation Formula to Spatial Reactor Kinetics Calculation with Adaptive Time Step Control," Nucl. Eng. Technol., V.43, p. 531, 2011

[17] H. J. Shim et al., "McCARD: Monte Carlo code for Advanced Reactor Deisgn and Analysis," Nucl. Eng. Technol., V.44, p. 161, 2012