Three-Dimensional Heterogeneous Variational Nodal Method for PWR Pin-by-pin Calculation and Control Rod Cusping Effect

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ABSTRACT

The Variational Nodal Method (VNM) is generalized for heterogeneous node by using finite sub-element technique within diffusion approximation in three-dimensional Cartesian geometry. Based on the code Violet-Het1D, a code named Violet-Het3D was developed to carry out Pressurized Water Reactor (PWR) pin-by-pin calculation and to handle the PWR control rod cusping effect. Instead of homogenizing the entire heterogeneous node caused by the partially inserted control rods, it explicitly describes the nodal heterogeneity by using tetrahedral mesh. Numerical results demonstrate its high accuracy for the pin-by-pin problem. For the control rod cusping effect, it shows better accuracy and efficiency than the flux-volume-weighted scheme.

Key Words: **Variational Nodal Method, heterogeneous, pin-by-pin, control rod cusping effect**

1. INTRODUCTION

Nodal methods play an important role in reactor core-analysis calculation due to its high computation efficiency and accuracy. However, traditional nodal methods require homogenized cross-section within each node. It introduces errors to calculate the differential worth of the control rod, and limits the computational efficiency when pin-by-pin problem is calculated.

Firstly, control rods keep moving along the axial direction within the Pressurized Water Reactor (PWR) core with a step size of about 2 cm, while the nodal size of neutronics simulation is usually about 20 cm. Thus, unavoidably a control rod assembly may be partly inserted into a node which means part of the node uses assembly-homogenized cross sections with control rods in while the other part uses assembly-homogenized cross sections with control rods out. The piece-wise distributed nodal cross sections can be simply homogenized by using the volume-weighted scheme which causes the numerically simulated curve of control rod differential worth being possessed by a lot of wiggles. Theoretically, it should be a smooth curve. This phenomenon is the so-called control rod cusping effect [1]. Since 1980s, many methods have been investigated to eliminate it, such as flux-volume-weighted method [2, 3] and adaptive mesh method [4]. The former has to obtain an approximated flux distribution, while the later has to regenerate the spatial mesh after each control rod movement to avoid the appearance of heterogeneous nodes.

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Secondly, traditional PWR core computation employs two-step scheme: assembly calculation and homogenization, whole core diffusion calculation and pin-power reconstruction within each assembly. To reduce the error introduced by homogenization, the pin-by-pin scheme has arisen. It solves the whole core problem with pin-cell homogenized cross section to eliminate the assembly homogenization and pin-power reconstruction. Therefore, many pin-by-pin calculation codes have been developed such as SCOPE2 [5] and EFEN [6]. However, as traditional nodal method requires homogenized cross-section in each mesh, the whole-core pin-by-pin problem should consist of millions of meshes, causing issues in both memory and efficiency. For example, a PWR can be divided into 10 million pin-size meshes. Together with the SP3 approximation and 4 energy groups, it needs 10 GB memory and the calculation time is about 24 hours [7] for a single CPU.

To overcome these disadvantages of traditional nodal methods mentioned above, traditional homogeneous nodal methods are expected to be generalized into heterogeneous nodal methods to maintain the computing efficiency with high accuracy. For the control rod cusping effect problem, if nodal method allows heterogeneity in a node, neither the flux-volume-weighted method nor the mesh regeneration would be needed to avoid the heterogeneous nodes. The control rod cusping effect is supposed to be directly eliminated by heterogeneous nodal method. For the pin-by-pin problem, a whole assembly or a quarter of an assembly can be treated as a node if heterogeneity is allowed in a node, so the computing efficiency increases with the decrease of the number of meshes.

Started from the above idea, this paper derives a finite sub-element method [8] based on VNM with diffusion approximation in three dimension Cartesian geometry after tested in one-dimensional case [9, 10]. Tetrahedron sub-elements are used to describe explicitly the heterogeneous nodes. A commercial program called Freefem++ [11] is employed to generate the sub-elements inside the nodes. Flux and source in the nodes as well as net current in the nodal surfaces are expanded by using liner finite trial functions. A code named Violet-Het3D was developed to treat heterogeneous node. In addition, a PWR pin-by-pin problem and a PWR control rod cusping effect problem are formulated to test the code. The capabilities and limitations of the code are then discussed.

2. THEORY

The three-dimensional within-group diffusion equation is:

$$\begin{cases} \nabla \cdot \boldsymbol{J}(\boldsymbol{r}) + \Sigma_t(\boldsymbol{r})\Phi(\boldsymbol{r}) = \Sigma_s(\boldsymbol{r})\Phi(\boldsymbol{r}) + S(\boldsymbol{r}) \\ \frac{1}{3}\nabla\Phi(\boldsymbol{r}) + \Sigma_t(\boldsymbol{r})\boldsymbol{J}(\boldsymbol{r}) = 0 \end{cases} \tag{1}$$

where Φ is the scalar flux ($cm^{-2}\,s^{-1}$), $\boldsymbol{J}$ is net current ($cm^{-2}\,s^{-1}$), Σ_t is the total cross section (cm^{-1}), Σ_s is the within-group scattering cross section (cm^{-1}), and S is the source term ($cm^{-3}\,s^{-1}$) including scattering and fission.

Same as the homogeneous VNM, the entire problem domain is decomposed into subdomains V_v

(nodes) and the functional can be written as a superposition of nodal contributions:

$$F\left[\Phi, J\right] = \sum_{v} F_v\left[\Phi, J\right] \tag{2}$$

However, to consider the nodal heterogeneity in this method, each node is further divided into a set of homogeneous sub-regions named sub-elements. That's the main difference between current VNM and this method. The nodal functional is then written as a superposition of sub-element functional:

$$F_v\left[\Phi, J\right] = \sum_{e} F_e\left[\Phi_e, J\right] \tag{3}$$

where the element functional is written as:

$$\begin{aligned} &F_e\left[\Phi_e, J\right] = \\ &\int_e dV\{D_e\left(\nabla\Phi_e\right)^2 + \left(\Sigma_{t,e} - \Sigma_{s,e}\right)\Phi_e{}^2 - 2\Phi_e S_e\} + 2\sum_{\gamma}\int_{\gamma}\Phi_{e,\gamma} J_{e,\gamma} d\Gamma \end{aligned} \tag{4}$$

The surface term in Eq. (4) only appears in those sub-elements adjacent to nodal interfaces because continuous trial functions are used within each node.

We expand the flux and source within the sub-element and net current along the sub-element's surfaces as:

$$\begin{cases} \Phi_e\left(\boldsymbol{r}\right) = \sum_{m=1}^{M} \varphi_{e,m} f_{e,m}\left(\boldsymbol{r}\right) \\ S_e\left(\boldsymbol{r}\right) = \sum_{m=1}^{M} s_{e,m} f_{e,m}\left(\boldsymbol{r}\right) \quad ,\boldsymbol{r} \in e \\ J_{e,\gamma}\left(\boldsymbol{r}\right) = \sum_{n=1}^{N} j_{e,\gamma,n} h_{e,\gamma,n}\left(\boldsymbol{r}\right) \end{cases} \tag{5}$$

Different from polynomial expansion in the current homogeneous VNM, $\boldsymbol{f}(\boldsymbol{r})$ and $\boldsymbol{h}(\boldsymbol{r})$ are the linear finite element trial functions [12] defined in the volume and on the surfaces. $\boldsymbol{\varphi}$, $\boldsymbol{s}$ and $\boldsymbol{j}$ are the unknown coefficients. M and N respectively represent the number of nodes within the sub-element and on its surface. For the cross sections in each element are homogeneous, the relationship between flux and source moments is written as:

$$s_{e,m} = \left(\Sigma_e + \frac{1}{k} v\Sigma_{f,e}\right)\varphi_{e,m} \tag{6}$$

Substituting Eq. (6) into the element functional in Eq. (4) yields the reduced functional:

$$F_e\left[\boldsymbol{\varphi}, \boldsymbol{j}\right] = \boldsymbol{\varphi}_e{}^{\mathrm{T}} \boldsymbol{A}_e \boldsymbol{\varphi}_e - 2\boldsymbol{\varphi}_e{}^{\mathrm{T}} \boldsymbol{F}_e \boldsymbol{s}_e + 2\boldsymbol{\varphi}_e{}^{\mathrm{T}} \boldsymbol{M}_e \boldsymbol{j}_e \tag{7}$$

where

$$A_{e,mm'} = \int_e \left\{ D_e \cdot \nabla f(\boldsymbol{r})_{e,m} \cdot \nabla f_{e,m'}(\boldsymbol{r}) + \left(\Sigma_{t,e} - \Sigma_{s,e} \right) f_{e,m}(\boldsymbol{r}) f_{e,m'}(\boldsymbol{r}) \right\} dV \tag{8}$$

$$F_{e,mm'} = \int_e f_{e,m}(\boldsymbol{r}) f_{e,m'}(\boldsymbol{r}) dV \tag{9}$$

$$M_{e,mn'} = \int_\gamma f_{e,m}(\boldsymbol{r}) h_{e,\gamma,n'}(\boldsymbol{r}) d\Gamma \tag{10}$$

To obtain the nodal functional, we should use the Boolean transformation matrix [13] Ξ_e to map the element trial function coefficients to the nodal expansion coefficients:

$$\boldsymbol{\varphi}_e = \Xi_e \boldsymbol{\varphi} \tag{11}$$

Substituting Eq. (11) into Eq. (7), and then substituting Eq. (7) into Eq. (2) leads to the nodal functional:

$$F_v[\boldsymbol{\varphi}, \boldsymbol{j}] = \boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{A} \boldsymbol{\varphi} - 2\boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{s} + 2\boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{M} \boldsymbol{j} \tag{12}$$

where

$$\boldsymbol{A} = \sum_e \Xi_e^T \boldsymbol{A}_e \Xi_e \tag{13}$$

$$\boldsymbol{s} = \sum_e \Xi_e^T \boldsymbol{F}_e \boldsymbol{s}_e \tag{14}$$

$$\boldsymbol{M} = \sum_e \Xi_e^T \boldsymbol{M}_e \tag{15}$$

As we obtain the nodal functional, the following derivation is same as that in homogeneous VNM. Taking the variation of the response matrix formulation, Eq. (12) with respect to $\boldsymbol{\varphi}$ and setting the variation to zero yields:

$$\boldsymbol{\varphi} = \boldsymbol{A}^{-1} \left(\boldsymbol{s} - \boldsymbol{M} \boldsymbol{j} \right) \tag{16}$$

The variation with respect to $\boldsymbol{j}$ yields the condition that

$$\psi_\gamma = \boldsymbol{M}_\gamma^{\mathrm{T}} \boldsymbol{\varphi} \tag{17}$$

be continuous across each nodal interface. Define the partial currents as:

$$j_\gamma^{\pm} = \frac{1}{4} \psi_\gamma \pm \frac{1}{2} j_\gamma \tag{18}$$

substituting Eq. (18) into Eq. (16) and Eq. (17) we can obtain the response matrix equation:

$$\boldsymbol{j}^{+} = \boldsymbol{B} \boldsymbol{s} + \boldsymbol{R} \boldsymbol{j}^{-} \tag{19}$$

$$\boldsymbol{\varphi} = \boldsymbol{H} \boldsymbol{s} - \boldsymbol{C} \left(\boldsymbol{j}^{+} - \boldsymbol{j}^{-} \right) \tag{20}$$

where

$$\boldsymbol{B} = \frac{1}{2}\left[\boldsymbol{G} + \boldsymbol{I}\right]^{-1}\boldsymbol{C}^{\mathrm{T}} \tag{21}$$

$$\boldsymbol{R} = \left[\boldsymbol{G} + \boldsymbol{I}\right]^{-1}\left[\boldsymbol{G} - \boldsymbol{I}\right] \tag{22}$$

$$G_{\gamma\gamma'} = \frac{1}{2}\boldsymbol{M}_{\gamma}^{\mathrm{T}}\boldsymbol{A}^{-1}\boldsymbol{M}_{\gamma'} \tag{23}$$

$$C_{\gamma}^{\mathrm{T}} = \boldsymbol{M}_{\gamma}^{\mathrm{T}}\boldsymbol{A}^{-1} \tag{24}$$

$$\boldsymbol{H} = \boldsymbol{A}^{-1} \tag{25}$$

Eq. (19) and Eq. (20) are used to update the moments of partial current and scalar flux. The moments of source are updated by Eq. (6).

3. RESULTS

A PWR pin-by-pin problem and a PWR control rod cusping effect problem were formulated to test the ability of the code Violet-Het3D for treating heterogeneous nodes.

3.1. Pin-by-pin Problem

The radial core configuration of the problem is shown in Fig. 1. Each pin is 1.26 cm in length and width, and the moderator region is 21.46 cm. In axial direction, the fuel region is 60 cm in height and there is a moderator region (9 cm thick) both at the top and the bottom of the core. The cross sections in each pin are homogenized. Ideally the neutron-transport equation should be solved in this problem. However in order to evaluate Violet-Het3D's ability of treating spatial heterogeneity, the neutron-diffusion equation was solved for demonstration purpose. The reference calculation takes each individual pin as a node in radial, while the Violet-Het3D treats an entire assembly as a single node with heterogeneous structure inside. Both calculations take 3 cm as the height of each node, so the entire problem is divided into 26 layers in total. In addition, it's a two-energy group problem.

The reference model treats each pin as a node (including reflector assembly), so the whole problem consists of 67626 nodes. And the reference solution is obtained by the code named Violet-Hom3D which uses the theory of homogeneous VNM. While the Violet-Het3D calculation only employs 234 nodes. As shown in Fig. 2, each assembly (including reflector assembly) in Violet-Het3D calculation is divided into tetrahedrons by the commercial program called Freefem which is not needed in the reference calculation. Tetrahedron is chosen for its good geometrical adaptability. And it can be found in Fig. 2 that each pin consists of 6 tetrahedrons which is enough to describe explicitly the heterogeneous assembly. Further refining the tetrahedrons will greatly decrease the computing effi-

ciency and obtain little improvement for the result. The results of keff are shown in table I and the power distribution is shown in Fig. 3. Table II shows the difference of the power distribution compared with the reference and Violet-Het3D obtains accurate results obviously.

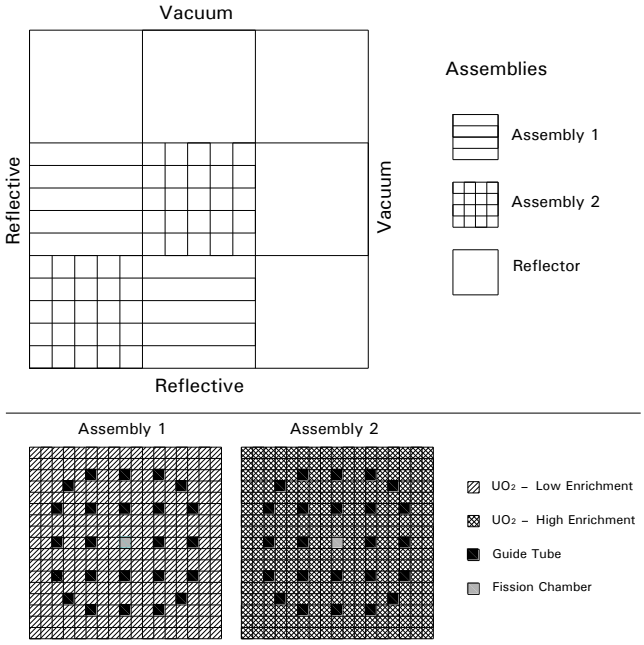

Fig. 1. Radial core and assembly configuration

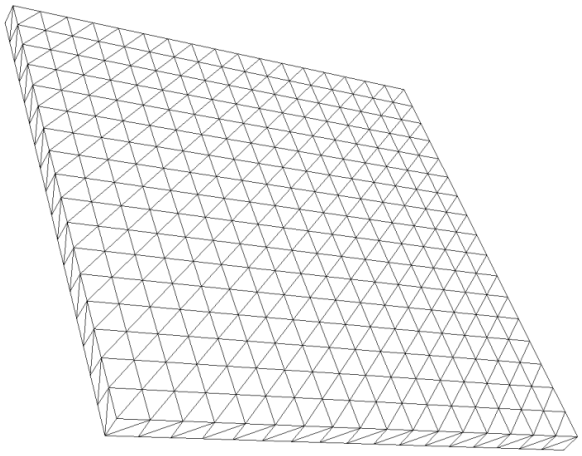

Fig. 2. Sub-elements configuration in each layer of the assembly

Table I. keff Comparison for the pin-by-pin problem

	Reference	Violet-Het3D	Error / pcm
k_{eff}	1.00438	1.00350	-88

Table II. Power Comparison of the pin-by-pin problem

Case	Reference	Violet-Het3D	Error / %
Maxpower	2.8410	2.8430	0.07
Minpower	0.0756	0.0748	-1.06
MaxError	-	-	1.5

The average error of power distribution is below 1.0% and the regions closed to moderator usually have low power and relatively high error. The positions of the maximum power, minimum power and maximum error are shown in Fig. 4. Violet-Het3D is supposed to be more efficient than the existing VNM for computing the pin-by-pin problem. However, as a result of the enormous number of nodes that had to be defined to model the complicate geometry of the assembly (648 nodes for each assembly in this problem), large response matrices are obtained. This will greatly increase not only the time of generating the response matrices, but also the time of iteration. In this problem, Violet-Het3D cost more time than the existing VNM. Improvements and acceleration methods are under study to reduce the computational time.

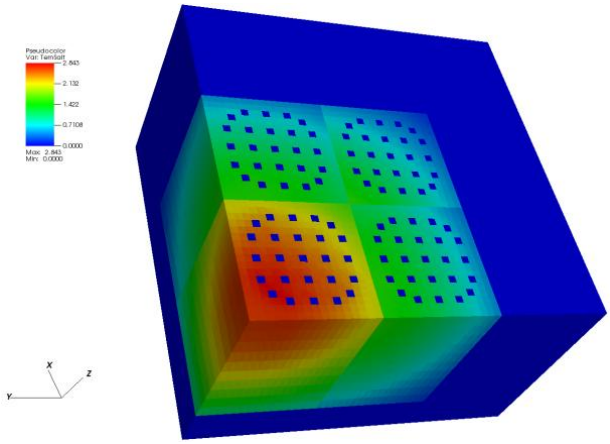

Fig. 3. Power distribution of the pin-by-pin problem

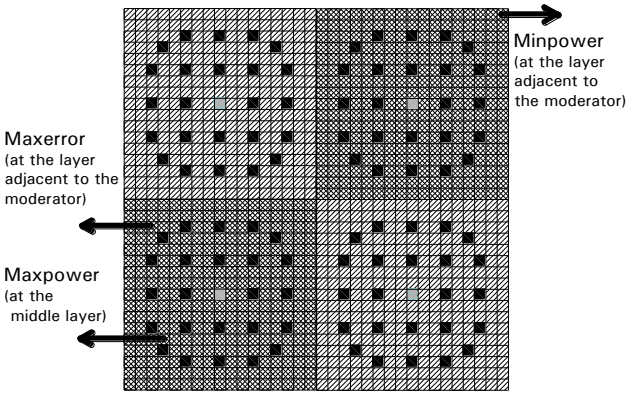

Fig. 4. Positions of the maximum power, minimum power and maximum error

3.2. Control Rod Cusping Effect

The configuration of the core is shown in Fig. 5 and Fig. 6 and the radial size of all the assemblies is 20×20 cm. The two-group macroscopic cross-sections of assemblies and reflector are already provided by lattice code. As indicated by Fig. 5, CR represents the assembly with control rod and it takes 1cm for every step from the top to the bottom of the core. Fig. 6 shows there are totally 272 steps for the control rod in the core.

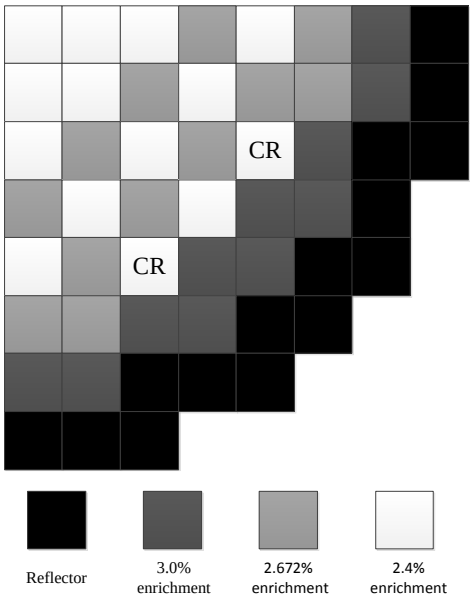

Fig. 5 Radial configuration of 1/4 reactor core

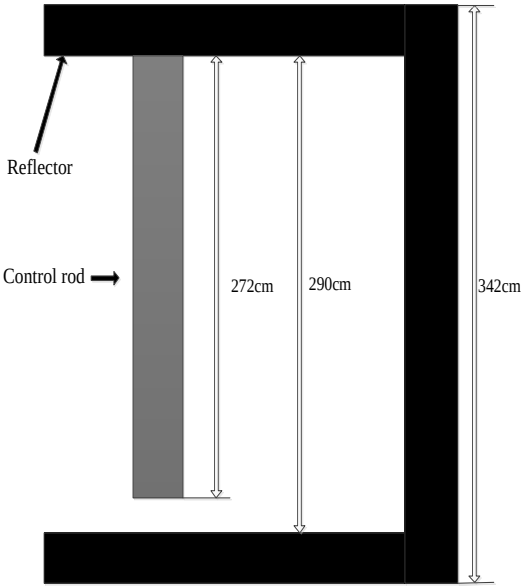

Fig. 6 Axial size of the reactor core

To obtain the reference of the control rod differential worth, we divide each assembly into 4 nodes in radial and take 1cm for the axial size. So the size of each node is 10×10×1 cm and heterogeneous nodes will not exist in this situation. Violet-Hom3D which applies the method of homogeneous VNM is used to the reference calculation.

Actually, in the core-analysis calculation, nodal size is usually about 10~20 cm in axial direction. In this problem, as indicated by Fig. 6, the axial size of the nodes should be 26 cm in the reflector region and 20 cm in the core except a layer of 10 cm at the bottom of the core. In this situation, heterogeneous nodes appear with the movement of the control rod as is shown in Fig. 7. To obtain the homogenous cross-section of the heterogeneous nodes, the easiest method is volume-weighted scheme. However, this scheme causes severe control rod cusping effect as is shown in Fig. 8. A more commonly used method is flux-volume-weighted scheme. It has to do the iteration between the one-dimensional calculation of the assembly with control rod in the axial direction and three-dimensional calculation of the core. The 3D dimensional calculation aims to provide radial leakage of the 1D calculation. And the 1D calculation aims to obtain the homogenized cross section for the 3D calculation. The iteration should do at least once to obtain acceptable accuracy. The result of this scheme is also shown in Fig. 8. We can find that the cusping effect is greatly weakened

but there are still a lot of small wiggles on the control rod differential worth curve. All the above calculations are done by Violet-Hom3D.

Violet-Het3D adopts the same coarse mesh mentioned above, for heterogeneity is allowed in this method, homogenization is not needed for the nodes with control rod partly inserted. The heterogeneous nodes are explicitly described by tetrahedrons (sub-elements): each node is divided into 10 layers with 24 tetrahedrons for each layer. The numerical result is also shown in Fig. 8. Obviously, Violet-Het3D obtains better results than volume-weighted and flux-volume-weighted schemes. It eliminates the cusping effect and obtains a smooth differential worth curve which agrees well to the reference. While there is still some difference between the reference and the curve obtained by Violet-Het3D especially at the top of the curve, it probably because the linear expansion approximation of the flux and source in the sub-element as indicated by Eq. (5). Increasing the number of sub-element in the nodes will improve the results.

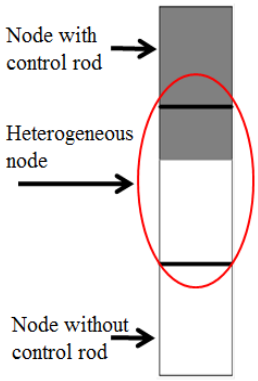

Fig. 7 Heterogeneous node caused by control rod

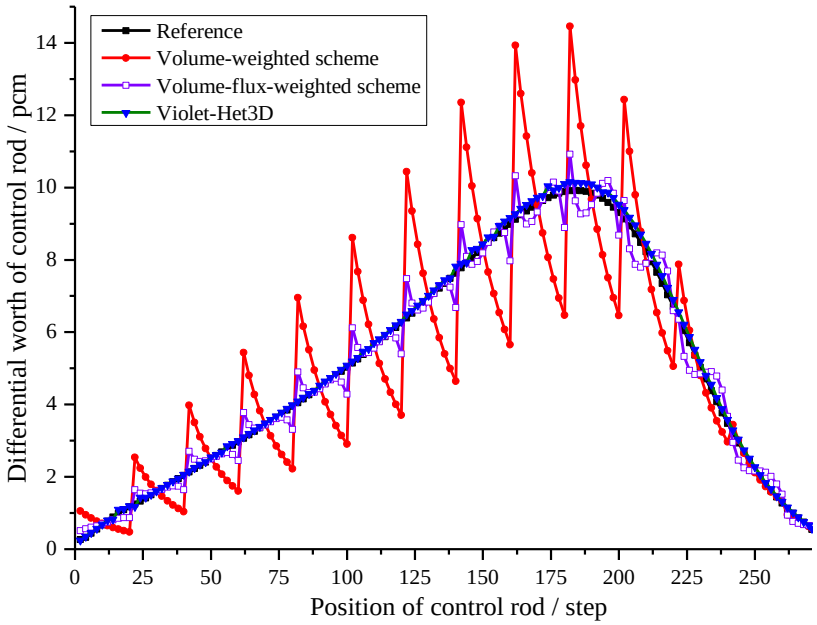

Fig. 8 Differential worth of control rod calculated by different scheme

Table III shows the computational time of different schemes. We can find the volume-weighted scheme costs the least time but the result is unacceptable. As the flux-volume-weighted scheme has to do the iteration between 3D and 1D calculation as least once, the computational time is more than twice as much as that of volume-weighted scheme. As indicated in Table III, Violet-Het3D costs much less time than the flux-volume-weighted scheme. It is because no 3D-1D iteration for the homogenized cross section is performed in Violet-Het3D. However, Violet-Het3D costs about 1.4 times as much time as volume-weighted scheme. This is because 99 nodes and 240 tetrahedrons are defined within each node in Violet-Het3D to describe the movement of control rods which makes the response matrices get larger than those in volume-weighted scheme. Larger response matrices slow down the power iteration of Violet-Het3D.

Table III. Computational time of different schemes

Schemes	Reference	Volume-weighted	Flux-volume-weighted	Violet-Het3D
Time /min	>1000	141.5	331.7	196.0

4. CONCLUSIONS

This paper derives a finite sub-element method based on VNM with diffusion approximation in three-dimension Cartesian geometry and a code named Violet-Het3D was developed to treat heterogeneous node. Two problems, a PWR pin-by-pin problem and a PWR control rod cusping effect problem were calculated.

The numerical results of the pin-by-pin problem show that high accuracy can be obtained by Violet-Het3D. The maximum relative error of the 3D pin power distribution is about 1.5% at the pin adjacent to the moderator region at the bottom of the core. More work should been done to improve the computing efficiency of Violet-Het3D.

The results of the control rod cusping effect problem show that without homogenization in the nodes with control rod partly inserted, Violet-Het3D obtains a smooth differential worth curve which agrees well to the reference. It costs more time than volume-weighted scheme but it's more efficient than flux-volume-weighted scheme.

Violet-Het3D will be expanded to solve the neutron-transport equation in the future and more improvements and acceleration methods should be done for this method.

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