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Stability, accuracy and numerical diffusion analysis of nodal expansion method for steady convection diffusion equation

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HIGHLIGHTS

- NEMs are innovatively applied to solve convection diffusion equation.
- Stability, accuracy and numerical diffusion for NEM are analyzed for the first time.
- Stability and numerical diffusion depend on the NEM expansion order and its parity.
- NEMs have higher accuracy than both second order upwind and QUICK scheme.
- NEMs with different expansion orders are integrated into a unified discrete form.

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ABSTRACT

The traditional finite difference method or finite volume method (FDM or FVM) is used for HTGR thermal-hydraulic calculation at present. However, both FDM and FVM require the fine mesh sizes to achieve the desired precision and thus result in a limited efficiency. Therefore, a more efficient and accurate numerical method needs to be developed. Nodal expansion method (NEM) can achieve high accuracy even on the coarse meshes in the reactor physics analysis so that the number of spatial meshes and computational cost can be largely decreased. Because of higher efficiency and accuracy, NEM can be innovatively applied to thermal-hydraulic calculation.

In the paper, NEMs with different orders of basis functions are successfully developed and applied to multi-dimensional steady convection diffusion equation. Numerical results show that NEMs with three or higher order basis functions can track the reference solutions very well and are superior to second order upwind scheme and QUICK scheme. However, the false diffusion and unphysical oscillation behavior are discovered for NEMs. To explain the reasons for the above-mentioned behaviors, the stability, accuracy and numerical diffusion properties of NEM are analyzed by the Fourier analysis, and by comparing with exact solutions of difference and differential equation. The theoretical analysis results show that the accuracy of NEM increases with the expansion order. However, the stability and numerical diffusion properties depend not only on the order of basis functions but also on the parity of the order. The numerical experiments are carried out to validate the above conclusions, which provide some significant guides for the development of the new NEMs. It can be concluded that NEMs have great potential to solve thermal hydraulic problems effectively, and can be used in the engineering design code.

1. Introduction

High temperature gas cooled reactor (HTGR) is characterized by the huge three-dimensional computational cost, drastic changes in temperature and flow distribution, multi-physics and multi-loop coupling complicated system and so on (Wang, 2011). The above characteristics increase the computational challenges. At the moment, for HTGR thermal-hydraulic calculation, the traditional finite difference method or finite volume method (FDM or FVM) is used. However, both FDM and FVM require fine mesh size to achieve the desired precision and thus result in a limited efficiency (Cleveland and Greene, 1986). Therefore, a more efficient and accurate numerical method for three-dimensional simulation needs to be developed.

Nodal expansion method (NEM) attracts many attentions due to its high efficiency and accuracy in the reactor physics analysis, and it has proved to be superior to FDM and FVM (Lawrence,

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1986). NEM is a kind of nodal method which combines the advantages of FDM and finite element method (FEM). As far as accuracy, the NEM employs piecewise continuous polynomial to approximate the solution, just the same way as the FEM. In addition, NEM generates quite sparse matrix structure as the FDM does. Therefore, NEM can achieve high accuracy even on the coarse meshes so that the number of spatial meshes and computational cost can be largely decreased (Hennart, 1986). In view of the advantages of NEM, we hope to extend NEM to solve the HTGR thermal hydraulic problems and finally to simultaneously and effectively solve multi-dimensional neutronic-thermal hydraulic coupling problem of HTGR (Deng, 2013). The convection diffusion equation is one of the fundamental equations in HTGR thermal hydraulic problems and many thermal hydraulic problems can be described through convection diffusion equation. However, for convection diffusion equation using NEM, false diffusion and unphysical oscillation behaviors are discovered in our research. So we want to learn the numerical properties of NEMs for thermal hydraulic problems in order to improve and implement NEM in engineering analysis code, which is relatively rare in the previous research.

Another nodal method, nodal integral method (NIM) has been developed to solve thermal hydraulic problem (Michael and Dorning, 2001; Wang, 2005; Singh, 2008), whose basic idea is that the solutions are analytically solved in certain condition. Recently, nodal integral expansion method (NIEM) has also been presented to solve one-dimensional, transient convection-diffusion equation, which combines some features of NEM and NIM (Lee, 2011). However, there exist a lot of time-consuming exponential terms in the derivation of the above two nodal methods, and the calculation of the pseudo-source terms is quite complicated.

Furthermore, stability, accuracy and numerical diffusion are important criterions of appraising the numerical methods. Stability and accuracy are always in conflict with each other. Specially, high order accuracy methods may lead to oscillatory while unconditionally-stable-methods may produce great errors because of false diffusion (Yu et al., 2011). So both the effect of stability and accuracy are considered rather than only one of them. In addition, when the numerical diffusion is less than the true diffusion, the numerical method may lead to unstable numerical solutions in the condition of coarse mesh or high velocity. On the contrary, when the numerical diffusion is greater than the true diffusion, the over-diffusive behavior of numerical solutions may be observed (Cai et al., 2014).

Therefore, the derivation process and the numerical property analysis of NEMs with different orders of basis functions for multi-dimensional steady convection diffusion equation are studied and developed. First, the formulations of NEM for multi-dimensional steady convection diffusion equation are presented in Section 2. Then, stability is analyzed by using Fourier analysis and exact solutions of difference equation in Section 3. Section 4 shows the theoretical analysis results of the numerical diffusion and numerical accuracy for NEMs with different orders of basis functions. At last, to verify the mathematical analysis, several numerical experiments are carried out in Section 5, a brief summary and discussion is presented in Section 6.

2. NEM formalism for multi-dimensional steady convection diffusion equation

The three-dimensional, steady state, convection diffusion equation in Cartesian geometry is written as:

$$U\frac{\partial\phi}{\partial x}+V\frac{\partial\phi}{\partial x}+W\frac{\partial\phi}{\partial x}-\Gamma\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}\right)=Q \tag{1}$$

where U, V, W are the velocity in the different coordinate direction, respectively; Γ is the diffusivity; Q is the source term.

The derivation process of NEM for three-dimensional steady convection diffusion equation is generally divided into three steps: first, the transverse integration process is employed to reduce a three-dimensional convection diffusion equation to three one-dimensional transverse-integrated equations; second, these solutions of one-dimensional transverse-integrated equations are approximated by an expansion of a series of Legendre polynomials and the expansion coefficients are determined by some constraint conditions, after that, a set of discrete equations are obtained in terms of nodal average variables; then, the nodal average variables can be easily obtained by the nodal balance equations, and the final system of discrete equations are presented. The derivations are discussed in details.

By applying the transverse integration strategy over node (i, j, k), the three transverse integrated equations can be written as:

$$F_r^K\frac{\mathrm{d}}{\mathrm{d}r}\phi_r^K(r)+\frac{\mathrm{d}}{\mathrm{d}r}J_r^K(r)=S_r^K(r)=Q_r^K(r)-L_r^K(r) \tag{2}$$

$$\phi_r^K(r)=\frac{1}{4h_\xi^K h_\eta^K}\int_{-h_\xi^K}^{h_\xi^K}\int_{-h_\eta^K}^{h_\eta^K}\phi^K\left(r,\xi,\eta\right)\mathrm{d}\xi\mathrm{d}\eta \tag{3}$$

$$J_r^K(r)=-\Gamma^K\frac{\mathrm{d}\phi_r^K(r)}{\mathrm{d}r} \tag{4}$$

$$Q_r^K(r)=\frac{1}{4h_\xi^K h_\eta^K}\int_{-h_\xi^K}^{h_\xi^K}\int_{-h_\eta^K}^{h_\eta^K}Q^K\left(r,\xi,\eta\right)\mathrm{d}\xi\mathrm{d}\eta \tag{5}$$

$$L_r^K(r)=\frac{1}{4h_\xi^K h_\eta^K}\int_{-h_\xi^k}^{h_\xi^K}\int_{-h_\eta^K}^{h_\eta^K}\left(F_\xi^K\frac{\partial\phi}{\partial\xi}-\Gamma^K\frac{\partial^2\phi}{\partial\xi^2}+F_\eta^K\frac{\partial\phi}{\partial\eta}-\Gamma^K\frac{\partial^2\phi}{\partial\eta^2}\right)\mathrm{d}\xi\mathrm{d}\eta \tag{6}$$

where $r = x, y, z \neq \xi \neq \eta$; $\xi = y, z, x$; $\eta = z, x, y$; $K = (i, j, k)$; $F_x^K = U^K$, $F_y^K = V^K$, $F_z^K = W^K$; U^K, V^K, W^K and Γ^K are the average values in the node (i, j, k). The node volume is $2h_x^{i,j,k}\times 2h_y^{i,j,k}\times 2h_z^{i,j,k}$ and the local origin is located in node center. $\phi_r^K(r)$ is the r-dependent transverse-integrated variable as shown in Fig. 1; $J_r^K(r)$ is the r-dependent diffusion current over the $\xi-\eta$ surface; the pseudo-source terms $S_r^K(r)$ are divided into two terms: transverse integrated true source term $Q_r^K(r)$ and transverse leakage term $L_r^k(r)$.

To solve Eq. (2), $\phi_r^K(r)$, $Q_r^K(r)$ and $L_r^K(r)$ within each node are approximated by an expansion of a series of Legendre polynomials.

$$\phi_r^K(r)\approx\sum_{n=0}^{N}a_{r,n}^K f_n^K(r) \tag{7}$$

$$Q_r^K(r)\approx\sum_{n=0}^{N_1=2}q_{r,n}^K f_n^K(r) \tag{8}$$

$$L_r^K(r)\approx\sum_{n=0}^{N_2=0}l_{r,n}^K f_n^K(r) \tag{9}$$