Application of the virtual density theory in fast reactor analysis based on the neutron transport calculation

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HIGHLIGHTS

- The virtual density theory is applied in the steady-state fast reactor code SARAX.
- New formulism of virtual density theory is proposed based on the SN nodal method.
- The transport-based virtual density method has good accuracy and efficiency.

ABSTRACT

The geometry distortion introduces one of the most important reactivity feedbacks in the fast reactor. To evaluate the reactivity caused by the geometry distortion, this paper presents a new approach applied in the steady-state fast reactor code SARAX. This approach is based on the discrete ordinates nodal method, first-order perturbation approximation and virtual density theory. In this way, the virtual material density is changed instead of changing the geometry in modeling the distortion. Compared with other methods to get geometry distortion reactivity, this method has better geometric adaptability and better efficiency in the multi-case evaluation. A series of verification are carried on, including the uniform expansion, the non-uniform expansion and the local geometry distortion. The results show that the virtual density method has good accuracy and efficiency in evaluating the geometry distortion reactivity.

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1. Introduction

The geometry distortion is a common phenomenon in the fast reactor, containing the core compaction, core expansion and local geometry distortion. During the normal or accidental transients occurring in a fast reactor, the thermal gradients will induce differential thermal expansion of the fuel and structure materials. And the differential thermal expansion results differential displacement. Besides the thermal expansion, the irradiation swelling and external mechanical force can also cause the geometry distortion.

As the primary reactivity feedback in a fast reactor, the assembly distortion is one of the most important contributions to achieve the inherent safety. Generally, the axial expansion and radial expansion can be simply evaluated by the direct eigenvalue calculation. Differently, evaluating the local geometry distortion is much more complicated. Since the local effect is usually accompanied with the irregular geometry. Theoretically, such effect can be simulated by the fine geometric modeling locally using the Monte Carlo method. However, the high-fidelity modeling at core level is not practical even based on current computational condition.

For the design work, the deterministic method is still widely applied for the fast reactor. The deterministic calculation is based on the spatial homogenization, which makes the modeling of local geometry distortion very difficult, especially for the irregular geometry.

To solve the problems, many methods have been proposed. Knutson proposed a method by treating the reactivity effect as the comprehensive contributions of fuel movement and sodium backfill in 1982 (Knutson, 1982). The assembly worth gradient for each core position and each direction should be pre-calculated in this method. Then, the reactivity was obtained by multiplying the assembly displacement and the worth gradient data. In 1986, Kamal and Orechwa proposed a similar method. They introduced the displacement reactivity worth to quantify the reactivity of assembly displacement (Kamal and Orechwa, 1986). Both methods assumed that the worth distribution was a cosine function. In 2013, Huo calculated the assembly bowing using the same method as Kamal and Orechwa, but the perturba-
tion theory was applied to calculate the displacement reactivity worth instead of the direct calculation (Huo et al., 2013).

For these methods, the geometry distortion calculation was still complicated. A plenty of calculations for each assembly and each direction should be carried on as pre-processing. This process was very time consuming if the neutron transport theory was applied. Besides, the accuracy for all of these methods was not so good. The relative error exceeded 12% even very small expansion was modeled in the previous tests.

In 2014, Reed proposed the virtual density theory (Reed, 2014a, b). It was pointed out that any geometry distortion can be counteracted by the equivalent material density change. This relationship allows evaluating the reactivity of geometry distortion by defining different material density change. Compared to other methods, the virtual density theory improved the computing efficiency greatly. By assuming the microscopic cross sections were not affected by the geometry change, the time-consuming pre-calculations were avoided.

Thanks to the fast development of computing technology, the neutron transport method is becoming more and more popular in the fast reactor core analysis. It overcomes the limitation of neutron diffusion in modeling the strong anisotropy of fast neutron (Yang et al., 2007). Based on this tendency, a new fast reactor analysis code SARAX (System for Advanced Reactor Analysis at Xi’an Jiao Tong University) has been developed based on the three-dimensional full core neutron transport calculation. By using the neutron transport theory for the core analysis, a more direct and efficient method to evaluate the geometry distortion reactivity should be considered.

In this paper, we introduce the virtual density theory into SARAX code for the reactivity analysis and extend the method to the transport theory. The special treatment of leakage term is abandoned compared to the diffuse theory. Two approaches are proposed to model the global and local geometry distortion according to their characteristics.

In Section 2, the virtual density theory based on the discrete ordinate ($S_0$) method is derived and its application is introduced for typical geometry distortion. In Section 3, the numerical tests for the global expansion and local distortion cases are carried on to verify the accuracy and show the capability of the new way for reactivity evaluation in the fast reactor. Section 4 gives the summation to close this paper.

2. Methods

2.1. SARAX code introduction

SARAX is a new code system developed for the fast reactor design and neutronics analysis. SARAX-FR is a part of SARAX, which is invoked for the core analysis calculation. This code reads the homogenized few-group cross sections from the output of Monte Carlo code OpenMC (Romano et al., 2015; Romano and Forget, 2013) or its own cross section generation code SARAX-FXS (Du et al., 2017).

With the interpolated few-group cross sections, the three-dimensional (3-D) neutron transport calculation is performed based on the $S_0$ nodal method (Lu and Wu, 2007). For each hexagonal assembly, 6 triangular meshes are divided.

2.2. Virtual density theory

The virtual density theory is based on the first order perturbation and alters the material density (isotropically or anisotropically) instead of explicitly changing the geometry in evaluating the reactivity caused by geometry distortion.

2.2.1. Formulation of virtual density theory

Reed (2014a,b) proposed a virtual density method based on the diffusion theory. To compare the difference, the diffusion-based equations is reviewed firstly. The perturbation equation can be written as:

$$\Delta \rho = \left( \phi^* \left( \frac{1}{V} \delta R_d + \delta S_d - \delta A_d - \delta L_d \right) \phi \right) \left\{ \phi^* \left| F_d \phi \right| \right\}$$

(1)

Here $F_d$, $S_d$, $A_d$, and $L_d$ are the diffusion operators for fission, scattering, absorption and leakage, respectively.

For the first 3 terms, there is little difference between the diffusion- and transport-based methods. However, special treatment was done to express the leakage term when the virtual density was applied in the diffusion equation, for which the leakage term is approximated by the Fick’s law. The leakage term in the diffusion formalism can be written as:

$$\langle \phi^* | \delta L_d \phi \rangle = -\int \langle \phi^* \nabla \cdot \delta D \nabla \phi \rangle \, dE \, dV$$

$$= -\int \langle \delta (\nabla \phi \cdot \delta D) \rangle \, dE \, dV + \int \langle \nabla \phi^* \cdot \nabla \phi D \rangle \, dE \, dV$$

(2)

Because the adjoint flux vanishes on the surface of distortion region and $\delta D$ vanishes beyond the extent of density change, the surface term is generally ignored. But this assumption is not rigorous since the diffusion coefficient could be discontinuous for the anisotropic distortion in the virtual density theory. In this case, the surface term is not zero and should be taken into account. Reed proposed a better way to solve this problem. The surface leakage diffusion quantities was derived and it was distinguished them from existing volume leakage quantities. The numerical tests showed good accuracy.

However, in current fast reactor analysis code, the neutron transport calculation is becoming the major choice for the core analysis. It is theoretically better to improve the accuracy for the more heterogeneous and anisotropic cores (Du et al., 2017). As a consequence, the geometry distortion reactivity calculation should be made consistent with the updated flux solver.

For calculating the geometry distortion reactivity, the transport-based equation will make the virtual density method more complete and easier to implement. Because based on the transport theory, the leakage term in Eq. (1) can be vanished during the derivation as in Eq. (3), so no special approximation or treatment is required. The first-order perturbation equation based on neutron transport equation can be expressed as:

$$\Delta \rho = \left( \phi^* \left( \frac{1}{V} \delta S + \delta A - \delta L \right) \phi \right) \left\{ \phi^* \left| F \phi \right| \right\}$$

(3)

Here $F$, $S$ and $A$ are the transport operators for fission, scattering and absorption, respectively.

For the perturbation terms, the operators in integral form are given as follows. As in Eqs. (4) through (6), the angular dependence of flux is explicitly expressed in the transport-based equations.

$$\langle \phi^* | \delta F \phi \rangle = \int \int \int z(E) \phi^* \, dE \, d\Omega \int \delta (\Sigma_{f}(r, E)) \phi(r, E, \omega') \, dE \, d\omega \, dV$$

(4)

$$\langle \phi^* | \delta S \phi \rangle = \int \int \int \phi^* \, dE \, d\Omega \int \delta (\Sigma_{s}(r, E, \Omega')) \phi(r, E, \Omega') \, dE \, d\Omega' \, dV$$

(5)

$$\langle \phi^* | \delta A \phi \rangle = \int \int \int \phi^* \phi \, dE \, d\Omega \, dV$$

(6)
In the same way, the base terms as defined as:

\[
\langle \phi^* | F | \phi \rangle = \int \int \frac{\mathcal{L}(E)}{4\pi} \phi^* dE d\Omega \int \int \phi \Sigma_r(r, E') \phi(r, E', \Omega') dE' d\Omega' dV
\]  
(7)

\[
\langle \phi^* | S | \phi \rangle = \int \int \int \int \phi^* dE d\Omega \int \int \int \Sigma_s(r, E, \Omega) - E, \Omega \phi(r, E, \Omega) dE' d\Omega' dV
\]  
(8)

\[
\langle \phi^* | A | \phi \rangle = \int \int \int \phi^* \Sigma_r dE d\Omega dV
\]  
(9)

In modeling the geometry distortion, we assume that the slight change of microscopic cross section can be ignored. So, if defining 
\[j = \frac{d}{dE} \frac{\Sigma_r}{\Sigma_s}
\]
then, Eq. (3) can be written as:

\[
\Delta \rho = \bar{\rho} \mathcal{L} \frac{\langle \phi^* \left( \frac{1}{\Sigma_s} F + S - A \right) \phi \rangle}{\langle \phi^* | F | \phi \rangle} = \bar{\rho} \mathcal{L} \frac{\langle \phi^* | L \phi \rangle}{\langle \phi^* | F | \phi \rangle}
\]  
(13)

where, the subscripts \(i\) and \(j\) stand for the radial and axial index, respectively.

If we define the shorthand notation as:

\[P = \frac{\langle \phi^* \left( \frac{1}{\Sigma_s} F + S - A \right) \phi \rangle}{\langle \phi^* | F | \phi \rangle}
\]
(14)

and,

\[L = \frac{\langle \phi^* | L \phi \rangle}{\langle \phi^* | F | \phi \rangle}
\]
(15)

The reactivity change is obtained as:

\[
\Delta \rho = \bar{\rho} \mathcal{L} \frac{\langle \phi^* | L \phi \rangle}{\langle \phi^* | F | \phi \rangle}
\]  
(16)

Substituting Eqs. (21) and (22) into Eq. (20), \(\varepsilon\) can be expressed as:

\[
\varepsilon = \frac{1}{f^2} - 1
\]  
(23)

Thus, the reactivity of isotropic distortion can be calculated using Eqs. (19) and (23). However, if the distortion is anisotropic, the geometry distortion would be different in each direction. Eq. (19) should be changed to:

\[
\Delta \rho = \sum_i \bar{\rho}_i \tilde{L}_i
\]  
(24)

where, \(i\) represents the different directions, and \(\tilde{L}_i\) is the leakage in direction \(i\).

In most cases, only the axial distortion and radial distortion need to be considered. So, Eq. (24) can be further written as:

\[
\Delta \rho = \varepsilon_r \tilde{L}_r + \varepsilon_z \tilde{L}_z
\]  
(25)

where, the subscripts \(r\) and \(z\) stand for the radial and axial index, respectively.

2.2.2. Application of virtual density theory

Three different kinds of geometry distortion are analyzed, including the uniform axial expansion, uniform radial expansion and non-uniform geometry distortion.

2.2.2.1. Uniform axial expansion. When the uniform axial expansion occurs, the height increases \((\kappa_z = \frac{z}{z_0})\) and the density decreases \((\kappa_d = \frac{1}{d})\) in the axial direction. The radius doesn’t change \((\kappa_r = 1)\) and the density decreases \((\kappa_d = \frac{1}{d})\) in the radial direction. Using Eq. (20), we can obtain that \(\varepsilon_r = 0\) and \(\varepsilon_z = \frac{1}{d} - 1\). So, the reactivity caused by the uniform axial expansion can be expressed as:

\[
\Delta \rho_{\text{axial}} = \left( \frac{1}{f^2} - 1 \right) \tilde{L}_r
\]  
(26)

2.2.2.2. Uniform radial expansion. When the uniform radial expansion occurs, the height doesn’t change \((\kappa_z = 1)\) and the density decreases \((\kappa_d = \frac{1}{d})\) in the axial direction. The radius increases \((\kappa_r = \frac{r}{r_0})\) and the density decreases \((\kappa_d = \frac{1}{d})\) in the radial direction. Using Eq. (20), we can obtain that \(\varepsilon_r = \frac{1}{d} - 1\) and \(\varepsilon_z = \frac{1}{d} - 1\). So, the reactivity caused by the uniform radial expansion can be expressed as:

\[
\Delta \rho_{\text{radial}} = \left( \frac{1}{f^2} - 1 \right) \tilde{L}_r + \left( \frac{1}{f^2} - 1 \right) \tilde{L}_z
\]  
(27)

2.2.2.3. Non-uniform geometry distortion. Generally, the non-uniform geometry distortion includes the non-uniform axial expansion and non-uniform radial expansion. The treatments of non-uniform axial expansion and axially non-uniform radial expansion are similar to the ways described above. The most challenging case is the local geometry distortion like assembly bowing, which can be converted into the assembly displacement at certain height. In this paper, two approaches are given to evaluate such reactivity.

Fig. 1 illustrates the first approach (method I), which describes the positional relationship of three adjacent assemblies in the core. Fig. 1(a) defines the original assembly array and the triangular meshes for calculating the nuclide density. The hexagonal assembly is divided into six regular triangular meshes, and the nuclide density in each mesh is obtained by volume weighting.
Fig. 1(b) and (c) show two cases of the assembly displacement. The intersection of the triangular meshes in one assembly is fixed at the center of this assembly. So, if the assembly moves, the triangular area changes accordingly.

In Fig. 1(b), the small displacement arises and the assembly is still in its original range. In this case, we adjust the triangular area and nuclide density according to the bold line, considering only the 6 triangular meshes in one assembly. Fig. 1(c) shows the other case, in which the displacement is larger and the assembly boundary exceeds the original range. So, the neighbor assembly is impacted. More meshes should be considered as in Fig. 1(c).

This method is a general method for all kinds of geometry distortion, including the non-uniform axial expansion and non-uniform radial expansion. However, if the local geometry distortion is very complicated, a lot of irregular triangular mesh should be considered for adjusting the triangular area and nuclide density.

For easier implementation, the second method is proposed (method II) especially for the assembly displacement. Fig. 2 illustrates this approach. The physical assembly displacement in Fig. 2(a) and (b) are the same as the ones in Fig. 1(b) and (c), respectively. But in method II, the mesh for adjusting the nuclide density will not be changed. So, the adjustment of triangular area is avoided. Based on the fixed meshes, the nuclide density is changed by mixing the part of assembly which moves inside or outside the original meshes.

The limitation of method II is that the geometry change cannot be too big to exceed the scope of original core size. Because if the assembly boundary exceeds the core size, there are no meshes remain for mixing the virtual material. Therefore, if the global axial or radial expansion arises, only method I works. In this paper, the non-uniform axial expansion and axially non-uniform radial expansion cases are calculated based on method I as in Sections 3.3 and 3.4, respectively. The local assembly displacement and assembly bowing cases are calculated by using method II.

For the local distortion problems, the contribution of each material should be considered separately to consider the different variation. So, Eq. (19) can be rewritten as:

$$
\Delta \rho_{\text{nodal}} = e_f \bar{P}_f + e_c \bar{P}_c + e_s \bar{P}_s
$$

where, $e_f$, $e_c$ and $e_s$ are density change of fuel, coolant and cladding, respectively.

Considering the density change in each mesh where the assembly displacement takes place, Eq. (28) can be applied to the whole core. The reactivity in each mesh can be calculated separately and then the total reactivity is obtained by summation. The expression is written as:

$$
\Delta \rho = \sum_{\text{Nodal}} \left( e_f \bar{P}_f + e_c \bar{P}_c + e_s \bar{P}_s \right)
$$

3. Numerical tests and verification

To verify the feasibility and accuracy of transport-based virtual density method, different geometry distortion is modeled in this paper. Simplified mini-core configuration is used in the tests. The assembly design comes from a previous design of FFBR (Xiao et al., 2015), which is illustrated in Fig. 3. The original design referred the published BN-600 sodium fast reactor (IAEA, 2013). For better breeding performance, the fuel composition was changed from the original oxide fuel to the U-Pu-Zr metal fuel, and the geometric design was slightly adjusted. Detailed parameters of geometry can be found in the literatures (Xiao et al., 2015; IAEA, 2013). The material composition was given in the previous paper (Xiao et al., 2015).

Based on the same assembly design, different mini-core models are established. The models consist of two types: one is the homogeneous model and the other one is the heterogeneous model. The former one considers only the homogeneous mixture in the assemblies. It is applied in Sections 3.1–3.4 for easy description of the core expansion. The core consists of 61 assemblies without consideration of the control assemblies. In Fig. 4, the homogeneous mini-core is illustrated. In Figs. 5 and 6, the same model is based on. The
heterogeneous mini-core is applied in Section 3.5. The 1/6 core geometry is illustrated in Fig. 7.

3.1. Uniform axial expansion

The whole core uniform axial expansion of 0.5%, 1.0% and 1.5% are tested. As the references, the OpenMC and SARAX-FR codes are performed to get the reactivity through direct calculation. The core is divided into ten axial planes and the S4 calculation is applied in running the SARAX-FR code.

As in Table 1, the results of SARAX-FR by direct calculation agree well with the OpenMC calculation. Based on the flux and adjoint flux from SARAX-FR, the virtual density calculation well recovers the solution of reactivity. The maximum relative error is less than 3%.

In this calculation, the OpenMC code spends 240 CPU hours to get all the results in Table 1. The SARAX-FR code spends 0.11 CPU hour in the direct calculation and 0.055 CPU hour in the virtual density calculation. The transport sweeping is carried on 4 times in the direct calculation for Table 1. However, only twice sweeping is required in the virtual density calculation to get the forward and adjoint flux. The CPU time is saved. Furthermore, the required time for the direct calculation will increase linearly with the number of cases to evaluate. But the time cost in the virtual density calculation will be kept. The benefit in efficiency will be significant in the multi-case evaluation.

3.2. Uniform radial expansion

In the uniform radial expansion tests, the expansion is also set to be 0.5%, 1.0% and 1.5%. Table 2 shows the results. The same conclusion can be obtained and the maximum relative error is less than 2.5%.

3.3. Non-uniform axial expansion

There are two kinds of non-uniform axial expansion, including the axially non-uniform axial expansion and the radially non-uniform axial expansion as illustrated in Fig. 5.

In the axially non-uniform axial expansion, the core is divided into five axial planes. Then, each plane expands by 1.0%, 1.1%, 1.2%, 1.3% and 1.4% from the bottom to the top. In the radially non-uniform axial expansion, we assume that the assemblies in the same ring have the same expansion, and each ring expands by 1.4%, 1.3%, 1.2%, 1.1% and 1.0% from the center to the periphery. Table 3 summarizes the results. For the non-uniform expansion, the direct calculation becomes more difficult to model due to the change of meshes. It can be seen that the virtual density calculation has good agreement in modeling the axially non-uniform axial expansion. The relative error is 2.46%. However, the relative error increases to 6.53% for the radially non-uniform axial expansion. It is caused by the larger flux error in the peripheral core from the SARAX-FR calculation.

3.4. Axially non-uniform radial expansion

The non-uniform radial expansion involves two cases: one is the axially non-uniform radial expansion, in which the radial expansion is uniform at the same core height but the expansion changes with the height; the other one is the assembly displace-

Table 1
Reactivity of uniform axial expansion.

<table>
<thead>
<tr>
<th>Expansion fraction</th>
<th>OpenMC</th>
<th>SARAX-FR</th>
<th>Virtual density</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$k_{ef}$</td>
<td>$\Delta p_{pcm}$</td>
<td>$k_{ef}$</td>
</tr>
<tr>
<td>Initial</td>
<td>1.00164 ± 0.00003</td>
<td>–</td>
<td>1.00307</td>
</tr>
<tr>
<td>0.5%</td>
<td>0.99540 ± 0.00003</td>
<td>–626</td>
<td>0.996901</td>
</tr>
<tr>
<td>1.0%</td>
<td>0.98925 ± 0.00003</td>
<td>–1250</td>
<td>0.990677</td>
</tr>
<tr>
<td>1.5%</td>
<td>0.98321 ± 0.00003</td>
<td>–1871</td>
<td>0.984553</td>
</tr>
</tbody>
</table>

Table 2
Reactivity of uniform radial expansion.

<table>
<thead>
<tr>
<th>Expansion fraction</th>
<th>OpenMC</th>
<th>SARAX-FR</th>
<th>Virtual density</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$k_{ef}$</td>
<td>$\Delta p_{pcm}$</td>
<td>$k_{ef}$</td>
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<td>–1871</td>
<td>0.984553</td>
</tr>
</tbody>
</table>

Table 3
Reactivity of non-uniform axial expansion.

<table>
<thead>
<tr>
<th>OpenMC</th>
<th>$k_{ef}$</th>
<th>$\Delta p_{pcm}$</th>
<th>Virtual density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>1.00164 ± 0.00003</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Axially non-uniform</td>
<td>0.99585 ± 0.00003</td>
<td>–585</td>
<td>–566</td>
</tr>
<tr>
<td>Radially non-uniform</td>
<td>0.99611 ± 0.00003</td>
<td>–554</td>
<td>–518</td>
</tr>
</tbody>
</table>
ment in the radial direction at different height. The latter one requires special treatment to consider the relative position change of assembly in the radial direction. It will be discussed in Section 3.5. In this section, only the results of axially non-uniform radial expansion are involved. The geometry distortion is illustrated in Fig. 6.

To calculate the reactivity of axially non-uniform radial expansion, the core is divided into five axial planes. Each plane expands by 1.4%, 1.3%, 1.2%, 1.1% and 1.0% from the top to the bottom. Table 4 shows the results of reactivity change. The relative error is 1.93% compared with the OpenMC direct calculation.

3.5. Assembly bowing

Assembly bowing is a typical non-uniform radial geometry distortion. It can be represented by defining the continuous local assembly displacement along the core height. Here, we consider a more realistic case, in which the heterogeneous mini-core is considered. The calculation consists of two steps: first, the SARAX-FXS module is run to generate the homogenized cross sections; then, the SARAX-FR module is run to perform the reactivity calculations based on the homogenized triangular meshes.
This method is based on the first order perturbation theory and use the virtual material density instead of explicitly changing the geometry in describing the assembly distortion. To well treat the anisotropy of fast neutron, the neutron transport theory is adopted. New formulism is proposed based on the $S_n$ nodal method. Arbitrary geometry distortion can be evaluated. Two different approaches are used to model the global and local geometry distortion, respectively. The flexible meshes are used for the uniform axial and radial expansion, non-uniform axial expansion and axially non-uniform radial expansion. The fixed meshes are applied for the local assembly displacement and assembly bowing.

A series of numerical tests are done to verify the virtual density calculations. The results show that the virtual density method has good accuracy in modeling the geometry distortion. Compared with the fine geometry modeling using the Monte-Carlo codes, the maximum relative error is less than 3% in modeling the uniform expansion, less than 7% in modeling most of the non-uniform expansion and less than 10% in modeling the assembly bowing.

Compared with the fine modeling by using the Monte-Carlo code, the new approach preserves the high efficiency of deterministic fast reactor codes and considers more rigorously than using the neutron diffusion approximation. Compared with the direct calculation, the virtual density calculation is more efficient for the multi-case evaluation since only twice transport sweeping is required no matter how many cases to calculate. Besides, compared with other methods for the geometry distortion evaluation, this method is more flexible for all kinds of distortion, especially for modeling the heterogeneous assembly bowing.

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