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Application of MCNP Perturbation Technique and Difference Method in AP1000

CHU Dongliang[1], HE Qing[2], HU Wenchao[3]

[1, 2] Key Laboratory of Condition Monitoring and Control for Power Plant Equipment, Ministry of Education, School of Energy Power and Mechanical Engineering, North China Electric Power University, Beijing 102206, P.R. China

[3]Nuclear and Radiation safety Center of MEP Beijing 100082, P.R. China

Abstract: ***The Monte Carlo N-Particle (MCNP) code is the internationally recognized code for calculating the k_{eff} for AP1000 system with specific nuclear material compositions, geometric structures and core size by the Monte Carlo method. For a PWR system, we calculated Δk_{eff} which arise from system nuclear material compositions, geometric structures and core size changes, by two different approaches, the MCNP perturbation technique and the MCNP difference method. When we simulate the core of AP1000 through the MCNP code, we find that as material compositions, geometric structures and core size changes in AP1000 system are small compared to the whole system, the Δk_{eff} results obtained from the MCNP perturbation technique are much more efficient and reliable than the results from the MCNP difference method. When material compositions, geometric structures and core size changes in AP1000 system are significant compared to the whole system, both the MCNP perturbation technique and the MCNP difference method can give satisfactory results.***

Keywords: MCNP; Perturbation Technique; Difference Method; AP1000; Coolant Density

1. Introduction

The Monte Carlo N-Particle (MCNP) code deals with transport of neutrons, gamma rays, and coupled transport, i.e., transport of secondary gamma rays resulting from neutron interactions in any complex geometric structure and nuclear material compositions [1]. MCNP code also has criticality calculation and the perturbation technique feature for critical systems, for example AP1000. MCNP code does not solve an explicit transport equation, but rather obtains answers by simulating individual particles and recording tallies of individual particle average behavior. The average behavior of particles in the physical system is then inferred from the average behavior of the simulated particles.

MCNP simulates the particle transport processes, tracks numerous particles, and calculates the k_{eff} for AP1000 with specific geometric structure and nuclear material compositions. MCNP is particularly useful for complex problems that cannot be modeled by computer algorithms that use deterministic methods. When the geometric structures, density or nuclear material compositions of AP1000 change, the k_{eff} of AP1000 also changes. To obtain the variation of k_{eff} of PWR corresponding to the reactor structure composition change of AP1000, one must calculate the k_{eff} before and after the nuclear structure compositions change separately, the difference of the two k_{eff} is the variation of k_{eff} of AP1000 before and after nuclear structure compositions change. This is the MCNP difference method [2].

When material composition change in AP1000 is significant compared to the reactor compositions in the whole AP1000, it is obvious that the MCNP difference method can give us satisfactory results. But when reactor structure change in any particular cell of AP1000 is small compared to the reactor structure compositions in the whole AP1000, the variation of k_{eff} obtained from this approach may not be reliable or is invalid. This comes from the fact that MCNP particle simulation technique is based on the Monte Carlo method, so the calculated variation of k_{eff} of AP1000 by the MCNP difference method may be less than the variance of k_{eff} itself. To solve this problem, MCNP introduced the perturbation technique to evaluate the response of the engineer values of AP1000 to the changes of AP1000 compositions. This is MCNP perturbation technique.

In the actual MCNP perturbation calculations, MCNP code does not really "perturb" the particle transport processes, it expresses its first- and second-order perturbation terms as the functions of macroscopic cross-sections and the track lengths of the particles in the unperturbed situation, and material macroscopic cross-section is related to material density linearly[3]. So in the perturbation calculations, MCNP code only needs to record the track lengths of the particles in the unperturbed transport processes, then by the relevant macroscopic cross-sections and recorded track lengths of the particles MCNP code generates the required perturbation results. This unique design of MCNP code make it easy and flexible enough for the user to use, it allows perturbations in cell material density, composition, or reaction cross-section data, and the perturbation calculations can be executed without actually changing cell material compositions of AP1000. Multiple perturbations can be applied in each run, and there is no limit to the number of perturbations in each run [4].

MCNP code calculates the perturbation up to the second-order perturbation. MCNP can generate first- and second-order perturbation terms separately enabling the user to determine the significance of including the second-order estimator for subsequent runs [1]. If the second-order results are more than 20-30% of the total, then higher order perturbation terms are necessary to accurately predict the change in the unperturbed tally. In such cases, the magnitude of the perturbation should be reduced to satisfy this condition. In the following of this

paper, we make calculation for density change of coolant in AP1000 by MCNP perturbation technique and MCNP difference method; then we compare the calculation results from the two different approaches, and discuss the limitations of two different approaches when they are applied in the calculations of PWR.

2. Structure of AP1000

The core of AP1000 has 157 assemblies, including fuel assemblies, control rod assemblies and burnable poison components, etc. The numbers of different fuel assembly in the core are shown in Table 1 and the distribution of each fuel assembly is shown in Figure 1.

Table 1: The type and quantity of fuel assembly

Name	Identifier	Type	Amount
Power control rod	G	Ash rod assembly	12
	N	Black rod assembly	16
Temperature control	R	Black rod assembly	8
Scram Rod	S	Black rod assembly	29
Burnable poison rod	B	B4C	34

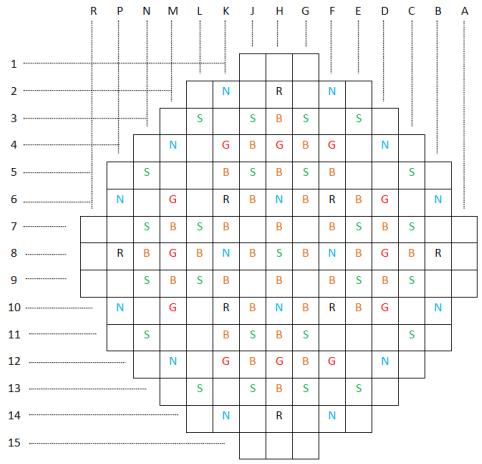

Figure 1: The distribution of control component rods and burnable poison assembly

We adjust the enrichment of fuel and the distribution of burnable poison rods to make the core critical and the average neutron density is 2.66×10^{14} n/cm^2. Core critical parameters are shown in Table 2.

Table 2: The main technical parameters of AP1000

Parameter	Design value
Core thermal power (MW)	3000
Height (cm)	366
Fuel assembly number	157
235U enrichment（%）	3.65%
Boron concentration (μg /g)	600
Cladding outside diameter (mm)	9.5
Cladding thickness (mm)	0.57
Space between of rods (mm)	12
UO2 density (g/cm3)	10.4
Coolant density (g/cm3）	0.73

We use the MCNP4C code to simulate AP1000, and then we calculated the k_{eff} of the reactor system seven times by MCNP4C code, each simulation calculation with different cycles or different neutron number. The seven k_{eff} we obtained by seven different MCNP runs are listed in Table 3.

Table 3 The k_{eff} from seven different runs

Neutron and cycle	k_{eff}	Variance
3000 n/cycles Total 500 cycles	1.00139	0.00063
5000 n/cycles Total 500 cycles	1.00117	0.00050
7000n/cycles Total 500 cycles	1.00098	0.00042
10000 n/cycles Total 500 cycles	1.00061	0.00036
20000 n/cycles Total 500 cycles	1.00074	0.00026
20000 n/cycles Total 700 cycles	1.00080	0.00022
20000 n/cycles Total 1000cycles	1.00083	0.00017

This article mainly studies the effects of the density changes to k_{eff}, so we change the density of coolant in AP1000. We made seven different MCNP runs for every change to test the reliability and the efficiency of the MCNP perturbation and MCNP difference method when applied in the k_{eff} calculation of AP1000. The following of this paper are the detailed calculations and the disadvantages and advantages of the MCNP perturbation technique and MCNP difference method.

3. Small Change of Coolant Density in AP1000

The temperature of coolant in AP1000 changes with the power variation, then the density of coolant will fluctuate. The density of borated coolant in this article is 0.73 g/cm^3, with the effect of power, the density of borated coolant is 0.74 g/cm^3.The density changes are small compared to the reactor core of the whole AP1000. In another words, this density change can be treated as small perturbation. Although the change of density is not large, the change will definitely affect k_{eff} of AP1000 in some degree. We use two different approaches to calculate the variation of k_{eff} of AP1000 before and after the density of coolant was changed. The first method is to calculate the k_{eff} of AP1000 before and after the coolant density were changed separately, the difference of the two k_{eff} is the variation of AP1000, the method also called the MCNP difference method. The second method is to calculate the variation of k_{eff} of AP1000 by MCNP perturbation technique directly, and then we compare the calculated Δk_{eff} results from two different approaches and discuss their advantages and disadvantages in calculation the variation of k_{eff}. The cycles and the neutron number used in seven different runs are the same as used in Table 3. The Δk_{eff} calculation results from MCNP different methods are listed in Table 4, and the Δk_{eff} calculation results from MCNP perturbation technique are listed in Table 5.

Table 4 Δk_{eff} calculation results from MCNP4C difference method

Neutron and cycle	0.73 (g/cm^3)	0.74 (g/cm^3)	Δk_{eff}
3000 n/cycles Total 500 cycles	1.00139	0.99909	-0.0023
5000 n/cycles Total 500 cycles	1.00117	1.00093	-0.0023
7000 n/cycles Total 500 cycles	1.00098	1.00093	-0.0023
10000 n/cycles Total 500 cycles	1.00061	0.99970	-0.00091
20000 n/cycles Total 500 cycles	1.00074	0.99888	-0.00186
20000 n/cycles Total 700 cycles	1.00080	0.99927	-0.00153
20000 n/cycles Total 1000cycles	1.00083	0.99925	-0.00158

Table 5 $\triangle$ k_{eff} calculation results from MCNP4C perturbation technique

Neutron and cycle	k_{eff}	Δk_{eff} 1st and 2nd perturbation	Δk_{eff} 2nd perturbation
3000 n/cycles Total 500 cycles	1.00139	-0.00140	-0.00001
5000 n/cycles Total 500 cycles	1.00117	-0.00149	-0.00001
7000 n/cycles Total 500 cycles	1.00098	-0.00149	-0.00001
10000 n/cycles Total 500 cycles	1.00061	-0.00145	-0.00001
20000 n/cycles Total 500 cycles	1.00074	-0.00154	-0.00001
20000 n/cycles Total 700 cycles	1.00080	-0.00153	-0.00001
20000 n/cycles Total 1000cycles	1.00083	-0.00151	-0.00001

The Δk_{eff} calculation results listed in Table 4 and 5 are from seven different runs, each run with different neutrons or different cycles. In Table 5, we also listed the results only including the second-order perturbation results. MCNP that has the ability to produce first-and second-order perturbation results separately enables the user to determine the significance of including the second-order estimator for subsequent runs. If the second-order results are a significant fraction (20~30%) of the total, then higher order terms are necessary to accurately predict the change in the unperturbed tally. In such case, the magnitude of the perturbation should be reduced to satisfy these conditions. Obviously, the second-order perturbation results presented in Table 5 are much less than 20% of the total, so the perturbation results in Table 5, which come from seven different runs each run with different neutrons of different cycles, are reliable.

The structure and the material compositions of the PWR which we used in Table 5, table 4 and table 3 are exactly the same. The slightly differences of k_{eff} in Table 5 and 4 come from the fact that we change the density of coolant for the MCNP perturbation calculations, the change of density does slightly affect the transport of the neutron. As the density change of coolant in AP1000 is small, it will only disturb the AP1000 slightly, that is to say, this situation is more suitable for the MCNP perturbation calculation. From the calculated Δk_{eff} results in Table 5, we can see that the seven Δk_{eff} results, which came from seven different runs with different cycles or neutrons by MCNP perturbation technique, are very stable. The Δk_{eff} result obtained from the 500 cycles each cycle with 3000 neutrons by MCNP perturbation technique is already good enough.

Based on the calculated Δk_{eff} results in Table 4, Table 5 and the analysis, we can conclude that when the density change is small compared to the density in AP1000 system, or the density change can be treated as small perturbation, the Δk_{eff} results obtained from the MCNP perturbation technique are much more efficient and reliable than the results from the MCNP difference method.

4. Significant Change of Coolant Density in AP1000

To further compare MCNP perturbation technique with MCNP difference method, we change the density of coolant from 0.73 g/cm^3 to 0.85 g/cm^3 in AP1000. The density change is large compared to the density of coolant in the AP1000 system. This density change will definitely affect k_{eff} of AP1000 system significantly. We also calculated the variation of k_{eff} of AP1000 before and after the density of coolant was changed by two different MCNP approaches. The first method is to calculate the k_{eff} of PWR before and after the density was changed separately, the difference of the two k_{eff} is the variation of k_{eff} of AP1000. The second method is that we use the MCNP perturbation technique to calculate the variation of k_{eff} of AP1000 after the density of coolant was changed directly. Then we compare the results from two different approaches and discuss their advantages and disadvantages in calculation of the variation of k_{eff} of PWR when the density change is significant. The cycles and the neutron number used in seven different runs are the same as those used in Table 4 and 5. The Δk_{eff} calculation results from MCNP difference method are listed in Table 6, and the Δk_{eff} calculation results from MCNP perturbation technique are listed in Table 7.

The geometry and material composition of AP1000 which we used in Table 6 and Table 7 are exactly the same. As the density change is large compared to the whole AP1000, the calculation results listed in Table 6 and 7 are from seven different runs, each run with different cycles and neutron number. In Table 7, we also listed only the second-order perturbation results separately. Obviously, the second-order perturbation results presented in Table 7 are much less than 10% of the total, so the perturbation results in Table 7 are also reliable [5].

Table 6. Δk_{eff} calculation results from MCNP4C difference method

Neutron and cycle	0.73 (g/cm^3)	0.85 (g/cm^3)	Δk_{eff}
3000 n/cycles Total 500 cycles	1.00139	0.98285	-0.01854
5000 n/cycles Total 500 cycles	1.00117	0.98276	-0.01854

7000 n/cycles Total 500 cycles	1.00098	0.98353	-0.01854
10000 n/cycles Total 500 cycles	1.00061	0.98326	-0.01735
20000 n/cycles Total 500 cycles	1.00074	0.98236	-0.01838
20000 n/cycles Total 700 cycles	1.00080	0.98247	-0.01833
20000 n/cycles Total 1000cycles	1.00083	0.98293	-0.0179

Table 7. Δk_{eff} calculation results from MCNP4C perturbation technique

Neutron and cycle	k_{eff}	Δk_{eff} 1st and 2nd perturbation	Δk_{eff} 2nd perturbation
3000 n/cycles Total 500 cycles	1.00139	-0.01822	-0.00161
5000 n/cycles Total 500 cycles	1.00117	-0.01822	-0.00161
7000 n/cycles Total 500 cycles	1.00098	-0.01895	-0.00124
10000 n/cycles Total 500 cycles	1.00061	-0.01859	-0.00127
20000 n/cycles Total 500 cycles	1.00074	-0.01940	-0.00105
20000 n/cycles Total 700 cycles	1.00080	-0.01940	-0.00101
20000 n/cycles Total 1000cycles	1.00083	-0.01914	-0.00110

From the results listed in Table 6 and 7, we can see that the seven calculated Δk_{eff} results, which come from seven different runs and different cycles or neutrons by perturbation technique and MCNP difference method, are all stable, the calculated Δk_{eff} results from seven different runs are very close to each other by every approach. Although there is a striking difference between the Δk_{eff} results obtained from two different MCNP approaches, this difference cannot decide which method is better when the density changes of coolant are large. We will study deeply on this difference in future. On the other hand, we find that the time to finish MCNP perturbation calculation in typical PC is much less than the time to finish MCNP difference method calculation.

Obviously, the second-order perturbation results presented in Table 7 are far less than fraction (20%-30%) of the total perturbation, so the perturbation results in Table7 are also reliable[6].

5. Conclusion

The MCNP code is powerful tool in neutron and other particle transport simulation calculation, when the composition of system are complicated and the deterministic method is unable to give satisfactory results, MCNP code is particularly useful to simulate the particle behavior and give the reliable results effectively.

We calculated the Δk_{eff} of the AP1000 as the density change by MCNP perturbation technique and MCNP difference method separately. When the density change is small compared to the density in AP1000, and the change of density can be treated as small perturbation, the Δk_{eff} results obtained from the MCNP perturbation technique are much more efficient and reliable than the results from the MCNP difference method.

As the density changes in AP1000 are large compared to the density of coolant in AP1000, and the change cannot be treated as small perturbation, both MCNP perturbation technique and the MCNP difference method give satisfactory and reliable results. Although there is a difference between the absolute value of Δk_{eff} obtained from two different MCNP methods, this is not can significantly affect the AP1000 system.

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