A k_{eff} Calculation Method by Monte Carlo

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Abstract

The effective multiplication factor (k_{eff}) is defined as the ratio between the number of neutrons in successive generations, which definition is adopted by most Monte Carlo codes (e.g. MCNP). Also, it can be thought of as the ratio of the generation rate of neutrons by the sum of the leakage rate and the absorption rate, which should exclude the effect of the neutron reaction such as (n, 2n)and (n, 3n). This article discusses the Monte Carlo method for k_{eff} calculation based on the second definition. A new code has been developed and the results are presented.

1. Introduction

Nuclear criticality safety is always a significant subject for the nuclear industry. And, with the closure of many experimental facilities and the development of numerical calculation, the nuclear criticality safety analysts increasingly depend on computer calculation to identify safe limits for the handling of fissile materials and design the nuclear reactor system. The Monte Carlo method[1], as a branch of numerical methods, has many merits including continuous-energy neutron interaction data instead of multi-group data, flexibility of complex geometry configuration and so on. And there are some Monte Carlo codes (e.g. MCNP[2]) having the ability of criticality calculation. The method adopted by these codes is based on the definition that k_{eff} is the ratio between the number of neutrons in successive generations. However, there is another definition of k_{eff}. This article introduces this definition into Monte Carlo method, and the relative algorithm are made and the code developed. And the calculation results are next presented. Finally, the conclusions are given.

2. Theory

The effective multiplication factor (k_{eff}) is defined as the ratio between the number of neutrons in successive generations. But, there is another definition, which can be derived from Boltzmann transport equation (without external sources):

$$\begin{aligned}
&\nabla\bullet\vec{\Omega}\varphi(\vec{r},E,\vec{\Omega})+\Sigma_t(\vec{r},E)\varphi(\vec{r},E,\vec{\Omega})\\
&=\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_s(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')\,f_1(\vec{r},E',\vec{\Omega}'\to E,\vec{\Omega})\\
&+\frac{1}{k_{eff}}\frac{\chi(\vec{r},E)}{4\pi}\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\nu(\vec{r},E')\Sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')\\
&+2\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_{(n,2n)}(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')\,f_2(\vec{r},E',\vec{\Omega}'\to E,\vec{\Omega})\\
&+3\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_{(n,3n)}(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')\,f_3(\vec{r},E',\vec{\Omega}'\to E,\vec{\Omega})+\cdots
\end{aligned}\qquad(1)$$

where, the functions f_1, f_2 and f_3 are the emitted neutron distribution function, so they satisfy the following equations:

$$\int_0^\infty dE\int_{4\pi}d\vec{\Omega}f_n(\vec{r},E',\vec{\Omega}'\to E,\vec{\Omega})=1\ \text{ where, }\ n=1,\ 2,\ 3\cdots\qquad(2)$$

And all the other symbols are conventional in the nuclear reactor physics. Integrate both sides of the formula (1) over the entire phase space,

$$\begin{aligned}
&\int_V dV\int_0^\infty dE\int_{4\pi}d\vec{\Omega}\nabla\bullet\vec{\Omega}\varphi(\vec{r},E,\vec{\Omega})+\int_V dV\int_0^\infty dE\int_{4\pi}d\vec{\Omega}\Sigma_t\varphi(\vec{r},E,\vec{\Omega})\\
&=\int_V dV\int_0^\infty dE\int_{4\pi}d\vec{\Omega}\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_s\varphi(\vec{r},E',\vec{\Omega}')\,f_1(\vec{r},E',\vec{\Omega}'\to E,\vec{\Omega})\\
&+\frac{1}{k_{eff}}\int_V dV\int_0^\infty dE\int_{4\pi}d\vec{\Omega}\frac{\chi(\vec{r},E)}{4\pi}\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\nu\Sigma_f(\vec{r},E')\varphi(\vec{r},E',\vec{\Omega}')\\
&+2\int_V dV\int_0^\infty dE\int_{4\pi}d\vec{\Omega}\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_{(n,2n)}\varphi(\vec{r},E',\vec{\Omega}')\,f_2(\vec{r},E',\vec{\Omega}'\to E,\vec{\Omega})\\
&+3\int_V dV\int_0^\infty dE\int_{4\pi}d\vec{\Omega}\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_{(n,3n)}\varphi(\vec{r},E',\vec{\Omega}')\,f_3(\vec{r},E',\vec{\Omega}'\to E,\vec{\Omega})\\
&+\cdots
\end{aligned}\qquad(3)$$

Considering the equations (2), the above expression can be simplied,

$$\begin{aligned}
&\int_V dV\int_0^\infty dE\int_{4\pi}d\vec{\Omega}\nabla\bullet\vec{\Omega}\varphi(\vec{r},E,\vec{\Omega})+\int_V dV\int_0^\infty dE\int_{4\pi}d\vec{\Omega}\Sigma_t\varphi(\vec{r},E,\vec{\Omega})\\
&=\int_V dV\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_s\varphi(\vec{r},E',\vec{\Omega}')\\
&+\frac{1}{k_{eff}}\int_V dV\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\nu\Sigma_f\varphi(\vec{r},E',\vec{\Omega}')\\
&+2\int_V dV\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_{(n,2n)}\varphi(\vec{r},E',\vec{\Omega}')\\
&+3\int_V dV\int_0^\infty dE'\int_{4\pi}d\vec{\Omega}'\Sigma_{(n,3n)}\varphi(\vec{r},E',\vec{\Omega}')\\
&+\cdots
\end{aligned}\qquad(4)$$

To utilize the relationship among various macroscopic cross section, formula (4) can be simplied further,

$$\begin{aligned}&\int_V dV\int_0^\infty dE\int_{4\pi} d\vec{\Omega}\nabla\bullet\vec{\Omega}\varphi(\vec{r},E,\vec{\Omega})\\&+\int_V dV\int_0^\infty dE\int_{4\pi} d\vec{\Omega}(\Sigma_c+\Sigma_f-\Sigma_{(n,2n)}-2\Sigma_{(n,3n)}-\cdots)\varphi(\vec{r},E,\vec{\Omega})\\&=\frac{1}{k_{eff}}\int_V dV\int_0^\infty dE\int_{4\pi} d\vec{\Omega}\nu\Sigma_f\varphi(\vec{r},E,\vec{\Omega})\end{aligned} \tag{5}$$

Finally, the expression of k_{eff} is obtained,

$$k_{eff}=\frac{\int_V dV\int_0^\infty dE\int_{4\pi} d\vec{\Omega}\nu\Sigma_f\varphi}{\int_V dV\int_0^\infty dE\int_{4\pi} d\vec{\Omega}\nabla\bullet\vec{\Omega}\varphi+\int_V dV\int_0^\infty dE\int_{4\pi} d\vec{\Omega}\Sigma_a{}'\varphi} \tag{6}$$

where, $\Sigma_a{}'=\Sigma_a-\Sigma_{(n,2n)}-2\Sigma_{(n,3n)}-\cdots$

So, if generation rate for fission neutrons, leakage rate and reaction rate of absorption (including capture and fission), (n,2n), (n,3n)⋯, could be obtained, k_{eff} will be calculated by the formula (6). Similarly with the approach adopted by MCNP, the conception of cycles is educed. But a cycle does not denote a generation any more, which is the life of a neutron from birth in fission to death by escape, parasitic capture or absorption for fission, a cycle denotes a certain time interval instead. Also, the first several cycles are ignored because the sources have not achieved equilibrium. After these cycles, the others are active cycles and the parameter *N* indicates the number of active cycles. In each active cycle *n*, the required physical quantities for calculating the k_{eff}^n by the formula (6) are estimated and then k_{eff}^n is obtained. For a certain reaction *x*, the estimator of the reaction rate R_x is,

$$R_x=\sum_{s=1}^{S}\sum_i Wd\Sigma_x, \tag{7}$$

The estimator of fission neutrons generation rate *F* is,

$$F=\sum_{s=1}^{S}\sum_i Wd\nu\Sigma_f \tag{8}$$

The estimator of leakage rate *L* is,

$$L=\sum_{s=1}^{S}\sum_j W \tag{9}$$

where,
S = number of source particle in the current cycle;
s = all source particle in the current cycle;
W = particle weight;
d = trajectory track length;
i = all track length segments for the source particle *n*;
j = all leakage neutrons for the source particle *n*.

The average k_{eff} estimator over N active cycles is defined,

$$\bar{k}_{eff} = \frac{1}{N}\sum_{n=1}^{N} k_{eff}^{n} \tag{10}$$

and the relative standard deviation is,

$$\sigma_{\bar{k}_{eff}} = \left(\frac{1}{N-1}\right)^{1/2}\left[\frac{1}{N}\sum_{n=1}^{N}\left(k_{eff}^{n}\right)^{2} - \left(\bar{k}_{eff}\right)^{2}\right]^{1/2} \tag{11}$$

3. Numerical results

To verify the accuracy of the code, several criticality benchmarks [3] are calculated and the results are compared with the reference. They are made up of five categories: critical assemblies utilizing ^{233}U, ^{235}U and ^{239}Pu. Table 1 contains a brief description of each of the criticality benchmarks, including its identifier (ID). The detailed information on the configuration and material specifications can be found from the references 3 and 4.

ID	Benchmark Description
U31	^{233}U Bare Metal Shpere
U32	1.0274 g/L Unreflested 69.19 cm Sphere of ^{233}U Nitrate Solution with Boron
U33	1.0153 g/L Unreflested 61.786 cm Sphere of ^{233}U Nitrate Solution with Boron
U51	ORNL-1 Uranyl nitrate in H_2O Sphere
U52	ORNL-2 Uranyl nitrate in H_2O Sphere
U53	ORNL-10 and CSEWG: T-5
Pu1	PU-SOL-THERM-011 Case 16-1,Bare Sphere
Pu2	PNL-5, Unreflected 20.25cm Sphere of Pu(43.43g/l) Nitrate Solution
Pu3	

Table 1 Criticality Benchmark Descriptions[3].

Tables 2 presents the benchmark k_{eff} values， the calculated results and the k_{eff} values[5] by the code MCNP5. It should be illuminated that the required neutron interaction data come from ENDF/B-VI. So, the values from the reference 5 are associated with the ENDF/B-VI.

ID	Benchmark k_{eff}	Calculated k_{eff}	MCNP[5]
U31	1.0000±0.0010	0.9962±0.0005	0.9926±0.0003
U32	1.0006±0.0033	0.9973±0.0008	0.9964±0.0005
U33	1.0006±0.0029	0.9961±0.0017	0.9974±0.0002
U51	1.0012±0.0026	0.9997±0.0014	Absent
U52	1.0007±0.0036	0.9964±0.0006	Absent
U53	1.0015±0.0026	1.0016±0.0010	0.9992±0.0002
Pu1	1.0000±0.0052	0.9970±0.0010	Absent
Pu2	1.0000±0.0052	0.9967±0.0009	Absent
Pu3	1.0000±0.0052	0.9955±0.0011	Absent

Table 2 Calculation Results for Benchmark.

Although the results are not completely consistent with the benchmarks, they are acceptable if the results by MCNP are accepted. And the difference between the benchmarks and the calculated results from two codes may be caused by the neutron interaction cross section, which should be discussed further.

4. Conclusion

From the numerical results, the new approach for calculating k_{eff} by Monte Carlo is effective. However, it is necessary to determine whether the results deviated slightly from the benchmarks are relative with the neutron cross section and whether there are other reasons.

5. ACKNOWLEDGMENTS

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6. References

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