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A deterministic and Monte Carlo coupling method for PWR cavity radiation streaming calculation

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ABSTRACT

PWR cavity radiation streaming calculation is important for the evaluation of the radioactive dose rate in structural materials. Discrete Ordinates (S_N) method has been widely used to solve shielding problems, but it is difficult to apply to a complex geometry. Monte Carlo (MC) method can treat the geometry exactly but requires very long computing time to obtain acceptable statistic deviations. Thus, an S_N–MC coupling method is adopted in order to combine the advantages of both S_N method and MC method in PWR cavity radiation streaming calculations. To develop this coupling method, two surface source models, the combined surface source model (CSSM) and the single surface source model (SSSM), are proposed and analyzed. From the numerical results two conclusions can be drawn. (1) The S_N–MC coupling method offers a speedup factor of 2–20 compared with the MC method to obtain the same statistic deviations. (2) In the S_N–MC coupling method, the CSSM is more efficient than the SSSM in reducing statistic deviations.

1. Introduction

Pressurized Water Reactor (PWR) cavity usually refers to the space between the reactor pressure vessel and concrete biological shield. Correspondingly, PWR cavity radiation streaming is the neutron and photon streaming upwards inside the reactor cavity. The reactor cavity radiation streaming calculation plays a very important role in the evaluation of the radioactive dose rate in structural materials (Regulatory Guide 1.190, 2001). In the field of nuclear engineering, Discrete Ordinates (S_N) and Monte Carlo (MC) methods are usually used to solve these shielding problems (Xie and Deng, 2005). As a deterministic method, the S_N method tends to be faster but cannot exactly handle the complex spatial geometry around the core. In contrast, the MC method can treat the geometry exactly but is extremely computationally expensive to obtain acceptable statistic deviations due to the dramatically attenuation of neutron flux (by 10 or even more orders of magnitude) in deep-penetration regions. Hence, neither the S_N nor the MC method can provide a good result with itself.

To solve the above problems, the idea of coupling of the S_N method and MC method has been proposed and implemented. DOMINO (Emmett et al., 1973) is a link code for coupling DOT (a two-dimensional S_N code) and MORSE (a Monte Carlo code) for radiation transport calculations. It transforms the angular flux as a function of energy group, spatial mesh interval and discrete angles into current, and subsequently into normalized probability distribution functions (PDFs). The objective of the coupling method is to take advantage of both S_N method and MC method in a complementary manner. During the past decades, this coupling method has been used for shielding calculations of ITER (Eggleston et al., 1998), AP1000 (Joel, 2009) and other nuclear facilities (Hu et al., 2003; Hagler and Fero, 2005; Chen and Fero, 2010). Furthermore, various investigations to extend this method to full three-dimensional model have been carried out in the past few years. Kurosawa (2005) developed a TORT (RSICC Computer Code Package CCC-650, 1998) and MCNP coupling method, but only for *xyz* geometries. Joel (2011) produced a link code capable of coupling the MC method and the S_N method with *rz*, $r\theta$, *xy*, *xyz*, and $r\theta z$ geometries. Han (2012a,b) also implemented the 3D S_N–MC coupling method in both Cartesian and cylindrical coordinates. However, these studies only enable the coupling calculation with the single surface source model (SSSM). In the SSSM, S_N code provides angular flux of one surface, a link code transforms the angular flux into PDFs, and MC code samples the source variables based on these PDFs. The SSSM decreases the MC calculation region in a particular direction, but cannot decrease the MC calculation region in other directions at the same time.

In this work, the application of the S_N–MC coupling method for PWR cavity radiation streaming calculation is investigated. Two models for the coupling of the S_N method and MC method are studied. One model, SSSM, uses single surface source as in the above literatures, while the other model, CSSM, uses combined surface source. Compared with the SSSM, the CSSM uses several

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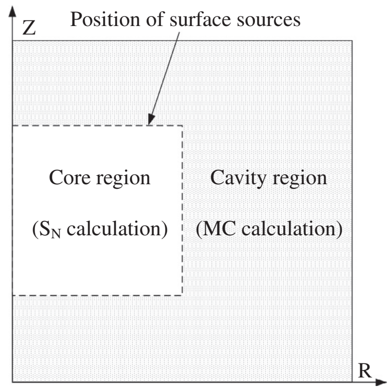


Fig. 1. Schematic model of the S_N–MC coupling method.

surface sources together to decrease the MC calculation region and is more efficient in reducing statistic deviations. Compared with the conventional MC method, both the SSSM and CSSM reduce the statistic deviations, leading to more accurate solutions at a lower computational cost.

The reminder of the paper is organized as follows. Section 2 and Section 3 exhibit the outline and methodology of the S_N–MC coupling method, respectively. Section 4 is dedicated to two test problems to verify the correctness of the S_N–MC coupling method. Section 5 presents the application of the coupling method for PWR reactor cavity radiation streaming calculation. Finally we draw some conclusions and make a few suggestions in Section 6.

2. Outline of the S_N–MC coupling method

Figs. 1 and 2 show the schematic model and the flow chart of the S_N–MC coupling method, respectively. As shown in Fig. 1, the core region with relatively simple geometry is calculated using the S_N method, and the complex cavity region is calculated using the MC method. In Fig. 2, a link code DO2MC is used to integrate the 2D S_N code DORT (RSICC Computer Code Package CCC-650, 1998) and the Monte Carlo transport code MCNP (Briesmeister, 2000) for coupling calculations. Essentially, DO2MC is a data processor for the angular flux produced by the S_N calculation and a source generator for the MC calculation.

The S_N–MC coupling method includes the following steps:

(1) Divide the problem into two parts and specify the positions of surface sources.

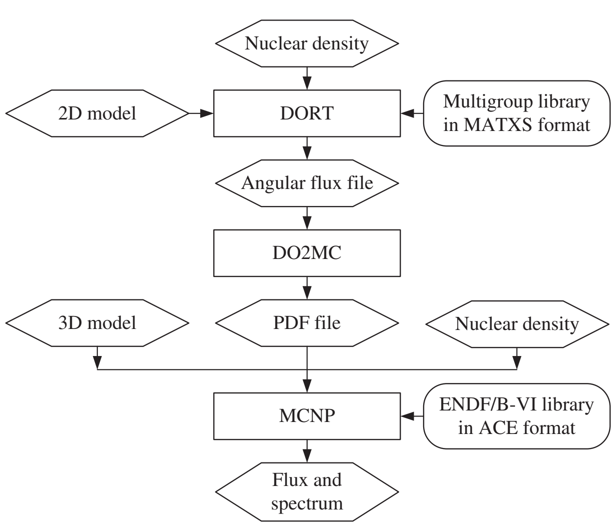


Fig. 2. Flow chart of the S_N–MC coupling method.

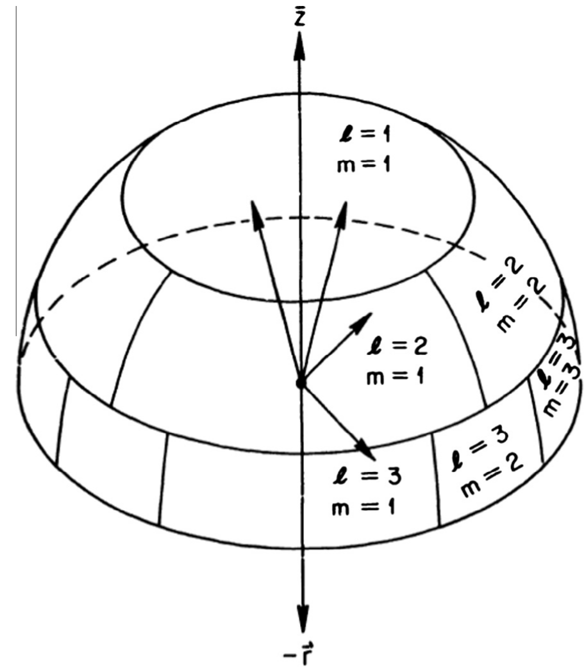


Fig. 3. Schematic representation of the upper hemisphere formed by the quadrature set (Emmett et al., 1973).

(2) Perform S_N calculation to obtain angular flux of surface sources.
(3) Transform angular flux into PDFs.
(4) Perform MC calculation to obtain flux and spectrum at detectors.

3. Methodology

In order to perform the S_N–MC coupling calculation, three key problems have to be solved: the PDFs of the surface sources, the segments of the angular distributions and the source variable sampling method.

3.1. Probability distribution functions (PDFs) of the surface sources

In the S_N–MC coupling method, the angular flux as a function of energy, spatial mesh interval and discrete angle is transformed into current and subsequently into normalized PDFs.

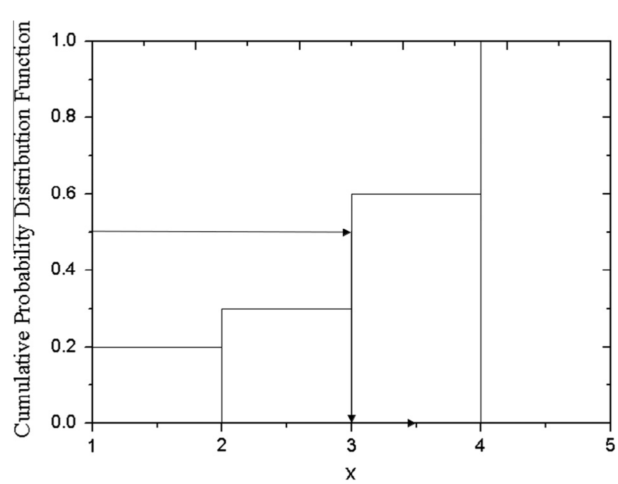


Fig. 4. Example of sampling a random variable from a cumulative PDF.

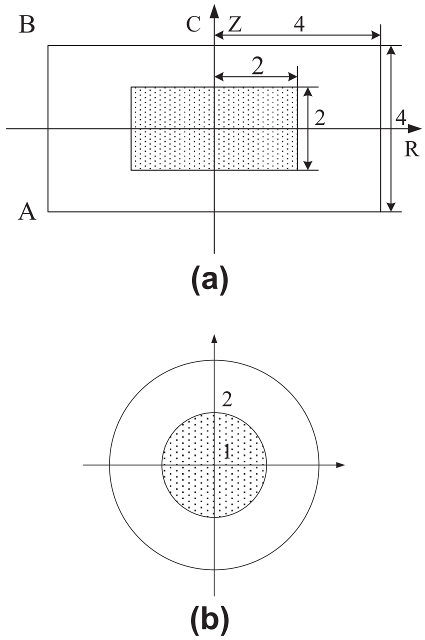


Fig. 5. Geometry of the two-region problem (a) axial cross section (b) radial cross section.

Table 1
Cross-sections of the two-region problem.

Region	Σ_t (cm^{-1})	Σ_a (cm^{-1})	Σ_s (cm^{-1})
1	1.0	0.5	0.5
2	0.8	0.4	0.4

The energy-, space- and angular-dependent flux is represented by $\varphi_{l,m,i,j,g,s}$, where s denotes surface, g denotes the energy group number, (i, j) denote the spatial mesh indices, l and m denote angular segments. The current through surface s of energy group g at spatial mesh interval (i, j) in direction (l, m) is:

$$E_{l,m,i,j,g,s} = \varphi_{l,m,i,j,g,s}|\varepsilon_{l,m}| \quad (1)$$

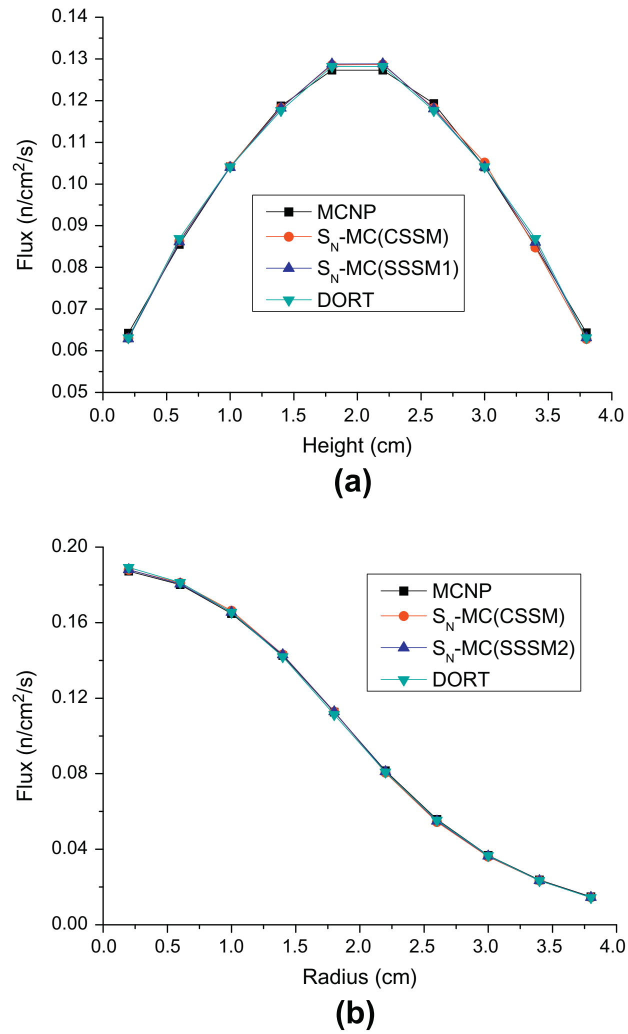


Fig. 7. Axial flux distribution along AB (a) and radial flux distribution along BC (b).

where $\varepsilon_{l,m}$ means one of $\mu_{l,m}$ or $\eta_{l,m}$, which is the direction cosine of the S_N quadrature set. Thus the current through surface s of energy

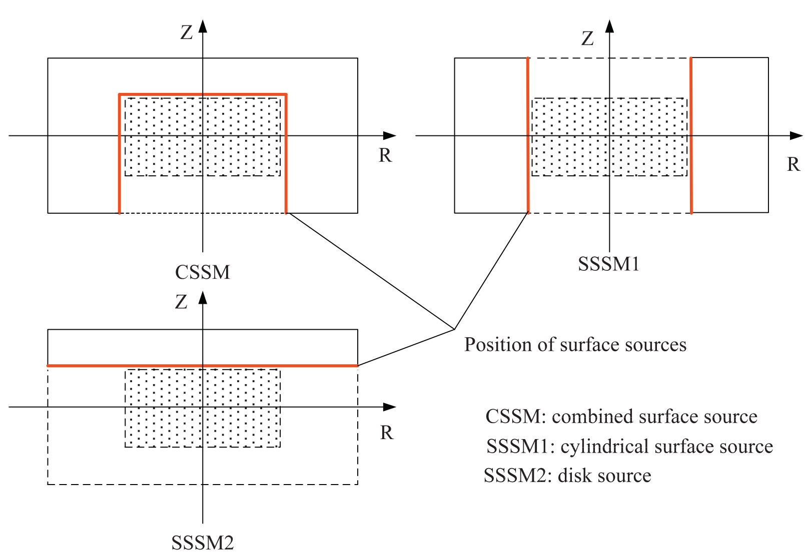


Fig. 6. S_N–MC coupling calculation models.

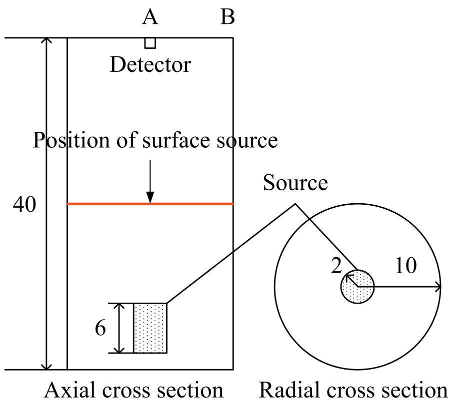


Fig. 8. Geometry of the homogeneous material problem.

group g at spatial mesh interval (i,j) of polar angle l can be obtained:

$$D_{l,i,j,g,s} = \sum_m E_{l,m,i,j,g,s}\omega_{l,m} \tag{2}$$

where $\omega_{l,m}$ is the weight of the S_N quadrature set. The scalar flux on surface s of energy group g at spatial mesh interval (i,j) is:

$$C_{i,j,g,s} = \sum_l D_{l,i,j,g,s} \tag{3}$$

Hence the energy spectrum on surface s is:

$$B_{g,s} = \sum_{i,j} C_{i,j,g,s}\Delta S_{i,j} \tag{4}$$

where $\Delta S_{i,j}$ is the area of spatial mesh interval (i,j). For the top or bottom surface, $\Delta S_{i,j} = \pi(r_{i+1}^2 - r_i^2)$; for the side surface, $\Delta S_{i,j} = 2\pi R(z_{j+1} - z_j)$, where R is the radius of the side surface. Then the number of particles crossing surface s is obtained:

$$A_s = \sum_g B_{g,s} \tag{5}$$

Finally, the number of particles crossing all the surfaces is obtained:

$$A = \sum_s A_s \tag{6}$$

$$A_t = A_n + A_r \tag{7}$$

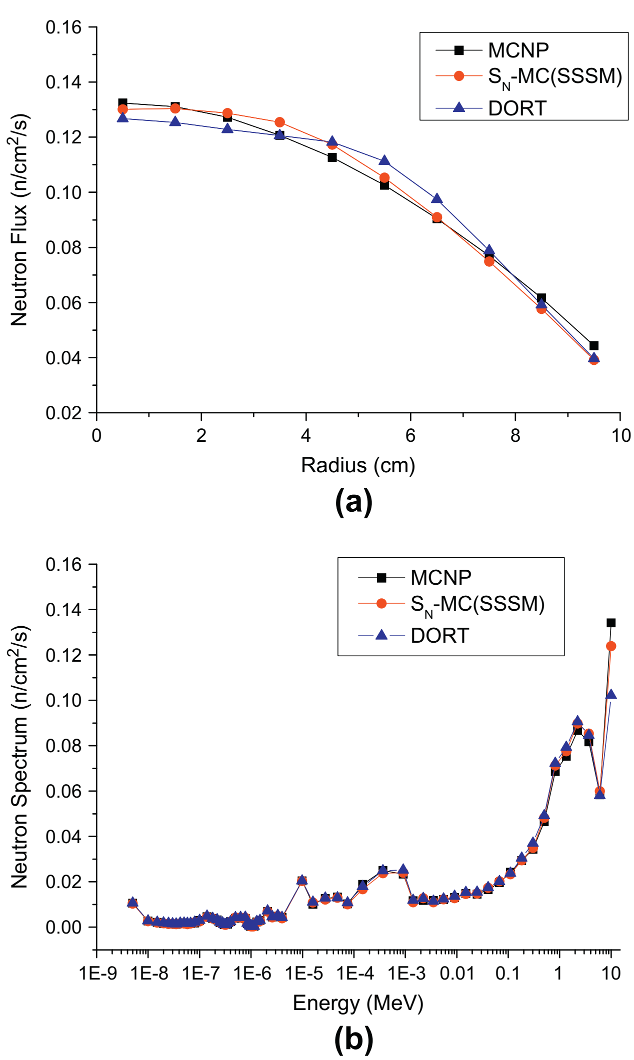


Fig. 9. Neutron flux distribution (a) and spectrum (b).

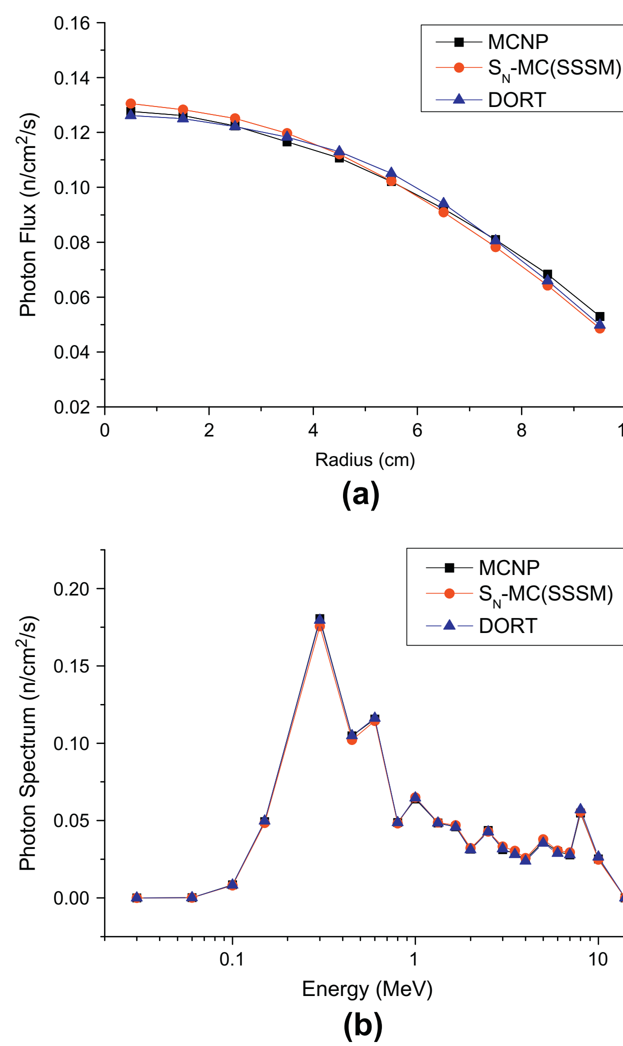


Fig. 10. Photon flux distribution (a) and spectrum (b).

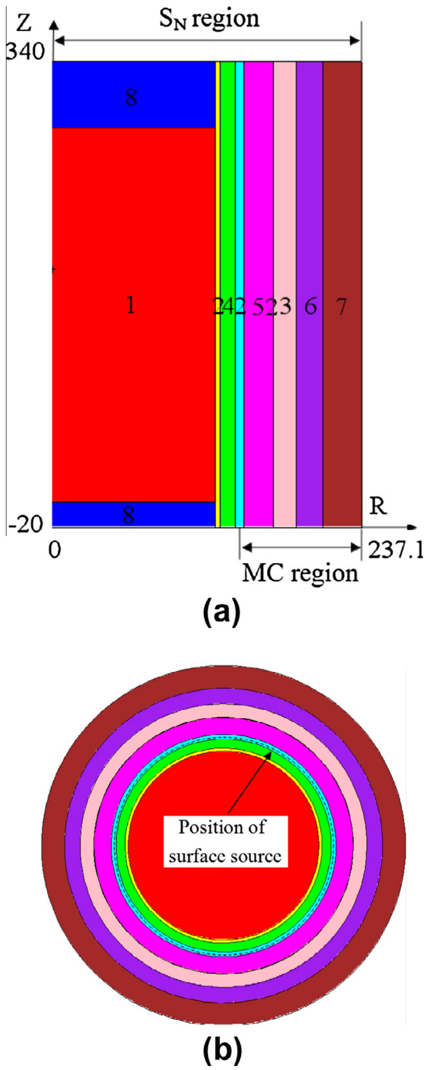


Fig. 11. Geometry of the PWR (a) axial cross section (b) radial cross section.

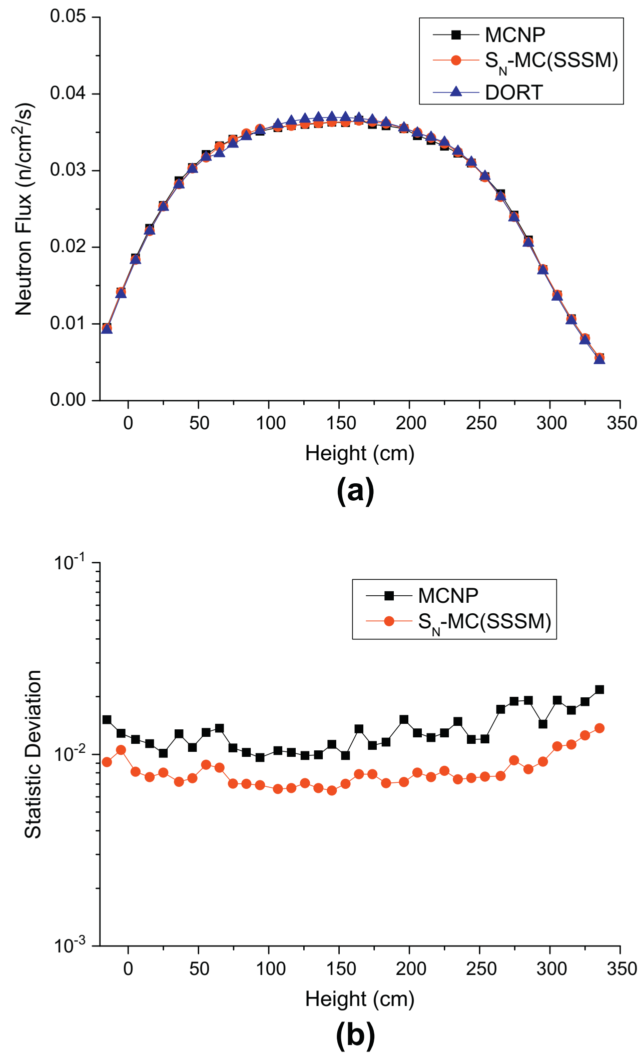


Fig. 12. Axial neutron flux distribution (a) and statistic deviations (b) of the cavity region.

Table 2
Materials inside and outside the core.

Region	Material
1	Reactor core
2	Baffle, barrel, pressure vessel liner
3	Pressure vessel
4	Bypass region
5	Downcomer region
6	Cavity
7	Biological shield
8	Top and bottom reflector

where A is the number of neutron or photon, A_t is the total number of neutron and photon, A_n and A_r represent number of neutron and photon crossing all the surfaces, respectively.

The summations in the above formulas are only about the directions along the surface normal and spatial intervals of the surface source. These arrays are normalized to form discrete PDFs as follows:

$$P_{l,m,i,j,g,s} = E_{l,m,i,j,g,s}\omega_{l,m}/D_{l,i,j,g,s} \tag{8}$$

$$P_{l,i,j,g,s} = D_{l,i,j,g,s}/C_{i,j,g,s} \tag{9}$$

$$P_{i,j,g,s} = C_{i,j,g,s}\Delta S_{i,j}/B_{g,s} \tag{10}$$

$$P_{g,s} = B_{g,s}/A_s \tag{11}$$

$$P_s = A_s/A \tag{12}$$

$$P_p = A_p/A_t \tag{13}$$

$P_{l,m,i,j,g,s}$: The azimuthal angle PDF for polar angle l for spatial mesh interval (i,j) and energy group g on surface s.

$P_{l,i,j,g,s}$: The polar angle PDF for spatial mesh interval (i,j) and energy group g on surface s.

$P_{i,j,g,s}$: The spatial PDF for energy group g on surface s.

$P_{g,s}$: The energy PDF for surface s.

P_s: The surface PDF for the combined surface source.

P_p: The particle PDF for the surface source.

Finally, these discrete PDFs are made cumulative for MCNP to sample source variables.

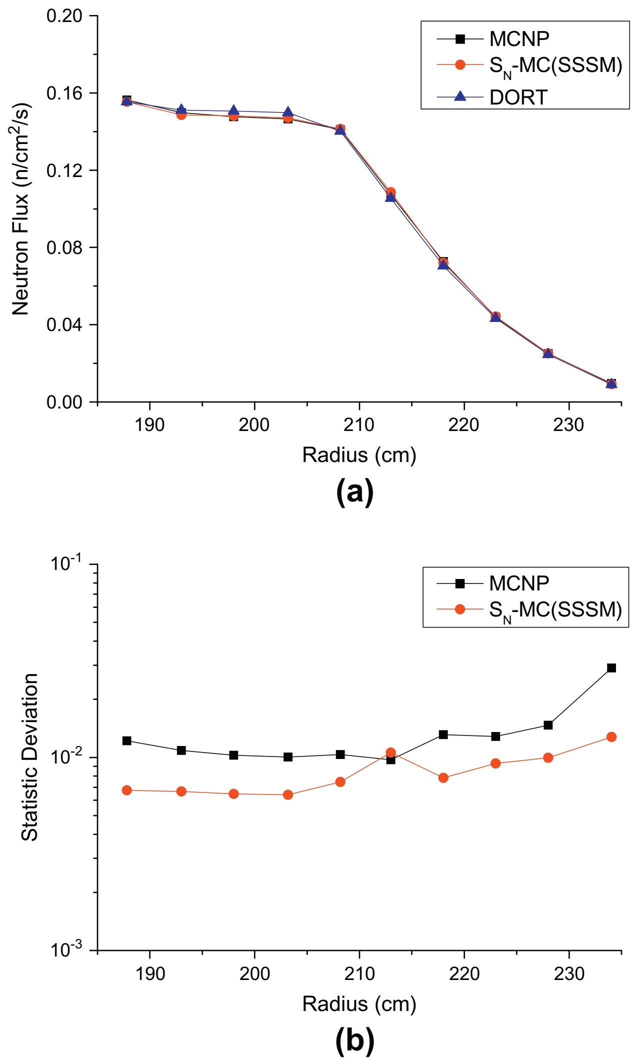


Fig. 13. Radial neutron flux distribution (a) and statistic deviations (b).

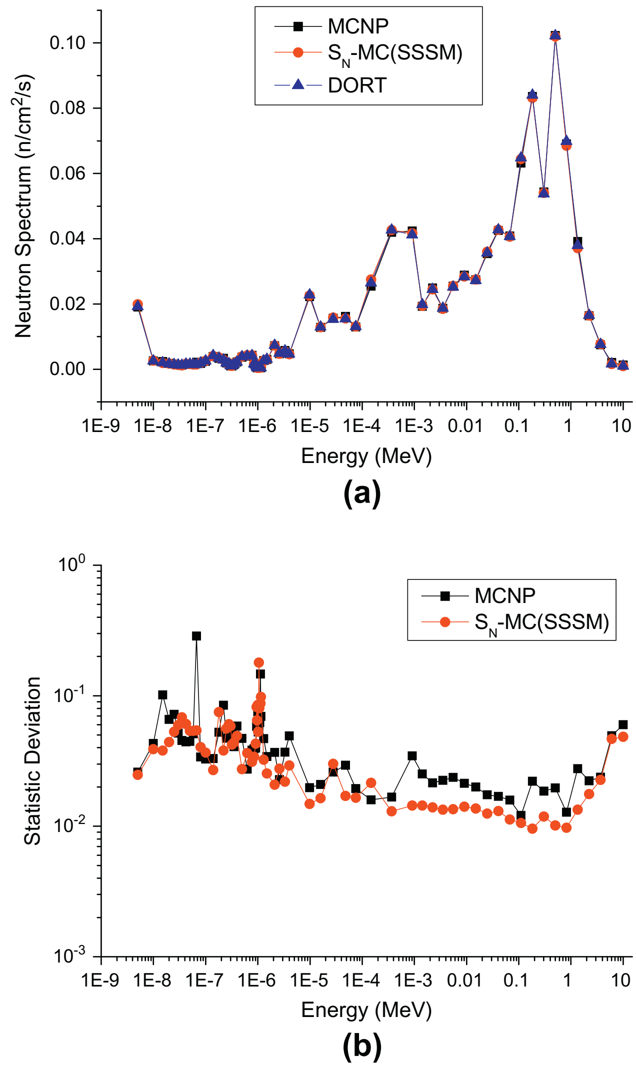


Fig. 14. Neutron spectrum (a) and statistic deviations (b).

3.2. Segments of the angular distributions

The quadrature set can be visualized as a unit directional sphere, and Fig. 3 depicts a schematic representation of the upper hemisphere.

The angular segments of each direction (l, m) are calculated utilizing the weights of quadrature set. Here we introduce an approximation that the segments of the angular distributions are continuous in the angular space. The azimuthal intervals are proportional to $\omega_{l,m}$, thus the segments of the azimuthal angle are obtained:

$$\frac{\phi_{l,m} - \phi_{l,m-1}}{2\pi - \pi} = \frac{\omega_{l,m-1}}{\sum_{m=1}^{M(l)} \omega_{l,m}}, \quad \phi_{l,1} = \pi \tag{14}$$

where $\phi_{l,m}$ is the mth azimuthal angle segment of polar angle level l, $M(l)$ denotes the number of azimuthal angles of polar angle level l.

By summing the weights over azimuthal intervals for each polar angle level, the segments of the polar angle cosines are obtained:

$$\frac{\eta_l - \eta_{l-1}}{1 - (-1)} = \frac{\sum_{m=1}^{M(l)} \omega_{l,m}}{\sum_{l=1}^{N} \sum_{m=1}^{M(l)} \omega_{l,m}}, \quad \eta_1 = -1 \tag{15}$$

where η_l is the lth segment of polar angle cosines, N is the number of polar angle levels.

3.3. Source variable sampling method

In the MC calculation, source particles are started with spaces, energies and directions sampled from the cumulative PDFs of the surface sources. A mapping and uniform sampling algorithm is used to calculate source variables. Suppose the probability of a random variable x is p_i when x equals to x_i, where $i = 1, 2, \ldots, I$, $\sum_{i=1}^{I} p_i = 1$. The cumulative PDF of x is defined as $c_j = \sum_{i=1}^{j} p_i$, $j = 1, 2, \ldots, I$.

Random variable x is sampled by the following procedure:

(1) Generate a random number $\xi_1 \in (0, 1]$.
(2) Determine j from $c_{j-1} < \xi_1 \leqslant c_j$.
(3) Generate a random number $\xi_2 \in (0, 1]$.
(4) Calculate $x = x_j^1 + \xi_2 \times (x_j^2 - x_j^1)$.

where x_j^1 and x_j^2 represent the lower and upper boundary value of discrete random variable x_j, respectively.

For example, in Fig. 4, if random number $\xi_1 = 0.5$, then the third discrete bin is chosen. If random number $\xi_2 = 0.5$, then $x = 3 + 0.5 \times (4 - 3) = 3.5$.

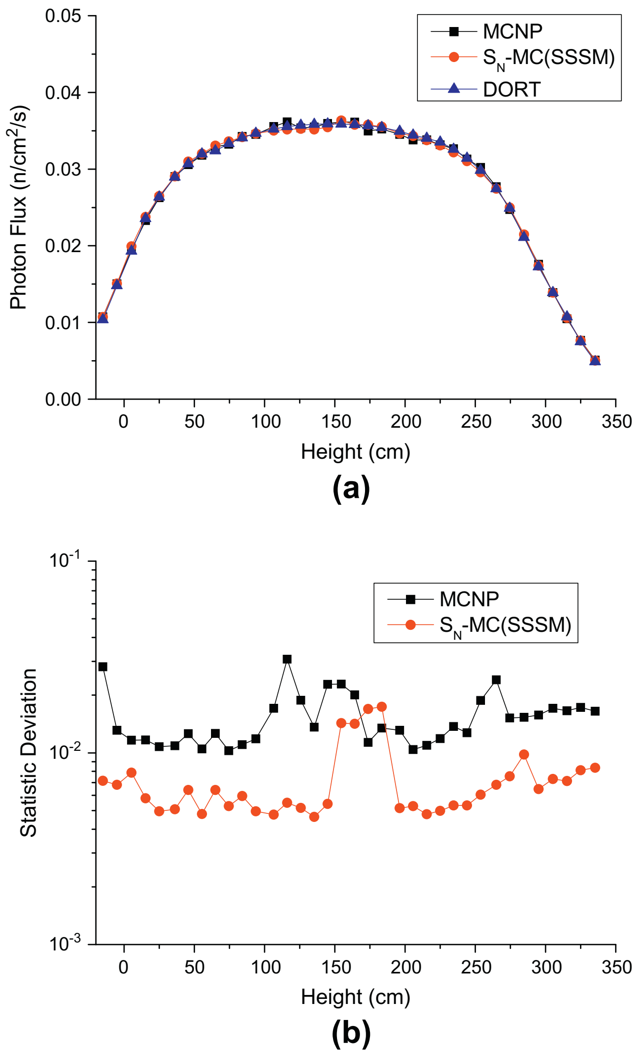


Fig. 15. Axial photon flux distribution (a) and statistic deviations (b).

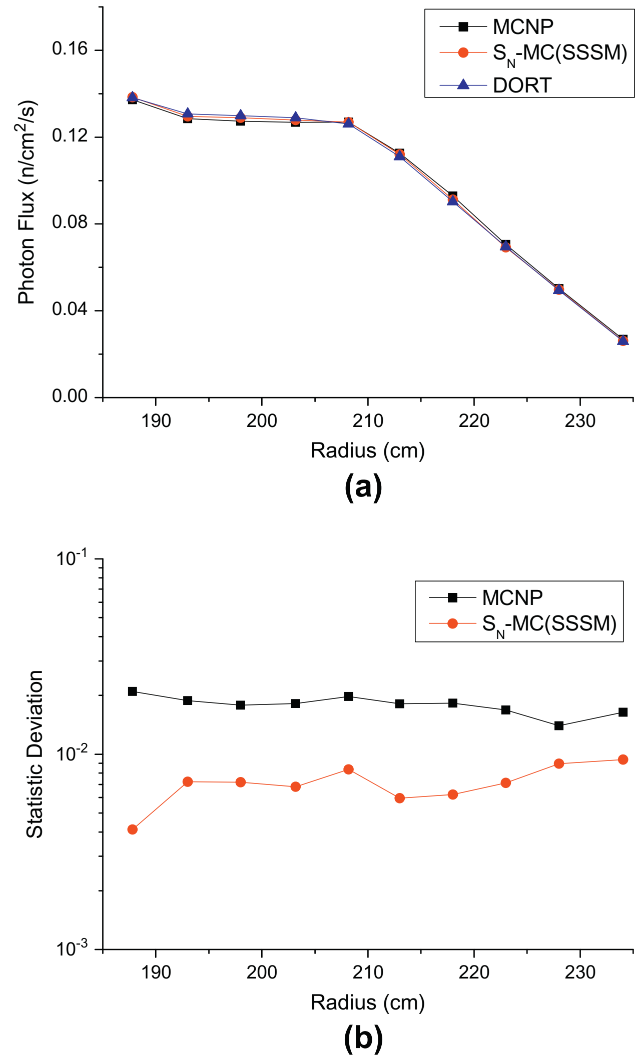


Fig. 16. Radial photon flux distribution (a) and statistic deviations (b).

4. Test calculations

Two test problems are calculated in this section. Since the purpose of these calculations is to verify the theoretical model of the coupling method instead of an actual application, the geometrical models of the problems are so defined to be suited to obtain accurate results by S_N and MC calculations independently. A two-region problem is designed to demonstrate the correctness of the CSSM and SSSM. A homogenous material problem is designed to demonstrate the correctness of the coupling method to deal with multigroup combined neutron/photon problems.

4.1. Two-region problem

The geometrical structure is illustrated by Fig. 5 with a length unit of cm, and the cross-sections are presented in Table 1. The goal of this problem is to obtain the flux distributions along AB and BC.

The whole region is considered in the S_N calculation in order to properly take albedo effects into account. In the S_N–MC coupling calculation, three surface source models are adopted. The first model uses a combined surface source (CSSM) emitting particles outwardly, the second model uses a cylindrical surface source (SSSM1) emitting particles outwardly, and the third model uses a disk source (SSSM2) emitting particles upwardly. Fig. 6 shows the S_N–MC coupling calculation models with three surface source models. The regions inside the surface sources are not considered in the MC calculation.

The results of the two region problem are exhibited in Fig. 7, where all results are normalized in the same way for the convenience of comparison. The principle of the normalization is to make the total flux to be one.

As can be seen in Fig. 7, the flux distribution obtained by the S_N–MC coupling method agrees well with those of the S_N method and MC method. This proves the correctness of the theoretical model of the coupling method. The MC calculation is performed once in the CSSM, and is performed two times in the SSSM. It indicates that recalculation can be avoided by the CSSM.

4.2. Homogenous material problem

The geometrical structure is illustrated in Fig. 8 with a length unit of cm. The material is a mixture of steel and water. The source is an isotropic neutron source with energy range (6.0655E+06–1.0000E+07) eV. The objective of this problem is to obtain the spectrum at the detector and flux distribution along AB.

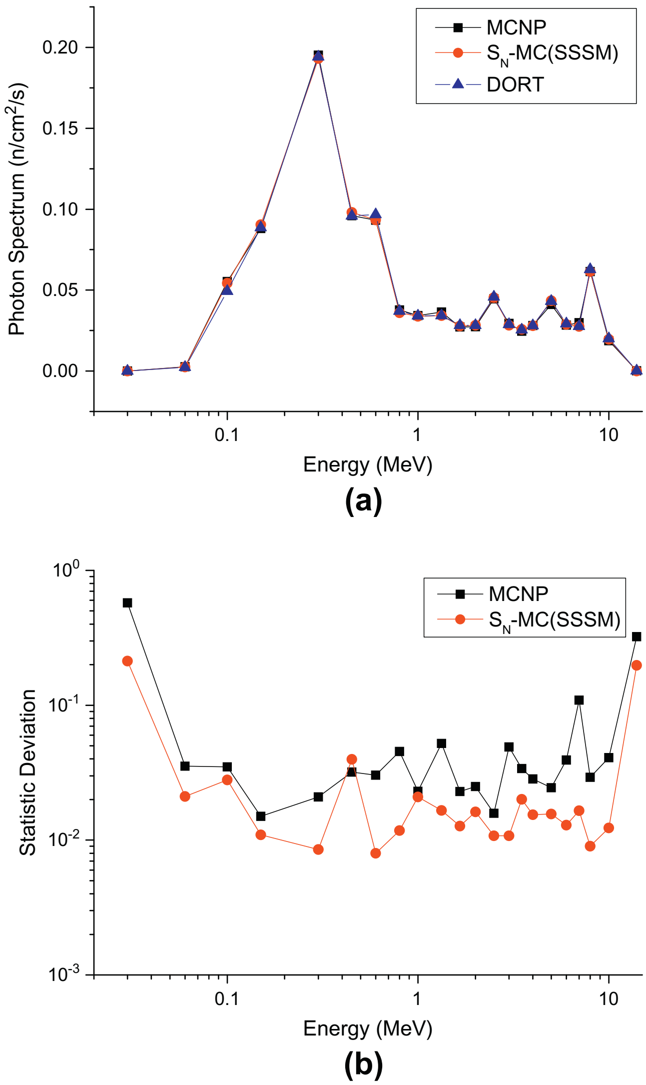


Fig. 17. Photon spectrum (a) and statistic deviations (b).

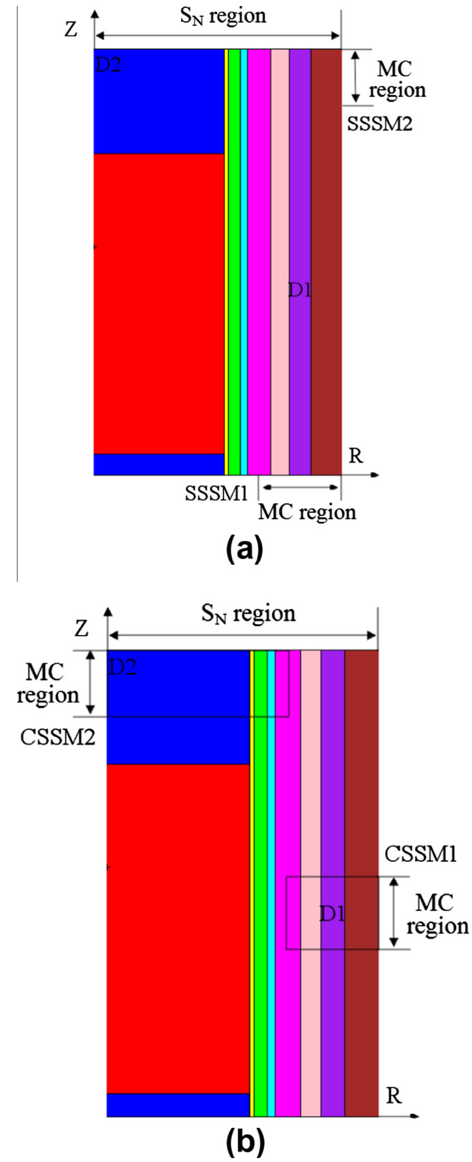


Fig. 18. S_N–MC coupling calculation models: SSSM (a) and CSSM (b).

Table 3
Computing time and speedup.

Code	MCNP as reference	S_N–MC			
		Total	DORT	DO2MC	MCNP
Time (min)	970.71	509.1	1.34	0.04	507.72
Speedup[a]	–	1.91	–	–	–

[a] Speedup = computing time of MCNP as reference/total computing time of S_N–MC.

In the S_N–MC coupling calculation, a disk source emitting particles upwardly are produced and the region below the disk source is not included. A 69 neutron groups and 22 photon groups cross-section library is used in all the calculations to eliminate the difference introduced by different libraries.

The results of the homogenous material problem are exhibited in Figs. 9 and 10. As can be seen from these figures, both of the neutron and photon flux distribution and spectrum obtained by the S_N–MC coupling method agree well with those of the S_N method and MC method. It demonstrates the validity of the coupling method to deal with multi-group combined neutron/photon problems.

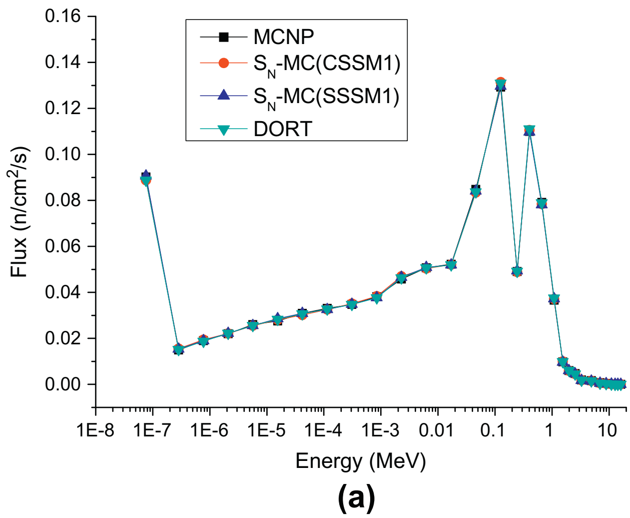
5. Application to PWR cavity radiation streaming calculation

5.1. Case 1

A representative model of a PWR cavity and surrounding geometry referring to the Qinshan Nuclear Power Plant in China is established. Fig. 11 shows the axial and radial cross sections of the PWR with a length unit of cm. Materials inside and outside the core for each region are given in Table 2. This problem is aimed to obtain the axial flux distribution and spectrum in the cavity region and radial flux distribution along mid-plane of the core region.

The model for S_N calculation is divided into 138 meshes in R direction and 130 meshes in Z direction, and a scheme of S_8 angular discretization is adopted. The same cross-section library as the homogenous material problem is used. In the S_N–MC coupling calculation, a cylindrical surface source model which emits particles outwardly is generated. Importance of the region inside the cylindrical surface source is set to be zero. Fmesh and En cards are used to tally the flux and spectrum of each tally region.

In order to evaluate the efficiency of the S_N–MC coupling method, another MC calculation model is established for reference in



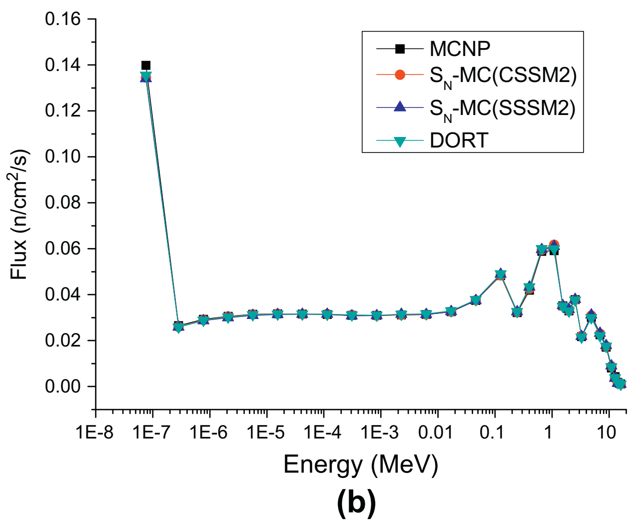


Fig. 19. Spectrum at detector 1(a) and 2(b).

which the whole region is considered. Geometry splitting/Russian roulette technique is adopted to obtain acceptable tally results with statistic deviations less than 10%.

The results are exhibited from Figs. 12–17. In particular, Figs. 12–14 show the flux distribution and spectrum of neutron, Figs. 15–17 show the flux distribution and spectrum of photon, respectively. As can be seen from these figures, the flux distribution and spectrum obtained by the S_N–MC coupling method agree well with those of the S_N method and MC method. In addition, the S_N–MC coupling method decreases the statistic deviations greatly in comparison with the MC method.

In addition to the flux and spectrum exhibited above, the computing time of the MC method and the S_N–MC coupling method are presented in Table 3. The total computing time of the S_N–MC coupling method consists of the computing time of DORT, DO2MC and MCNP. It can be seen from Table 3 that the computing time of the S_N–MC coupling method is reduced in comparison with that of the MC method.

5.2. Case 2

In order to prove the advantages of the CSSM over the SSSM, we compare the CSSM and the SSSM in this section. Fig. 18 shows the S_N–MC coupling calculation models. Compared with case 1, the geometrical model is 50 cm longer in the *z* direction. The aim is to obtain neutron spectrum at two detector (D1 and D2) locations.

Table 4
Computing time, speedup and statistic deviations.

Model	Time (min)				Speedup[a]	ASD[b]	
	DORT	DO2MC	MCNP	Total		Detector 1	Detector 2
MCNP as reference	–	–	594.95	–	–	0.036	0.025
CSSM	1.49	0.02	31.46	32.97	18.05	0.033	0.024
SSSM	1.49	0.03	45.57	47.09	12.63	0.034	0.024

[a] Speedup = computing time of MCNP as reference/total computing time of S_N–MC.
[b] ASD = average statistic deviations.

In the S_N–MC coupling calculation, four surface source models (CSSM1, CSSM2, SSSM1, SSSM2) are generated. In the reference MC calculation, both geometry splitting/Russian roulette and source energy biasing techniques are used to reduce statistic deviations. A 30 group multi-group neutron library is used in all the calculations to eliminate the difference introduced by different libraries.

Fig. 19 shows the spectrum of detector 1 and 2. As can be seen from these figures, the spectrum obtained by the S_N–MC coupling method agrees well with those of the S_N method and the MC method. Table 4 shows the computing time, speedup and statistic deviations. Compared with the reference MC calculation, both the CSSM and the SSSM have a speedup of over 10 to obtain the same statistic deviations. Compared with the SSSM, the CSSM defines interfaces closer to the detectors and transports more particles to the detectors, therefore costs less computing time to obtain the same statistic deviations.

6. Conclusion

In this work, a deterministic and Monte Carlo coupling method for PWR cavity radiation streaming calculation is studied. A link code DO2MC has been developed and verified. The main conclusions are as follows:

(1) Compared with the MC method, the S_N–MC coupling method has a speedup of 2–20 to obtain the same statistic deviations.
(2) In the coupling method, the CSSM is more efficient than the SSSM in reducing statistic deviations.

Because the 2-D RZ S_N method in the S_N–MC coupling method is not appropriate for problems with significant azimuthal variations, we will attempt to develop a 3-D S_N–MC link code to integrate the 3D S_N method and the MC method for coupling calculations. Furthermore, a parallelization of both S_N and MC calculation are under development to improve the computational efficiency.

Acknowledgments

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