Development of three dimensional discrete ordinates-Monte Carlo coupled system*

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The radiation shielding calculations of large nuclear facilities are complicated due to their bulk shields and complex geometries. A program system based on three-dimensional discrete ordinates (S_N)-Monte Carlo (MC) coupled method has been developed to solve this kind of shielding problems. S_N method is used to treat the deep penetration problem in the bulk shield, and MC simulation is performed with complex geometry. The coupled method is implemented in the interface program to calculate the probability of particle variables from the S_N angular flux distribution. A special source routine is written and linked to MC code to processed these probability arrays and sample the particle variables to generate source for the use of MC code. The H. B. Robinson Unit 2 pressure vessel benchmark was used to validate the S_N -MC coupled program system. The specific activities for the six dosimeters in the surveillance capsule were calculated. Satisfactory agreements were obtained from the comparisons of S_N -MC coupling scheme with the program system is suitable to treat three dimensional shielding problems with satisfactory accuracy.

Keywords: Discrete ordinates, Monte Carlo, Coupled, Benchmark validation, Shielding

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I. INTRODUCTION

Radiation shielding calculation of large scale nuclear facilities is complicated due to the bulk shield and complex geometry. Discrete ordinates (S_N) and Monte Carlo (MC) methods are commonly used in the design of radiation shielding. MC method is able to treat the complex geometry, but time-consuming in dealing with the deep penetration problems. S_N method has great computational efficiency, but it is quite costly in computer memory. Therefore, for the shielding analysis of a large and complex system, the coupled method which combines the advantages of both the MC and S_N approaches is very suitable. The MC method is used to simulate the particle transport in the complex geometry, and the S_N method is used to treat the deep penetration problems in the bulk shield.

The existing S_N -MC coupled codes include DOT-DOMINO-MORSE [1] and DORT-PROBGEN-MCNP [2]. However, these codes cannot support full three-dimensional geometry. Masahiko Kurosawa developed TORT-MCNP [3] for the calculation of neutron flux around a core of BWR, but it only for Cartesian geometry. In this work, a program system has been devised to make full three-dimensional S_N -MC coupling calculations in both Cartesian and Cylindrical geometry. The validation calculation of the H. B. Robinson Unit 2 (HBR-2) pressure vessel benchmark problem [4] is presented and discussed.

II. S_N -MC COUPLED METHOD

To perform the S_N -MC calculation, the model is divided into two parts. The one part of the model is the bulk shield region with simple geometry, and the other part is the complex geometry. The discrete ordinates method has advantage in treating the deep penetration problem with simple geometry. The MC method is able to treat the complex geometry, but time-consuming in dealing with the deep penetration problem. In order to eliminate the weakness of the single method, an interface program is developed to transform the angular fluxes from S_N solution into normalized probability distributions. The normalized probability distributions calculated by interface program are as follows:

$$p(i) = \frac{\sum_{g=1}^{G} \sum_{m=1}^{M} w_m \psi(r_i, E_g, \Omega_m) |\lambda_m| A_i}{\sum_{i=1}^{I} \sum_{g=1}^{G} \sum_{m=1}^{M} w_m \psi(r_i, E_g, \Omega_m) |\lambda_m| A_i},$$
(1)

$$p(g/i) = \frac{\sum_{m=1}^{M} w_m \psi(r_i, E_g, \Omega_m) |\lambda_m| A_i}{\sum_{g=1}^{G} \sum_{m=1}^{M} w_m \psi(r_i, E_g, \Omega_m) |\lambda_m| A_i}, \quad (2)$$

$$p(m/g/i) = \frac{w_m \psi(r_i, E_g, \Omega_m) |\lambda_m| A_i}{\sum_{m=1}^M w_m \psi(r_i, E_g, \Omega_m) |\lambda_m| A_i}, \quad (3)$$

where $\psi(r_i, E_g, \Omega_m)$ represents the angular flux in the spatial mesh i for energy group g and direction m. I is the total number of spatial mesh, G is the total number of energy groups, M is the total number of directions. λ_m means direction cosine with respect to a set of orthogonal coordinate axes. w_M is the corresponding directional weight. A_i means the area of the spatial mesh i. The probability of any spatial mesh, p(i), is calculated by Eq. 1 based on the radio of the

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total number of particles crossing at that location to the total number of particles crossing the entire common surface. p(g/i) in Eq. 2 is the normalized energy spectrum. Eq. 3 defines the probability for every angle used in the discrete ordinates method. That is, if the calculation used an S8 quadrature scheme, then there would be 80 probabilities, each corresponding to a unique direction.

$$\sum_{i=1}^{j-1} p_i \le \xi \le \sum_{i=1}^{j} p_i.$$
(4)

The space bin is chosen by Eq. 4, and ξ means a random number. The energy and angular bin selection were conducted in the same fashion as shown in Eq. 4, and the final energy and direction were sampled randomly from within the selected bin.

III. PROGRAM SYSTEM

The flow chart of three-dimensional S_N -MC coupled program system was shown in Fig. 1. The coupled program system consists of three-dimensional S_N code, S_N -MC interface program, MC source subroutine and MC code.



Fig. 1. Flow chart of the program system for three-dimensional coupled S_N -MC.

In practical application, a common surface is first specified in both S_N mesh model and the MC model. In S_N calculation, the angular fluxes (as a function of mesh interval, energy group and discrete direction) on the common surface are stored in a BNDRYS formatted file. In MC simulation, this surface is specified as the source. The interface program reads the BNDRYS-format file generated by S_N , and then uses the equation given in Section 2 to generate the necessary probability distributions. The MC source subroutine is linked to MC code to generate MC source particles variables by using the probability. The Cartesian (X, Y, Z) and Cylindrical (R, θ, Z) can be selected in the calculation by the coupling method.

IV. CALCULATION RESULTS AND DISCUSSION

The HBR-2 benchmark was adopted to validate the capability of the 3D S_N -MC coupling methodology. The specific activities for the six dosimeters were calculated. The dosimeters were irradiated during cycle 9 in the surveillance capsule. The surveillance capsule is located on the mid-place of the HBR-2 core. The experimental measurements and results of DORT code are included in the benchmark documentation. The 45 °sector of 3D calculated model is displayed in Fig. 2. As shown in Fig. 2, the model was separated to S_N mesh model and the MC model. The inner surface of core barrel is specified as the common surface. TORT [5] and MCNP [6] were used via the program system for S_N and MC model calculation, respectively. The S_N model was analyzed with the TEXT10 library, which have 30 neutron and 12 gamma energy groups. The point-wise cross-section files generated from ENDF/B-VI data library [7] were used in the MCNP calculations.



Fig. 2. (Color online) 3D horizontal cross section model of HBR-2 reactor.

For S_N calculation, the order of scattering expansion is P3, and the angular quadrature set is S8. The mesh grids for the S_N model are $110 \times 36 \times 48$. The angular fluxes on the common surface, calculated by TORT, were stored in a BNDRY format file, and then the interface program and the source subroutine were employed to generate the source particles of MCNP. The MC model describes the detailed geometry and material compositions of surveillance capsule mounting on the thermal shield. The neutron flux values and activities at the dosimeter position of the surveillance capsule are calculated by S_N -MC coupled method. It is seen from Fig. 3 that the S_N -MC neutron spectrum appears to be in relatively

| | Tuble 1. Tubles of calculated to inclusive (0/11) specific activities. | | | | | | | |
|-----------|--|---------------------|-----------------------|-----------------------|---------------------------|----------------------|-------------------|--|
| | ${}^{237}{ m Np}(n,f)$ | 238 U (n, f) | ${}^{58}{ m Ni}(n,p)$ | ${}^{54}{ m Fe}(n,p)$ | ${}^{46}\mathrm{Ti}(n,p)$ | 63 Cu (n,a) | Average | |
| Code | ¹³⁷ Cs | ¹³⁷ Cs | ⁵⁸ Co | 54 Mn | ⁴⁶ Sc | ⁶⁰ Co | | |
| DORT | 0.90 | 0.85 | 0.96 | 0.93 | 0.85 | 0.90 | $0.89 {\pm} 0.04$ | |
| S_N -MC | 1.06 | 0.96 | 1.01 | 1.03 | 1.01 | 1.09 | $1.03 {\pm} 0.04$ | |
| TORT | 1.12 | 1.07 | 1.00 | 0.99 | 1.03 | 1.05 | $1.04 {\pm} 0.04$ | |

Table 1. Ratios of calculated-to-measured (C/M) specific activities.

good agreement with the DORT-BUGLE96 solution in HBR-2 benchmark report.



Fig. 3. (Color online) Neutron spectrum of the surveillance capsule.

The ratios of the calculated specific activities by different codes with the measurements were shown in Table 1. The average ratios of calculated-to-measured (C/M) for the six dosimeters in the surveillance capsule for DORT, S_N -MC and TORT are 0.90±0.04, 1.03±0.04 and 1.04±0.04, respec-

tively. The C/M of DORT and TORT come from [4] and [8], respectively. Table 1 shows that the S_N -MC calculated specific activities are quite similar to the TORT results and the experimental measurements. As to be expected from the neutron flux comparisons, the S_N -MC calculated specific activities are larger than the DORT results. The necessary simplification of certain features for the HBR-2 reactor, the different codes and cross-section library differences can all be the contributing factors.

V. CONCLUSIONS

A program system has been developed to implement the coupled S_N -MC scheme by integrating the 3D S_N code TORT, the MC transport code MCNP, the coupling interface program and source subroutine. The program system is able to deal with the shielding problem with bulk shield and complex geometry in large dimensions. The HBR-2 benchmark problem has been performed to validate the program system. Good agreements were obtained by comparing with the measurements and the results of other codes. The successful application demonstrates that the coupling scheme with the program system is a powerful computational tool for three-dimensional shielding analysis of complex and large nuclear facilities.

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