Development of three dimensional discrete ordinates-Monte Carlo coupled system post-print

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Abstract

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 (SN)-Monte Carlo (MC) coupled method has been developed to solve this kind of shielding problems. SN 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 SN 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 SN-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 SN-MC results with those obtained from measurement and other computer codes. The result demonstrates that the SN-MC coupling scheme with the program system is suitable to treat three dimensional shielding problems with satisfactory accuracy.

Full Text

Preamble

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Development of Three-Dimensional Discrete Ordinates-Monte Carlo Coupled System

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Radiation shielding calculations for large nuclear facilities are complicated due to their bulk shields and complex geometries. A program system based on the three-dimensional discrete ordinates (SN)-Monte Carlo (MC) coupled method has been developed to solve this class of shielding problems. The SN method is used to treat deep penetration problems in bulk shields, while MC simulation handles complex geometries. The coupled method is implemented in an interface program that calculates the probability distribution of particle variables from the SN angular flux distribution. A specialized source routine was written and linked to the MC code to process these probability arrays and sample particle variables for generating sources in the MC code. The H. B. Robinson Unit 2 pressure vessel benchmark was used to validate the SN-MC coupled program system. Specific activities for six dosimeters in the surveillance capsule were calculated. Satisfactory agreement was obtained when comparing SN-MC results with measurements and other computer codes. The results demonstrate that the SN-MC coupling scheme with this program system is suitable for treating three-dimensional shielding problems with satisfactory accuracy.

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

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Introduction

Radiation shielding calculations for large-scale nuclear facilities are complicated due to bulk shields and complex geometries. Discrete ordinates (SN) and Monte Carlo (MC) methods are commonly used in radiation shielding design. The MC method can treat complex geometry but is time-consuming for deep penetration problems. The SN method offers high computational efficiency but requires substantial computer memory. Therefore, for shielding analysis of large and complex systems, a coupled method that combines the advantages of both MC and SN approaches is highly suitable. The MC method simulates particle transport in complex geometries, while the SN method treats deep penetration problems in bulk shields.

Existing SN-MC coupled codes include DOT-DOMINO-MORSE [**?**] and DORT-PROBGEN-MCNP [**?**]. However, these codes cannot support full three-dimensional geometry. Masahiko Kurosawa developed TORT-MCNP [**?**] for calculating neutron flux around a BWR core, but it only supports Cartesian geometry. In this work, a program system has been devised to perform full three-dimensional SN-MC coupling calculations in both Cartesian and cylindrical geometries. The validation calculation of the H. B. Robinson Unit 2

(HBR-2) pressure vessel benchmark problem [**?**] is presented and discussed.

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II. SN-MC Coupled Method

To perform SN-MC calculations, the model is divided into two parts: a bulk shield region with simple geometry and a region with complex geometry. The discrete ordinates method is advantageous for treating deep penetration problems with simple geometry. The MC method can treat complex geometry but is time-consuming for deep penetration problems. To eliminate the weaknesses of each single method, an interface program is developed to transform the angular fluxes from the SN solution into normalized probability distributions.

The normalized probability distributions calculated by the interface program are as follows:

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

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

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

where $\psi(r_i, E_g, \Omega_m)$ represents the angular flux in spatial mesh i for energy group g and direction m. I is the total number of spatial meshes, G is the total number of energy groups, and M is the total number of directions. λ_m denotes the direction cosine with respect to a set of orthogonal coordinate axes, w_m is the corresponding directional weight, and A_i is the area of spatial mesh i. The probability of any spatial mesh, $p(i)$, is calculated by Eq. (1) based on the ratio of the total number of particles crossing 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 uses an S_8 quadrature scheme, there would be 80 probabilities, each corresponding to a unique direction.

The interface program uses the equations given above to generate the necessary probability distributions. The MC source subroutine is linked to the MC code to generate MC source particle variables using these probabilities. Both Cartesian (X, Y, Z) and cylindrical (R, θ, Z) geometries can be selected in the calculation by the coupling method. The space bin is chosen by:

$$\sum_{j=1}^{i-1} p_j \leq \xi \leq \sum_{j=1}^{i} p_j, \tag{4}$$

where ξ is a random number. The energy and angular bin selections are conducted in the same fashion as shown in Eq. (4), and the final energy and direction are sampled randomly from within the selected bin.

III. Program System

The flow chart of the three-dimensional SN-MC coupled program system is shown in Fig. 1 [Figure 1: see original paper]. The coupled program system consists of a three-dimensional SN code, an SN-MC interface program, an MC source subroutine, and an MC code.

IV. Calculation Results and Discussion

The HBR-2 benchmark was adopted to validate the capability of the 3D SN-MC coupling methodology. The specific activities for six dosimeters were calculated. The dosimeters were irradiated during cycle 9 in the surveillance capsule, which is located on the mid-plane of the HBR-2 core. Experimental measurements and DORT code results are included in the benchmark documentation.

The 45° sector of the 3D calculated model is displayed in Fig. 2 [Figure 2: see original paper]. As shown in Fig. 2, the model was separated into an SN mesh model and an MC model, with the inner surface of the core barrel specified as the common surface. TORT [**?**] and MCNP [**?**] were used via the program system for SN and MC model calculations, respectively. The SN model was analyzed with the TEXT10 library, which has 30 neutron and 12 gamma energy groups. Point-wise cross-section files generated from the ENDF/B-VI data library [**?**] were used in the MCNP calculations.

In practical application, a common surface is first specified in both the SN mesh model and the MC model. In the SN 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 SN and then processes it to generate the source particles for MCNP.

For SN calculation, the order of scattering expansion is P_3, and the angular quadrature set is S_8. The mesh grids for the SN 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 source subroutine were employed to generate the source particles for MCNP. The MC model describes the detailed geometry and material compositions of the surveillance capsule mounted on the thermal shield. Neutron flux values and activities at the dosimeter positions of the surveillance capsule were calculated by the SN-MC coupled method.

As seen from Fig. 3 [Figure 3: see original paper], the SN-MC neutron spectrum appears to be in relatively good agreement with the DORT-BUGLE96 solution in the HBR-2 benchmark report.

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

Dosimeter	SN-MC
^{237}Np(n,f) ^{137}Cs	0.89$±$0.04
^{238}U(n,f) ^{137}Cs	1.03$±$0.04
^{58}Ni(n,p)	1.04$±$0.04
^{54}Fe(n,p)	
^{46}Ti(n,p)	
^{63}Cu(n,a)	
Average	

The ratios of calculated specific activities by different codes with measurements are shown in Table 1. The average ratios of calculated-to-measured (C/M) for the six dosimeters in the surveillance capsule for DORT, SN-MC, and TORT are 0.90 ± 0.04, 1.03 ± 0.04, and 1.04 ± 0.04, respectively. The C/M values for DORT and TORT come from [**?**] and [**?**], respectively. Table 1 shows that the SN-MC calculated specific activities are quite similar to the TORT results and experimental measurements. As expected from the neutron flux comparisons, the SN-MC calculated specific activities are larger than the DORT results. Necessary simplifications of certain features for the HBR-2 reactor, differences in codes, and cross-section library differences can all be contributing factors.

V. Conclusions

A program system has been developed to implement the coupled SN-MC scheme by integrating the 3D SN code TORT, the MC transport code MCNP, the coupling interface program, and source subroutine. The program system is able to deal with shielding problems involving bulk shields and complex geometry in large dimensions. The HBR-2 benchmark problem has been performed to validate the program system. Good agreement was obtained by comparing with 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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Note: Figure translations are in progress. See original paper for figures.