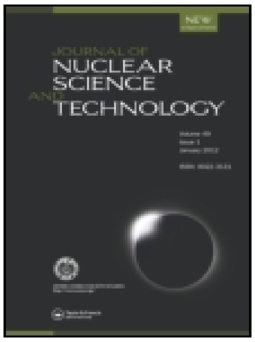

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Development of SCINFUL-QMD Code to Calculate the Neutron Detection Efficiencies for Liquid Organic Scintillator up to 3 GeV

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The Monte Carlo code, designeted SCINFUL-QMD, has been developed to calculate neutron detection efficiency up to 3 GeV for liquid organic scintillators such as NE-213. The existing Monte Carlo code, SCINFUL, is known to reproduce a response function and detection efficiency at incident neutron energies below 80 MeV. We incorporate the quantum molecular dynamics plus statistical decay model (QMD+SDM) into SCINFUL to extend the upper limit of incident neutron energy to 3 GeV. The results by SCINFUL-QMD are compared with experimental data and those of CECIL. The SCINFUL-QMD exhibits an increase in detection efficiency above 300 MeV. This tendency agrees with one of the experimental data. The increase is achived by taking charged pion production into account.

***KEYWORDS**: neutorn, 3 GeV, detection efficiency, NE-213, liquid organic scintillator, SCINFUL, QMD, Monte Carlo*

I. Introduction

For the neutron Time-of-Flight (TOF) measurement, the neutron detection efficiency of liquid organic scintillators is essential to determine the absolute yield. Many experiments in the energy region up to 100 MeV have been performed to obtain the neutron detection efficiency for various organic scintillators. However, the experimental data for the high energy neutron detection efficiency up to several GeV are very scarce. The existing Monte Carlo codes, SCINFUL[1)] and CECIL,[2)] are often used for calculating the neutron detection efficiency. The SCINFUL is known to reproduce well the response function and detection efficiency for the NE-213 (liquid) and the NE-110 (solid) organic scintillators. However, the upper limit of incident neutron energy is set at 80 MeV. In contrast, the CECIL code is capable of calculating the response function up to a few GeV. Thus, the CECIL has been used to determine the neutron detection efficiency above 100 MeV.[3,4)] Unfortunately, this code treats a lesser number of reaction channels than the SCINFUL, and considers the light output only for p and α. In addition, the total cross section adopted in this code are assumed constant above 200 MeV. It is, therefore, of interest to develop a new code applicable to the calculation in the higher-energy region.

The quantum molecular dynamics plus statistical decay model (QMD+SDM)[5)] successfully simulates the nuclear reactions in the higher-energy region. We incorporate the QMD+SDM into the SCINFUL code to develop a new code that can calculate the neutron detection efficiency up to 3 GeV. This code is hereafter designated the SCINFUL-QMD. The calculation results by the SCINFUL-QMD are compared with the experimental data and those by the CECIL.

II. Calculation Model

1. SCINFUL

The SCINFUL code is designed to provide the full response anticipated for neutron interactions in either liquid or solid cylindrical organic scintillators by means of the Monte Carlo method. The incident neutron energy range is set at 0.1 to 80 MeV. The SCINFUL treats 39 reaction channels, starting from 11 initial channels. These initial reaction channels are listed in **Table 1**.

Table 1 Reaction Channels in the SCINFUL and the CECIL codes

SCINFUL	CECIL
$\mathrm{H}(n,n)$	$\mathrm{H}(n,n)$
$\mathrm{C}(n,n)$	$\mathrm{C}(n,n)$
$\mathrm{C}(n,\gamma)$	$\mathrm{C}(n,\gamma)$
$\mathrm{C}(n,\alpha)$	$\mathrm{C}(n,\alpha)$
$\mathrm{C}(n,3\alpha)$	$\mathrm{C}(n,3\alpha)$
$\mathrm{C}(n,np)$	$\mathrm{C}(n,np)$
$\mathrm{C}(n,2n)$	
$\mathrm{C}(n,p)$	
$\mathrm{C}(n,d)$	
$\mathrm{C}(n,t)$	
$\mathrm{C}(n,{}^3\mathrm{He})$	

The neutron detection efficiencies of the NE-213 calculated by the SCINFUL are shown in **Fig. 1** with the experimental data[6–8)] and the results by the CECIL. Below 40 MeV, the SCINFUL code reproduce the experimental data very well. In contrast, the values by the CECIL are higher than both the experimental data and the predictions by the SCINFUL. This overestimation by the CECIL code is mainly related to the overestimation of the $\mathrm{C}(n,x\alpha)$ spectrum.[7)] In the higher-energy region, the SCINFUL shows the good agreement with the value of reference 7. However, the SCINFUL underestimates the values of reference 8.

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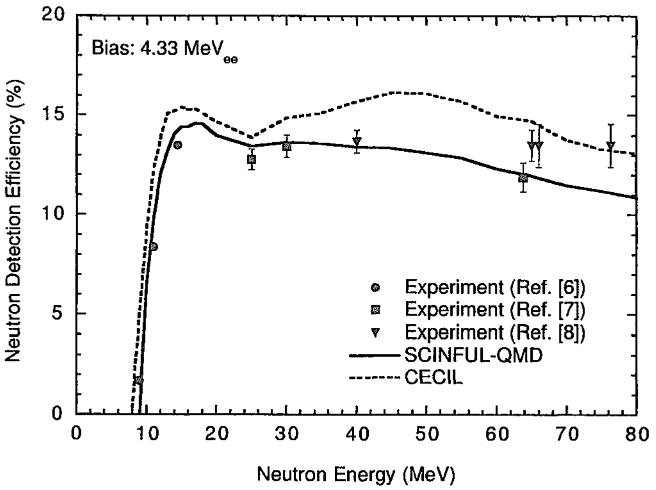

Fig. 1 Neutron detection efficiencies of the NE-213 (12.7 cm in diameter and 12.7 cm long) at 4.33 MeVee bias setting

2. QMD+SDM

The simulation code divides the nuclear reaction into two stages, i.e., the dynamical and the statistical processes, according to their typical collision times. The QMD method is utilized for the dynamical process and the SDM for the subsequent statistical process.

The QMD method is a semiclassical simulation method that approximates the nucleon wave nature by the use of a Gaussian-type function. For effective two-body interaction, this method employs the Skyrme type interaction including the Coulomb and symmetry terms. The behavior of individual nucleons is calculated along the time evolution. The SDM describes the light-particle evaporation by using the Monte Carlo method until no particles are emitted. This method does not treat gamma-ray emissions.

The QMD+SDM is widely used to describe various nuclear reactions. The validation of this model has been confirmed in reference 5 for incident energies from 100 MeV to 3 GeV.

3. SCINFUL-QMD

We combined the SCINFUL code with the QMD+SDM to simulate nuclear reactions above 150 MeV. Below 150 MeV, the SCINFUL-QMD calculates nuclear reactions by expansion of the reaction cross section data in the SCINFUL. In further study, we will use the evaluated nuclear data to simulate nuclear reactions up to 150 MeV . The computational scheme of the SCINFUL-QMD is given in **Fig. 2**.

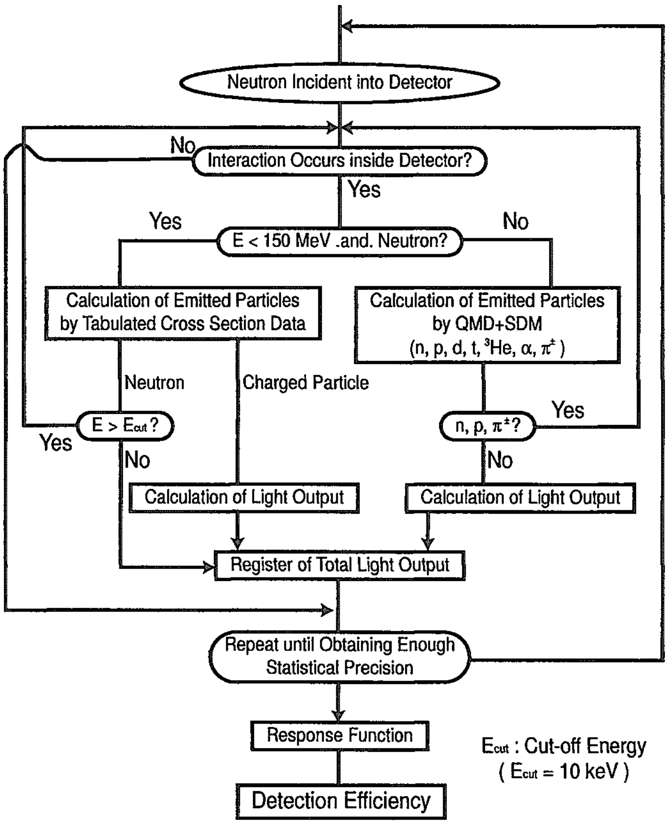

Fig. 2 Computational scheme and flow of the SCINFUL-QMD code

In the neutron transport simulation by the Monte Carlo technique, total cross sections of H and ^{12}C are utilized to provide the probability of the interaction. The CECIL code adopts the constant values of total cross section above 200 MeV. On the other hand, the SCINFUL-QMD code has data set of the total cross sections up to 3 GeV. All cross sections adopted in this code are shown in **Fig. 3** with the experimental data.[9–12] The interactions with carbon are dominant in the higher-energy region. If an interaction is certain to occur, information on the reaction such as the coordinates of the collision point, the energy of the colliding neutron and the target element is stored. Then the nuclear reaction is calculated. Two different methods are employed in the SCINFUL-QMD. For neutrons at incident energies below 150 MeV, tabulated cross section data are used to choose among the types of reactions that are energetically taking place. At energies of 80 to 150 MeV, the cross section data used in the SCINFUL were extrapolated. In the next version of the SCINFUL-QMD, the cross section data in this energy region will be revised. The energies and kinematics of the chosen reaction are determined by the Monte Carlo sampling. Above 150 MeV, nuclear reactions are simulated by the QMD+SDM. We take *n, p, d, t,* ^{3}He, α and $\pi^{\pm}$ as emitted particles in the QMD+SDM. For *n, p,* and $\pi^{\pm}$, the Monte Carlo choice is utilized again to check whether the interaction takes place inside the scintillator. The light outputs for charged particles are determined by reference to tables on the conversion of kinetic energy into light output. This tabulated light output data are taken from the original SCINFUL code. The sum of these light outputs is accumulated as the total light output for one neutron injection. The calculation is repeated until a specified statistical precision is obtained.

The response function is constructed using the total light output for incident neutrons. The detection efficiency is determined by integrating the response function above a bias energy, which is expressed by electron-equivalent value (MeVee).

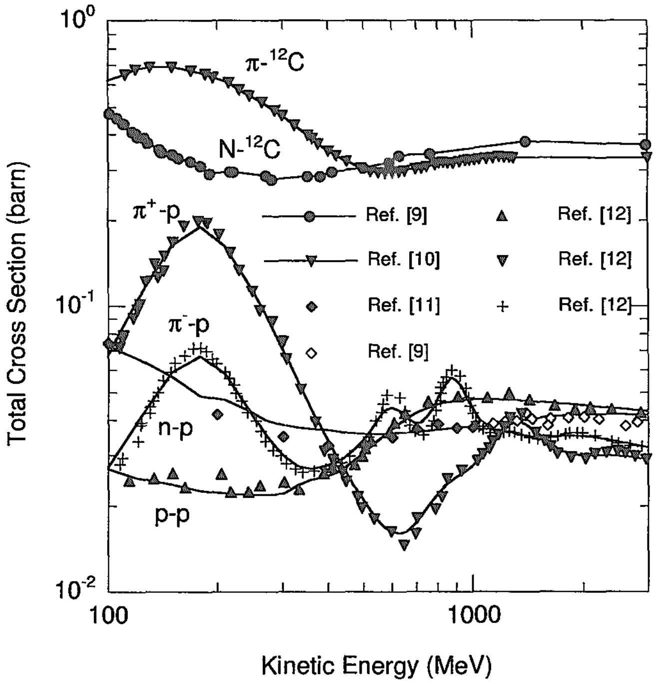

Fig. 3 Total cross sections adopted in the SCINFUL-QMD code. The character N stands for nucleon.

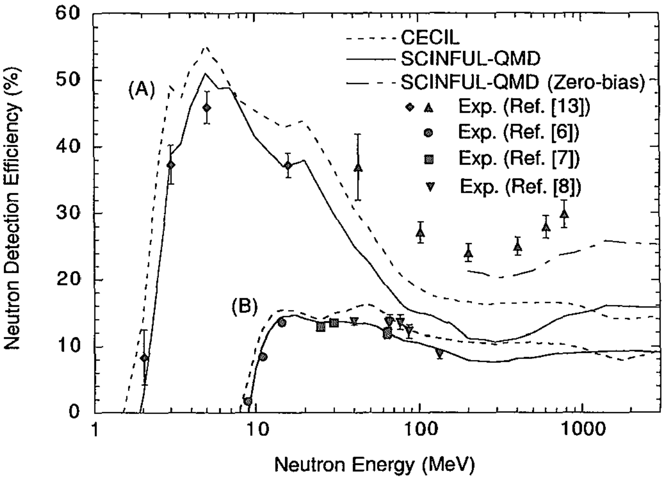

Fig. 4 Neutron detection efficiencies up to 3 GeV. (A) NE-213 (12.7 cm in diameter and 17.78 cm long) at 0.45 MeVee bias setting. (B) NE-213 (12.7 cm in diameter and 12.7 cm long) at 4.33 MeVee bias setting.

III. Comparison between Calculation and Experiment

The neutron detection efficiencies calculated by the SCINFUL-QMD up to 3 GeV are shown in **Fig. 4** with the experimental data[6–8, 13] and the results by the CECIL. Figure 4 includes two size of scintillators, i.e. (A) a 12.7 cm in diameter by 17.78 cm long the NE-213 liquid organic scintillator at 4.33 MeVee and (B) a 12.7 cm in diameter by 12.7 cm long one at bias level of 0.45 MeVee.

At the status (A), the results by the SCINFUL-QMD agree with the experimental data below 20 MeV. In the higher-energy region, the SCINFUL-QMD reproduces the tendency of the experimental data. However, the absolute values of the experimental data are larger than the predictions of the SCINFUL-QMD. The total cross sections determine the mean free path in the scintillator, and their values, adopted in the SCINFUL-QMD, are considered to be accurate. The QMD+SDM simulates the nuclear reactions in this energy region adequately. Nevertheless, the experimental data are still larger than the those along the dotted curve computed by the SCINFUL-QMD code at zero level bias. On the other hand, at the status (B), the results by the SCINFUL-QMD generally agree with the experimental data. This agreement is kept even in the higer-energy region within 20 %. Hence we may say that the absolute values in reference 13 may contain some unclarified effect.

The results by the CECIL code are larger than those by the SCINFUL-QMD. This can be explained by the fact that the CECIL employs too large a cross section of $C(n, x\alpha)$ to reproduce the light output. The SCINFUL-QMD code shows an increase in detection efficiencies above about 300 MeV. This increase is caused by the production of charged pions and rising total cross sections for ^{12}C. In contrast, the detection efficiencies by the CECIL indicates no increase in this region. The reason is that the code neglects charged pion production and assumes that the total cross sections are constant above 200 MeV.

IV. Conclusion

The SCINFUL-QMD code was developed to calculate neutron detection efficiencies up to 3 GeV. The CECIL code assumes that total cross sections are constant above 200 MeV and neglects pion production reaction. The SCINFUL-QMD code has the total cross sections up to 3 GeV and considers pion production, and the effect by the modification is observed as an increase in the detection efficiencies above 300 MeV. Accordingly, we consider that the detection efficiencies by the SCINFUL-QMD code are more accurate than those by the CECIL code.

At energies of 80 to 150 MeV, the reaction cross sections adopted in the SCINFUL-QMD were extrapolated from those in the original SCINFUL code. To obtain further accuracy, evaluation of the cross sections up to 150 MeV is required.

The results by the SCINFUL-QMD code were compared with the experimental data. For a 12.7 cm in diameter by 12.7 cm long NE-213, the detection efficiencies by the code agree with the experimental data. For a 12.7 cm in diameter by 17.78 cm long the NE-213, however, the experimental data are considerably larger than the predictions by the SCINFUL-QMD and the CECIL in the high energy region above 40 MeV. Additional experiments are expected.

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