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**SCINFUL-QMD : Monte Carlo Based Computer Code to  
Calculate Response Function and Detection Efficiency of a  
Liquid Organic Scintillator for Neutron Energies up to 3 GeV**

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SCINFUL-QMD: Monte Carlo Based Computer Code to Calculate Response Function and Detection  
Efficiency of a Liquid Organic Scintillator for Neutron Energies up to 3 GeV

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The Monte Carlo based computer code SCINFUL-QMD has been developed to evaluate response function and detection efficiency of a liquid organic scintillator for neutrons from 0.1 MeV to 3 GeV. This code is a modified version of SCINFUL that was developed at Oak Ridge National Laboratory in 1988, to provide a calculated full response anticipated for neutron interactions in a scintillator. The upper limit of the applicable energy was extended from 80 MeV to 3 GeV by introducing the quantum molecular dynamics incorporated with the statistical decay model (QMD+SDM) in the high-energy nuclear reaction part. The particles generated in QMD+SDM are neutron, proton, deuteron, triton,  $^3\text{He}$  nucleus, alpha particle, and charged pion. Secondary reactions by neutron, proton, and pion inside the scintillator are also taken into account. With the extension of the applicable energy, the database of total cross sections for hydrogen and carbon nuclei were upgraded. This report describes the physical model, computational flow and how to use the code.

Keywords: SCINFUL-QMD, Response Function, Detection Efficiency, Liquid Organic Scintillator, NE213, BC501A, High-energy Neutron, Quantum Molecular Dynamics, Monte Carlo.

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SCINFUL-QMD: 液体有機シンチレータに対する中性子エネルギー3GeV までの  
応答関数および検出効率計算コード

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(2006年10月3日受理)

高エネルギー中性子に対する液体有機シンチレータの応答関数および検出効率を計算するために、シンチレータ中の3次元粒子輸送を模擬できるモンテカルロコード SCINFUL-QMD を開発した。本コードは、1988年に米国オークリッジ国立研究所にて開発された SCINFUL コードを高エネルギー領域に拡張したものであり、適用エネルギー上限は 3GeV である。150MeV 以上の高エネルギー核反応計算には、量子分子動力学 (QMD) に統計崩壊模型 (SDM) を接続した核反応模型 QMD+SDM を採用した。QMD+SDM で考慮している放出粒子は、中性子・陽子・重陽子・三重陽子・ $^3\text{He}$  原子核・アルファ粒子・パイオンである。このうち、中性子・陽子・パイオンに関しては、シンチレータ内での二次反応も考慮した。さらに、適用エネルギー上限の拡張に伴い、有機シンチレータを構成する水素および炭素原子核の全断面積データを更新した。本レポートでは、SCINFUL-QMD コードの物理モデル、計算の流れとともに、使用方法について記す。

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## 1. Introduction

Liquid organic scintillators, such as NE213 and BC501A types, have been widely used for neutron spectroscopy, since they have comparatively high detection efficiency and a good property for the discrimination of neutrons from gamma rays. In neutron spectroscopy by the use of the liquid organic scintillator, response functions and detection efficiencies are indispensable to determine the absolute magnitude and shape of the energy spectrum.

In the field of neutron engineering, the energy of interest is up to about 3 GeV because the ratio between income and outgoing energies for neutron production becomes worse in higher energy region. Therefore, the upper energy targeted in the neutron spectroscopy is also set around 3 GeV. Many experiments have been performed to determine the response function and detection efficiency of liquid organic scintillators in the neutron energies below 80 MeV. Experimental data for higher energy neutrons ( $> 80$  MeV), however, are very scarce due to the experimental difficulty to produce the monoenergetic neutron beam and the impracticality of measuring them for various shapes of the scintillators in various neutron energies. For these reasons, the response function and the detection efficiency have been estimated using Monte Carlo based computer codes.

The SCINFUL<sup>1)</sup> and the CECIL<sup>2)</sup> codes have been used for these purposes. Although SCINFUL is known to reproduce the experimental data well, the upper limit of incident neutron energy is set at 80 MeV by the restriction of the physical model and the nuclear data compiled in the code. On the other hand, CECIL is capable of calculating the response function up to a few giga-electron volts, and has been used for estimation above 80 MeV. While nuclear reactions caused by high-energy-neutron incidence into the scintillator are very complex, the physical model employed in CECIL is quite simplified, *e.g.* the number of reaction channels in CECIL is less than that in SCINFUL, the light outputs are considered only for proton and alpha particle, and the data of cross sections above 200 MeV are constant. It is therefore of great interest to develop a new Monte Carlo based computer code that is applicable to the calculation up to 3 GeV.

The quantum molecular dynamics (QMD) model<sup>3)</sup> was developed in 1980s to describe the behavior of nucleons and mesons inside a nucleus, and the formation of various fragments. The model successfully simulates the direct process of nuclear reaction, and the statistical decay model (SDM)<sup>4)</sup> is capable of treating the sequential fission and evaporation processes. Thus, we incorporated QMD+SDM model<sup>4)</sup> into SCINFUL as a high-energy nuclear-reaction part to extend the upper limit of the code from 80 MeV to 3 GeV. This modified version of SCINFUL was named SCINFUL-QMD<sup>5)</sup>.

In this report, we describe the overview of the SCINFUL-QMD code in Section 2. Section 3 is devoted to introducing the physical models in the code. The comparison with the experimental results and the predictions of CECIL are shown in Section 4. In Section 5, we give the user guide for installation of the code, preparation of input data, execution of the calculation, and examples of output files. The summary of this report is given in Section 6.

## 2. Overview of Code

SCINFUL-QMD is designed for a liquid organic scintillator of NE213 and BC501A types in the shape of a right circular cylinder. The code simulates the scintillator response to neutrons from 0.1 MeV to 3 GeV using the Monte Carlo technique.

Before introducing the detailed algorithm of the program, we first review some basic concepts of the neutron detection with an organic scintillator. It should be noted that the neutron does not stimulate the scintillator directly. A neutron must interact with the scintillation material by producing at least one charged particle. Figure 1 is schematic illustrations of neutron detection. For neutrons below 10 MeV, the detection is primarily caused by a neutron scattering with a hydrogen nucleus, and a subsequent interaction of the recoil proton with the scintillation material. These interactions make the molecules excited, and photons are emitted from the molecules via de-excitation processes. Sequentially, the photons are converted to photoelectrons at the photocathode of a photomultiplier tube (PMT) as exhibited schematically in Figure 1 (a).

Figure 1 (b) shows another method of neutron detection; it is especially observed in the energy region above a few tens of MeV. When a neutron causes nuclear reactions inside the carbon target, one or more charged particles can be generated. These charged particles stimulate the scintillation material to produce photons.

The organic scintillator schematically presented by Figure 1 (c) consists of the hydrogenous radiator and the carbon target. A neutron is detectable with the processes described above in a wide neutron energy range. The output pulses from the PMT do not have a unique relationship with the incident neutron energy. They have a fluctuation of the pulse height from nearly zero to the maximal value even for the same energy neutrons because the types and energies of the charged particles depend on the types of nuclear reaction and some particles may escape from the scintillator with some energy.

SCINFUL-QMD simulates the behavior of the particles inside a scintillator considering the geometrical configuration, and gives the expected distribution of the light outputs from PMT.

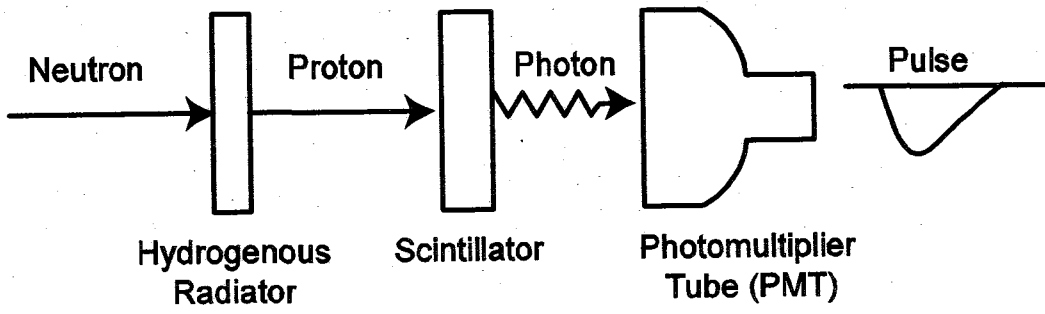
### 2.1 Main Routine

The computational flow of a main routine in SCINFUL-QMD is shown in Figure 2. The first part of the calculation is dedicated to sampling of the first collision of the incident neutrons. The interaction probability derived from the total cross section determines whether the first collision takes place inside the scintillator. If the interaction occurs, the type of nuclear reaction is chosen according to the reaction cross section for each channel. All information of the interaction is recorded for the sequential steps.

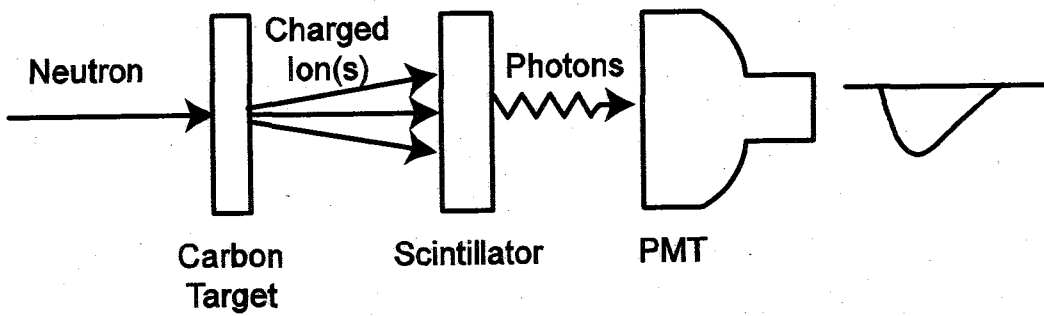
The second part is a main part of the calculation. The energetics and kinematics of the nuclear reaction chosen at the first part of the calculation are computed here using the physical models described in the Section 3. Once the simulation of the reaction is completed, the transport process just described above



(a) Proton Recoil:



(b) Interaction with Carbon:



(c) Combined

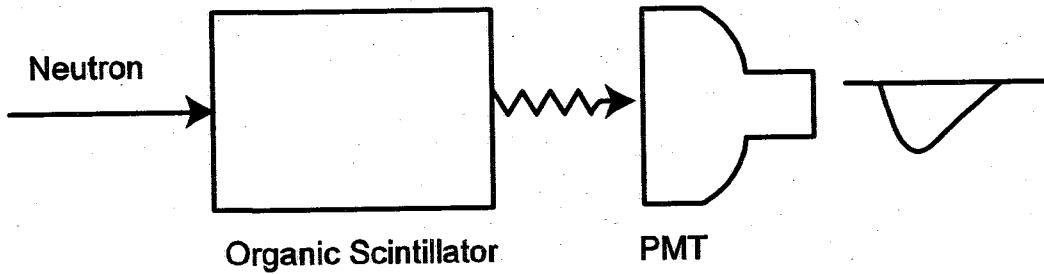


Figure 1. Schematic illustration of neutron detection. This figure is cited from Ref. 1

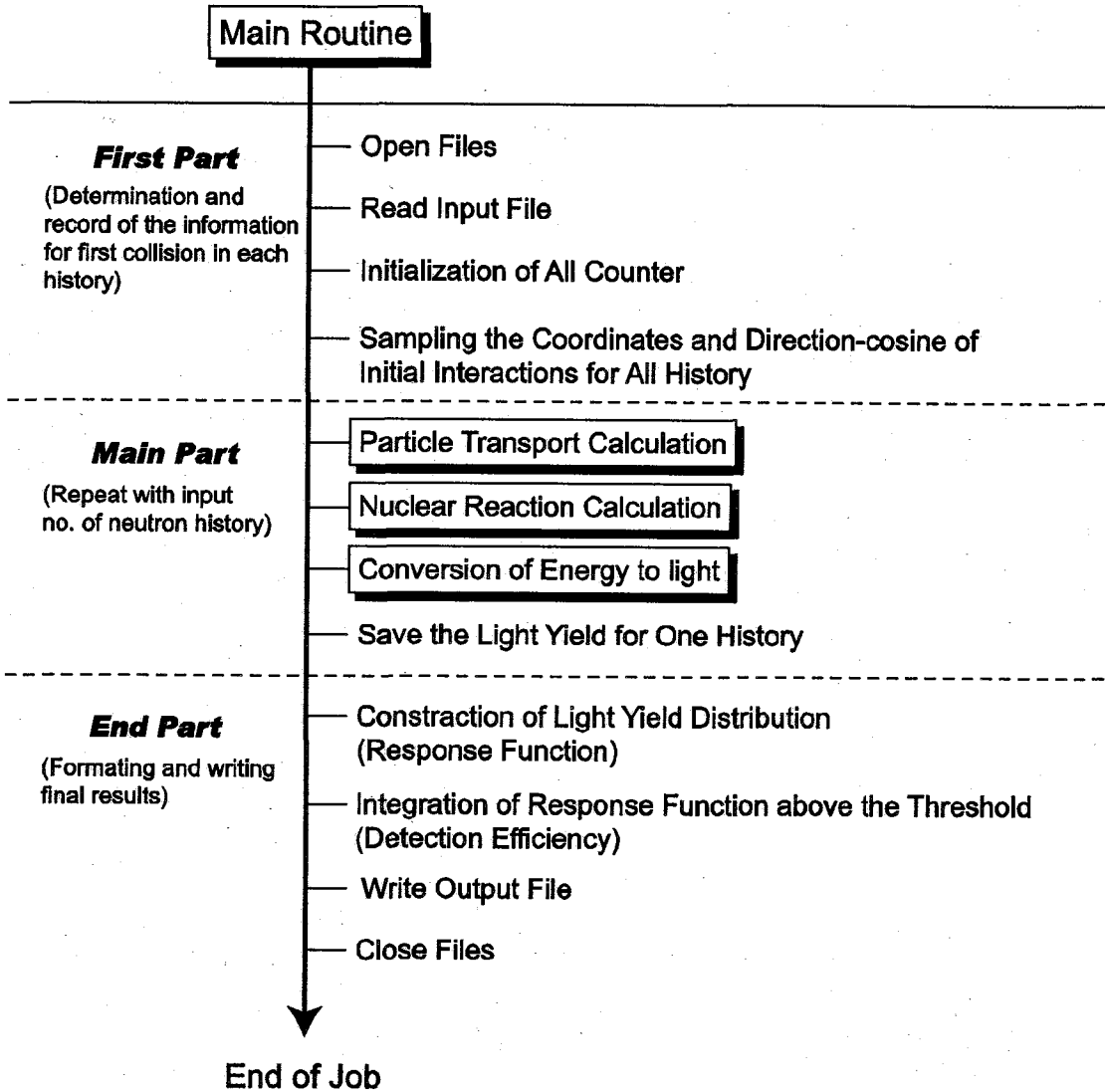


Figure 2. Flow of main routine in SCINFUL-QMD

is retried for the secondary particles generated by the primary reaction; namely to determine a new probability for interaction, determine a new path length to the surface of the scintillator along the scattered path, and determine whether an interaction takes place inside the scintillator. If an interaction occurs, the program computes the energetics and kinematics and again judges the further interaction.

The last part of the calculation is devoted to formatting and outputting of the simulation results. The light outputs for each history are scored in the corresponding light-unit bin, and construct the response function. By integrating the response function above the bias defined by user, the neutron detection efficiency is also obtained.

## 2.2 Particle Transport Calculation

In SCINFUL-QMD, the transport and reaction processes are considered for not only incident neutrons but also the emitted particles from nuclear reaction. The extra-nuclear cascade inside the scintillator is examined for neutrons, protons and charged pions. The flight path of the particle is determined by Monte Carlo method with the total cross section for hydrogen and carbon nuclei. The algorithm of the particle transport calculation is explained below.

Figure 3 shows the flow of the particle transport calculation. Microscopic cross sections for hydrogen and carbon nuclei,  $\sigma_H$  and  $\sigma_C$ , are sampled from the database up to 3 GeV according to the type of the particle and its kinetic energy. Figure 4 depicts the data of cross sections employed in the code together with the experimental data<sup>6-9)</sup>. Macroscopic cross sections,  $\Sigma_H$  and  $\Sigma_C$ , are derived by the following equation,

$$\Sigma_H = N_H \sigma_H, \quad \Sigma_C = N_C \sigma_C$$

where  $N_H$  and  $N_C$  indicate atom density of hydrogen and carbon, respectively. The values for hydrogen and carbon are  $4.833 \times 10^{-2}$  and  $3.984 \times 10^{-2}$  (atoms/barn)/cm in the NE213-type liquid organic scintillator. The probability of the interaction with hydrogen is expressed as,

$$P = \frac{\Sigma_H}{\Sigma_H + \Sigma_C}$$

The probability to go forward a certain distance without any interactions is given as,

$$D = \exp(-\Sigma_t L)$$

where  $\Sigma_t$  means the total macroscopic cross section, *i.e.* the sum of  $\Sigma_H$  and  $\Sigma_C$ , and  $L$  is the path length from

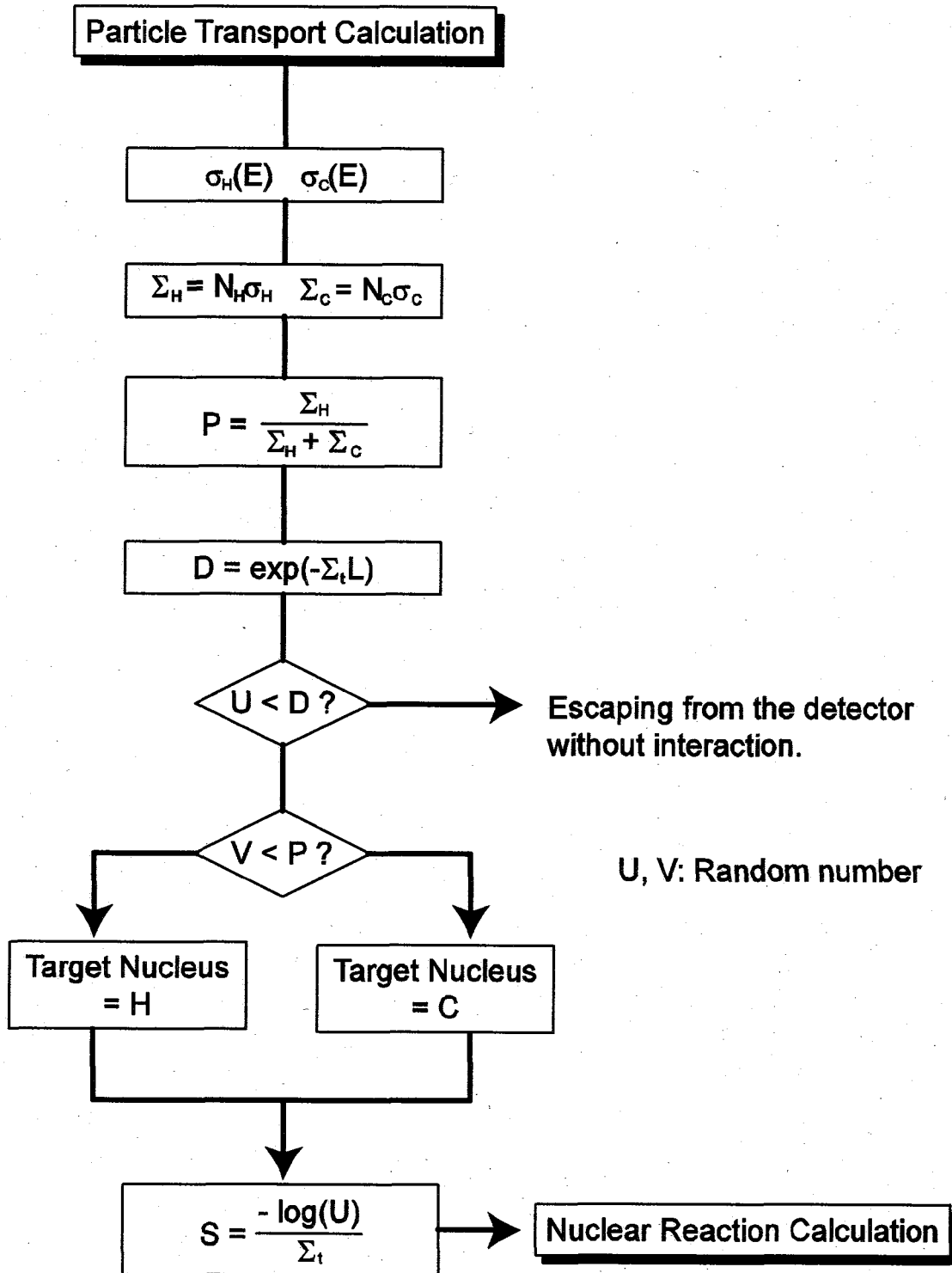


Figure 3. Flow of particle transport calculation

the current position to the surface of the scintillator on the scattered direction.

The next step is the sampling whether the interaction occurs or not by use of the probability  $D$  and a random number  $U$ . In the case of occurring interaction, the determination of the target nucleus and the path length to the interaction spot is taken place. The probability  $P$  is used to determine the target nucleus together with a new random number  $V$ . The path length to the interaction spot  $S$  is given as the following expression,

$$S = \frac{-\log(U)}{\sum_i}$$

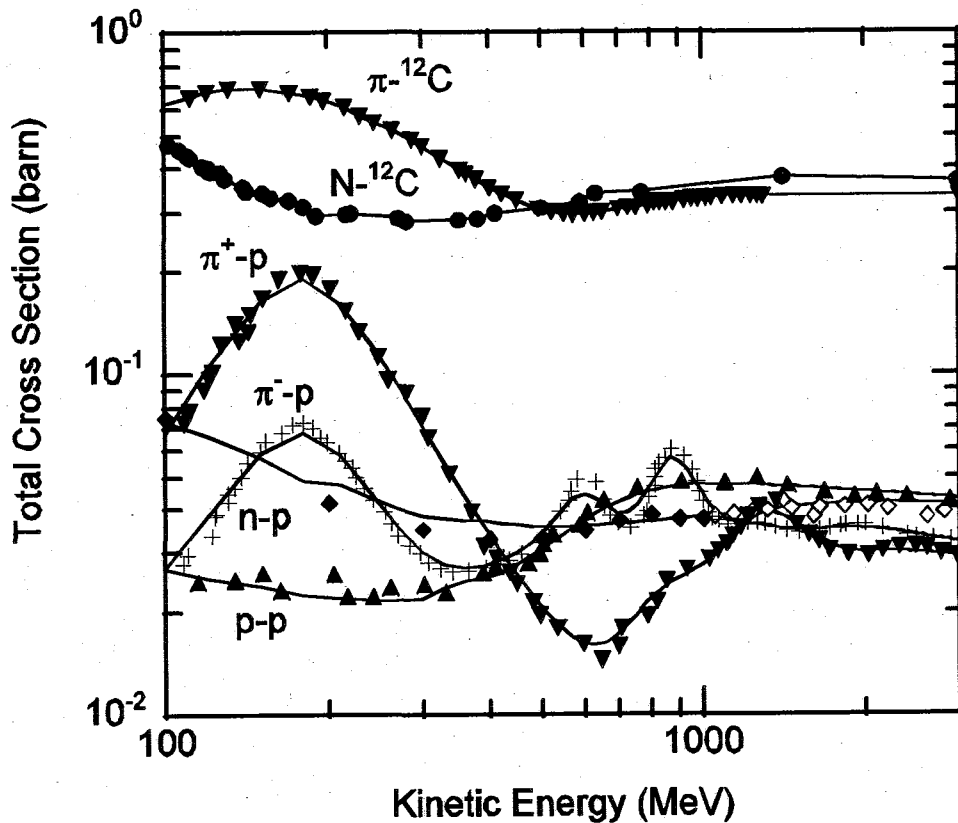


Figure 4. Total cross sections for hydrogen and carbon up to 3 GeV. Solid lines indicate the values adopted in SCINFUL-QMD. Marks express the experimental data cited from Ref. 6-9. N denotes a nucleon

2.3 Nuclear Reaction Calculation

The flow of the nuclear reaction calculation is shown in Figure 5. When a neutron enters into the scintillator and sequentially causes a collision, the routines for the nuclear reaction calculation are called. SCINFUL-QMD has two types of physical model. The QMD+SDM model is chosen to simulate the nuclear reaction if the kinetic energy  $E$  is larger than the switching energy  $E_{swt}$ , and when the  $E$  is smaller than the  $E_{swt}$ , the SCINFUL model is implemented. The details of these models are described in Section 3. The default value of the switching energy is set at 150 MeV, and this value can be easily changed by modifying source files. When the kinetic energy of neutron decreases below the cut-off energy defined in the input file, the history for one neutron is terminated.

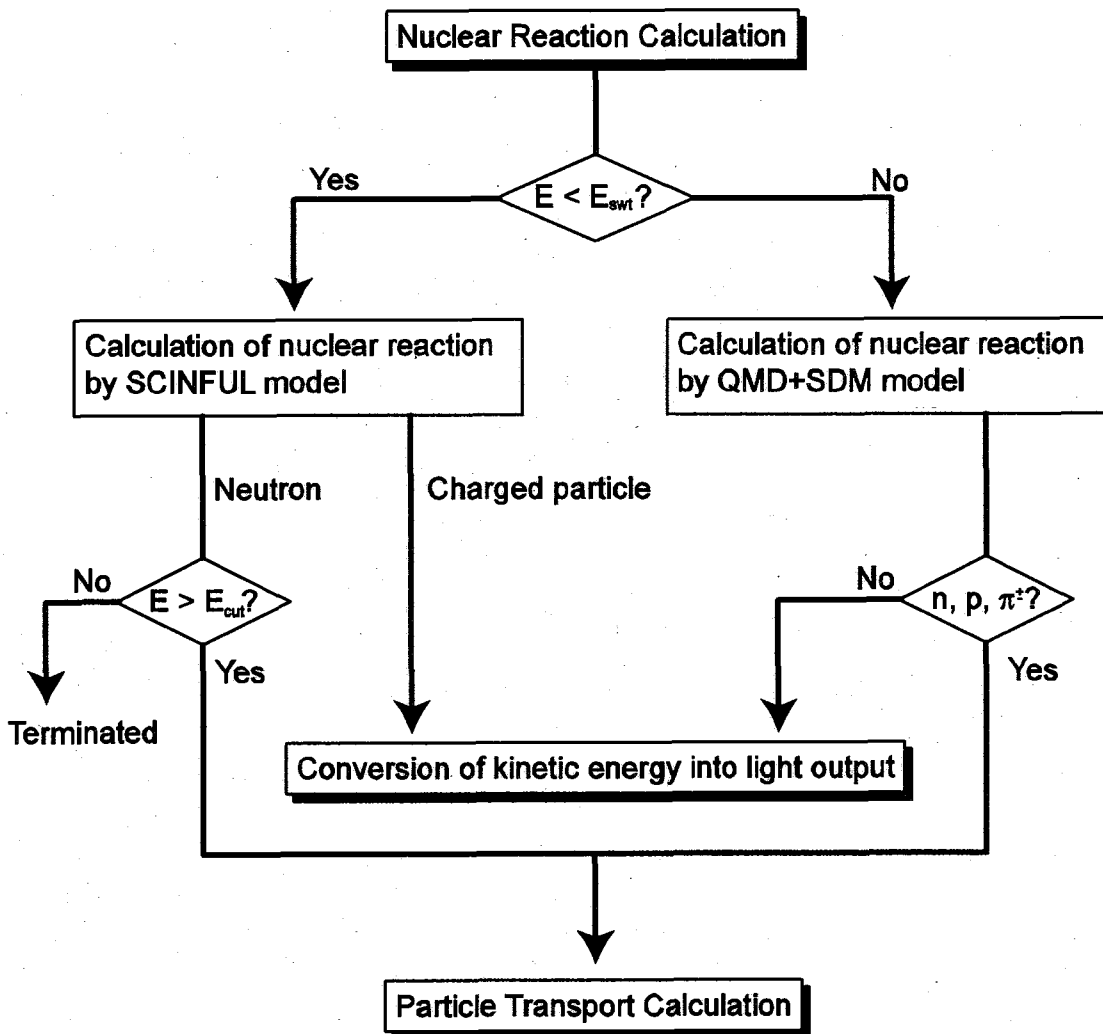


Figure 5. Flow of nuclear reaction calculation

## 2.4 Conversion of Kinetic Energy into Light Output

The final phase of the neutron detection process is the absorption of the energy of charged particles and the concomitant creation of fluorescent light by excitation of molecules of the scintillation material. Because the fluorescence and the quenching processes inside the scintillator are very complicate, the quantification of the light output remains as one of the least understood parts of the neutron detection process. In the simulation, the light outputs are derived directly by the kinetic energies of charged particles.

In order to develop the new function to convert the kinetic energy into the light output, we have measured the light outputs for proton, deuteron, triton,  $^3\text{He}$  nucleus, and alpha particle. The detail of the experiment is described elsewhere<sup>10)</sup>. SCINFUL-QMD employs this light-output function. In addition, the light-output database of the original SCINFUL<sup>1)</sup> and the light-output function for proton and deuteron proposed by Nakao *et al.*<sup>11)</sup> are also selectable. The values for deuteron in the SCINFUL database are revised by Meigo *et al.*<sup>12)</sup> Figures 6 through 10 show the light outputs of the charged particles compiled in SCINFUL-QMD.

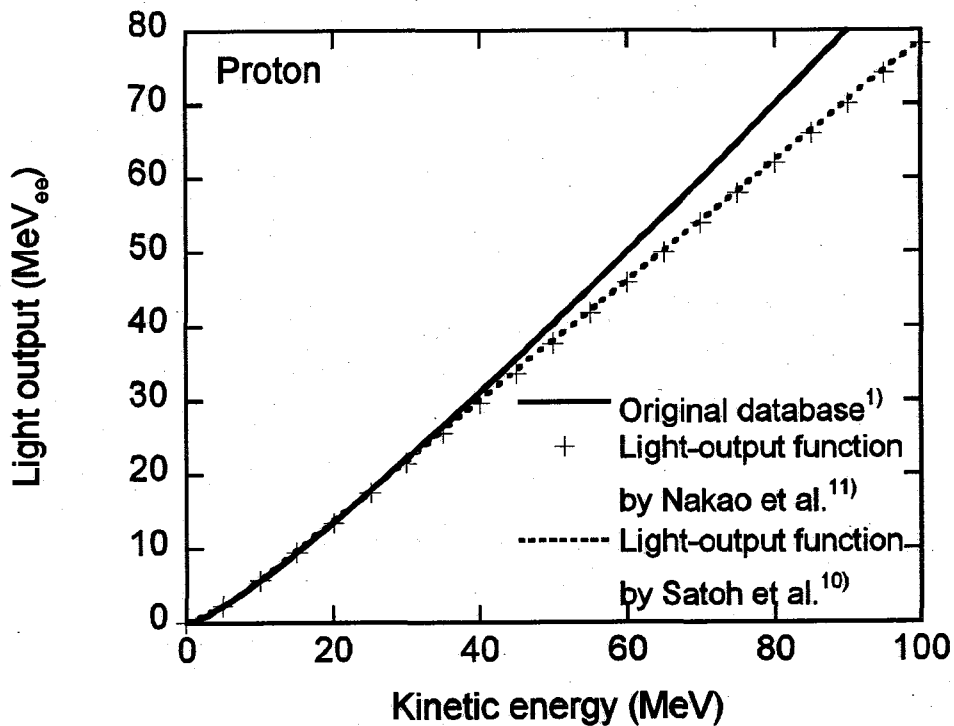


Figure 6. Light output of proton

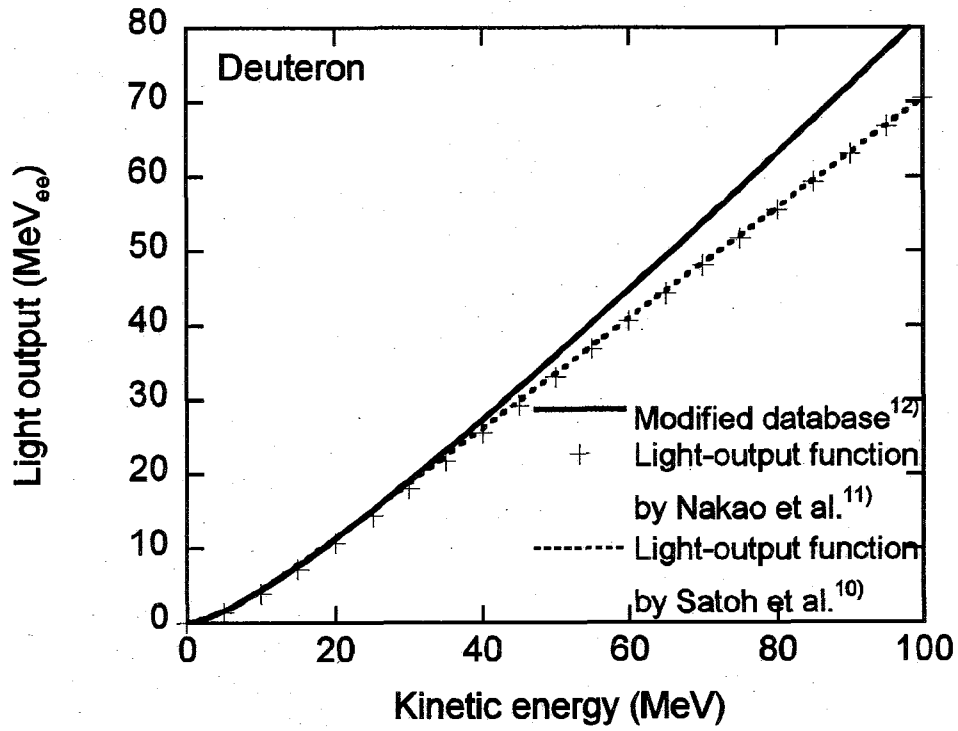


Figure 7. Light output of deuteron

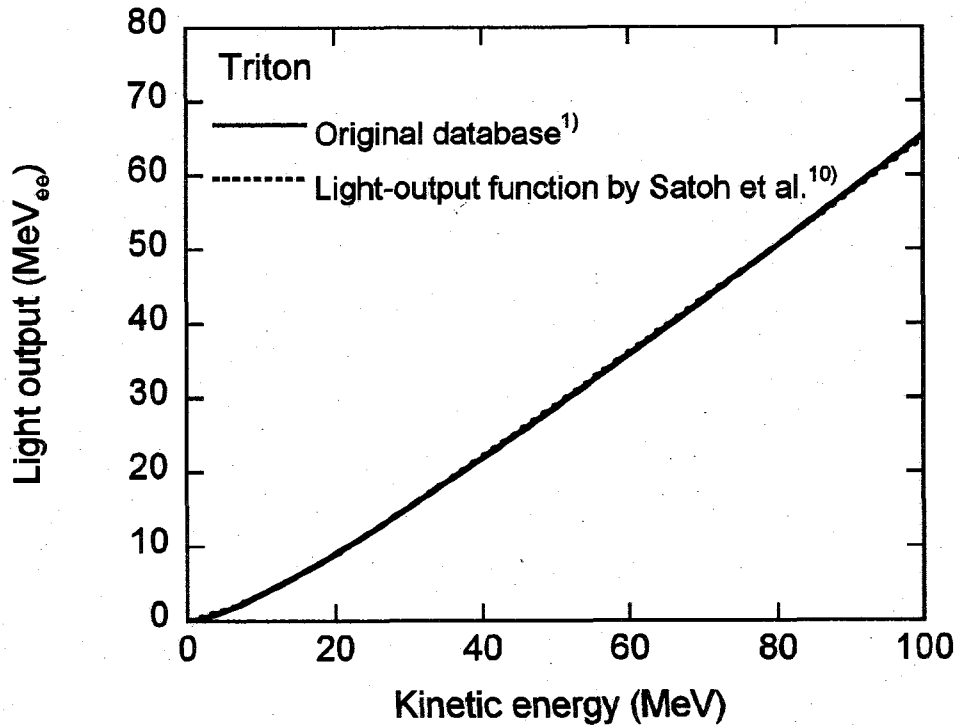


Figure 8. Light output of triton



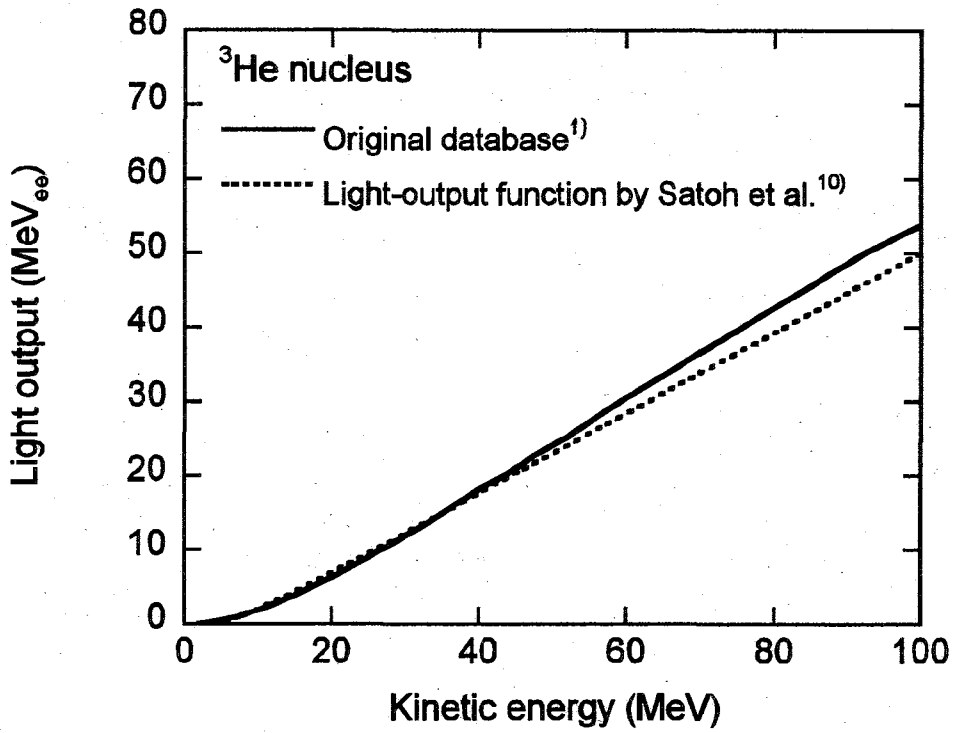


Figure 9. Light output of <sup>3</sup>He nucleus

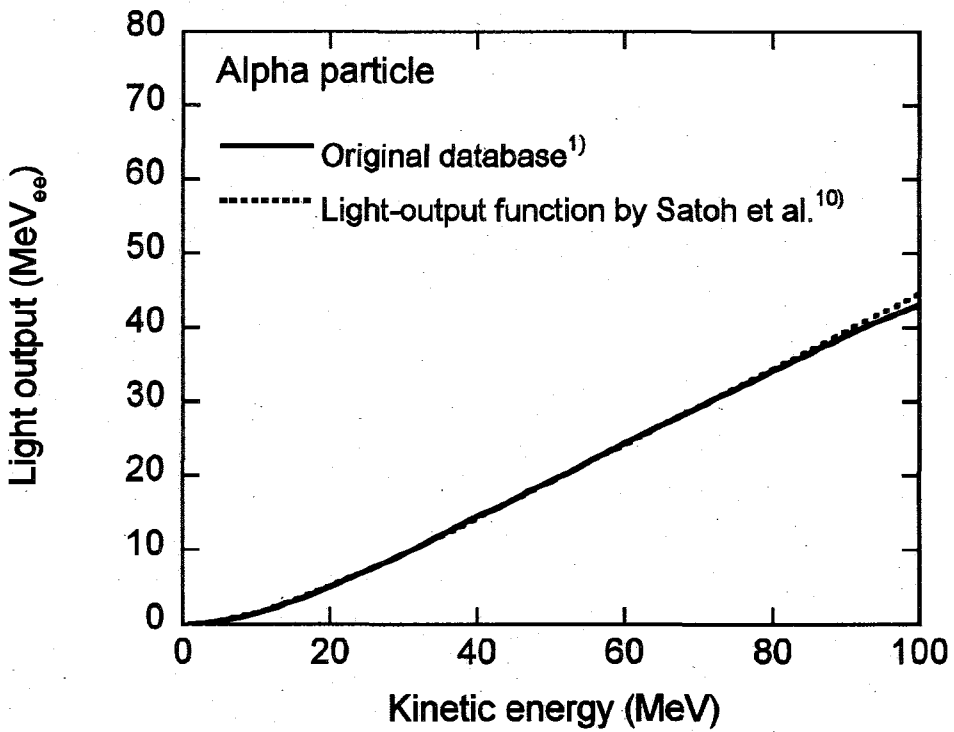


Figure 10. Light output of alpha particle

### 3. Physical Model in the Code

SCINFUL-QMD employs two types of physical model, SCINFUL and QMD+SDM, to reproduce the various nuclear reactions in wide energy range. These models are selected according to the kinetic energy of incident neutrons. In this section, we give a brief description about the physical models of the SCINFUL-QMD code. The details are described elsewhere<sup>1,4)</sup>.

#### 3.1 SCINFUL Model

The physical model of the original SCINFUL code<sup>1)</sup>, here we refer as SCINFUL model, is based on multibody-breakup theory. In the SCINFUL model, the simulation of nuclear reaction is started from 11 initial reaction channels listed in Table 1, and follows the sequential decay process of the residual nucleus. In Table 1, the initial reaction channels in CECIL<sup>2)</sup> are also listed. It is obvious that the SCINFUL model treats more initial channels than those employed in CECIL. To determine the initial type of reaction, cross section data are utilized. The energy dependency of the cross sections for each reaction channel is shown in Figure 11.

Table 1. List of initial reaction channels in SCINFUL and CECIL

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

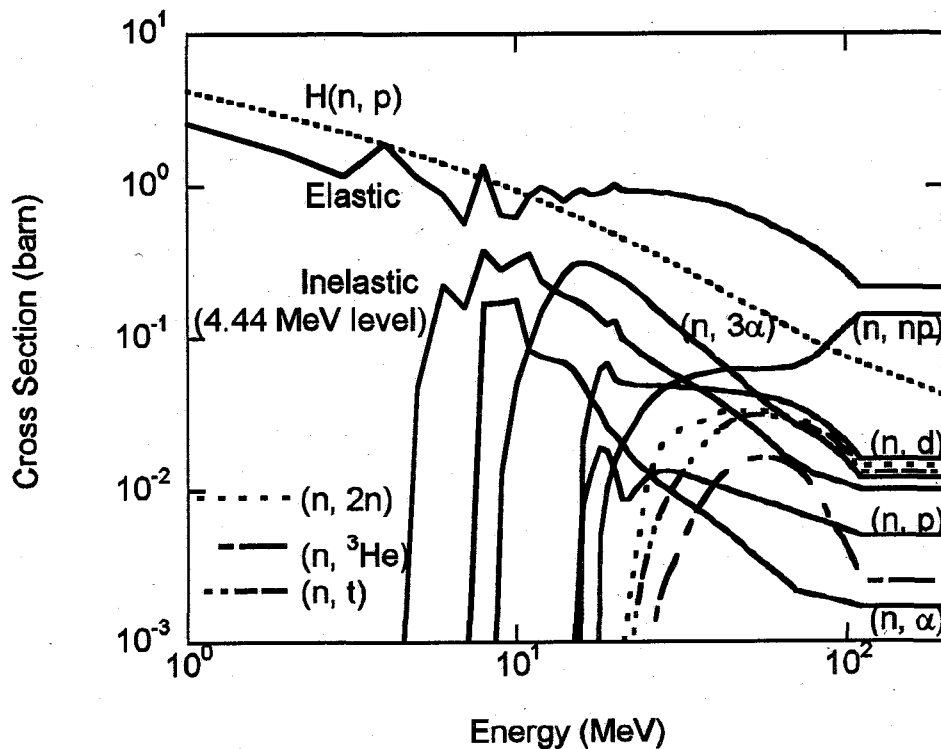
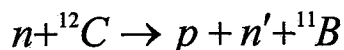


Figure 11. Reaction cross sections adopted in SCINFUL model

In order to explain the concept of the SCINFUL model, we use the  $n+^{12}\text{C} \rightarrow p+n'+^{11}\text{B}$  reaction as a typical example.



- I:  $n+^{12}\text{C} \rightarrow ^{13}\text{C}$  (Compound nucleus)
- II:  $^{13}\text{C} \rightarrow p+^{12}\text{B}^*$  (Excited)
- III:  $^{12}\text{B}^* \rightarrow n+^{11}\text{B}$  (Ground state) .or.  $\rightarrow n+^{11}\text{B}^*$  (Excited)
- IV:  $^{11}\text{B}^* \rightarrow \gamma+^{11}\text{B}$  (If possible)

At the first step, an incident neutron makes an excited compound nucleus with  $^{12}\text{C}$  nucleus. Then, the compound nucleus breaks up to a proton and an excited  $^{12}\text{B}$  nucleus. The total available energy of this first decay process is limited, because the  $^{12}\text{B}^*$  nucleus must retain a sufficient energy to cause the subsequent decay by a neutron emission. The outgoing proton and the recoil nucleus share the available energy. The

kinetic energy of the outgoing proton is determined using Monte Carlo technique with the energy distribution evaluated by the TNG code<sup>13)</sup>, which is a multistep statistical code based on the Hauser-Feshbach theory, and the energy of the corresponding recoil nucleus is also deduced.

The next step is to compute the decay process of the excited  $^{12}\text{B}$  nucleus to a neutron and a  $^{11}\text{B}$  nucleus. The energetics and kinematics are determined in the same manner just described above, except for the total available energy and the probability distribution. If the  $^{11}\text{B}$  nucleus is able to shift into a more stable state by emitting gamma rays, the process is also executed in the code.

We especially mention that the data of the total and the angular differential cross sections for n-p scattering were revised by Meigo<sup>12)</sup>. Figure 12 shows the angular differential cross section for the n-p scattering. The original SCINFUL calculates the total n-p cross-section using the Gammel formula<sup>14)</sup>, and the calculated values become lower in above 50 MeV with increasing neutron energy. Therefore, Meigo replaced the total n-p cross section with the values of the phase-shift analysis by Arndt<sup>15)</sup> which reproduce the experimental data<sup>16-18)</sup> better than the original.

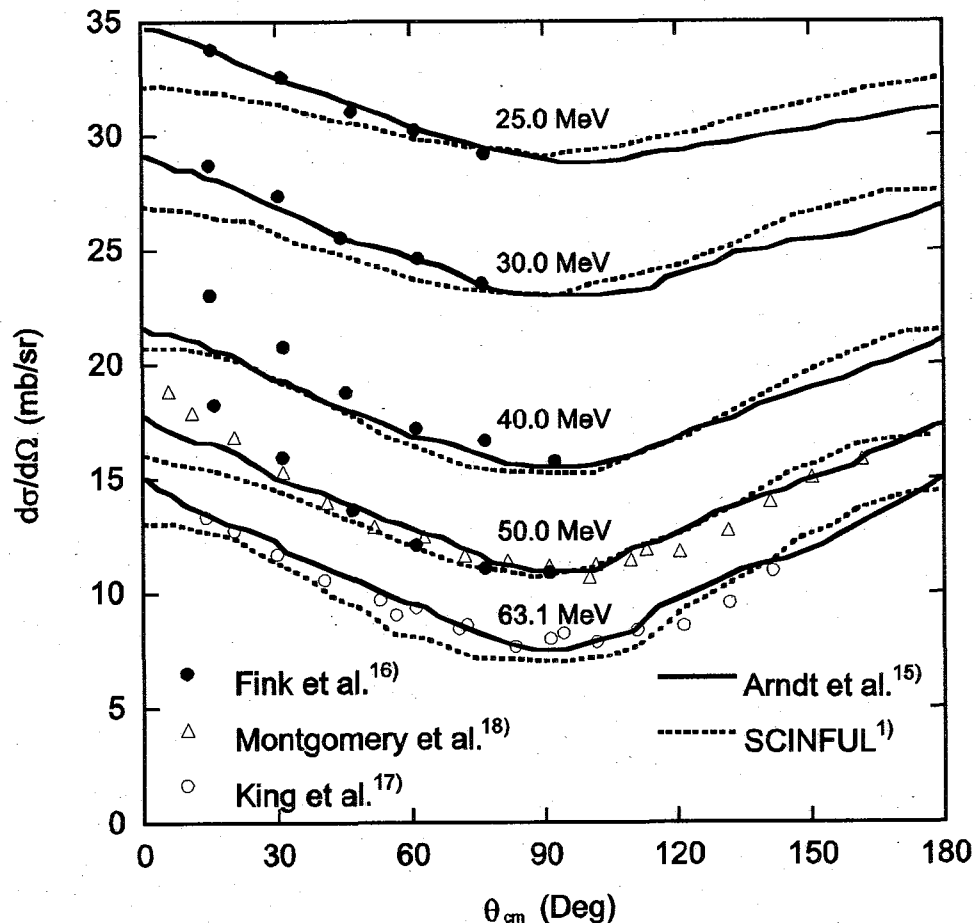


Figure 12. Angular differential cross sections for n-p scattering compared with the experimental data<sup>16-18)</sup> and phase-shift analysis given by Arndt<sup>15)</sup>

### 3.2 Quantum Molecular Dynamics (QMD) Model

The Quantum Molecular Dynamics (QMD) model<sup>3,4)</sup> is based on a microscopic dynamical n-body theory tailored to describe the formation of fragments in various nuclear reactions with a unified way. The concept of QMD model is quite similar to the classical Molecular Dynamics (MD) approach which is widely used in chemistry and astrophysics. "Quantum" in the name of QMD means a quantal extension for conventional MD.

Nucleons are represented as Gaussian-wave packets in position and momentum space. The behavior of each nucleon is described by Newtonian equations along the time evolution considering the mean-field potential in the nucleus. In the QMD model incorporated into the SCINFUL-QMD code, the Skyrme, the Coulomb, and the symmetry forces are included as for the effective potential<sup>4)</sup>. The time evolution of the system is affected by not only the Newtonian equation but also the two-body collision term. Since QMD simulation neglects the asymmetry of the wave function, the fermionic nature of the nucleons can not be treated correctly. Whenever a collision occurs, Pauli Exclusion Principle is mimicked by estimating the probability that the other nucleons already occupy the final phase spaces of the scattering nucleons. All channels included in the collision term are listed in Table 2, where  $B$  and  $N$  denote a baryon and a nucleon, respectively. Only one-pion-production channels are considered, because the contribution of two or more pions production is relatively low in the energy region up to 3 GeV.

Table 2. List of collision channels treated in QMD model

No.	collision channels		
1.	$B_i + B_j$	$\longrightarrow$	$B_i + B_j$
2.	$N + N$	$\longrightarrow$	$N + \Delta$
3.	$N + \Delta$	$\longrightarrow$	$N + N$
4.	$N + N$	$\longrightarrow$	$N + N^*$
5.	$N + N^*$	$\longrightarrow$	$N + N$
6.	$N + \pi$	$\longrightarrow$	$\Delta$
7.	$N + \pi$	$\longrightarrow$	$N^*$
8.	$\Delta + \pi$	$\longrightarrow$	$N^*$

### 3.3 Statistical Decay Model (SDM)

At the end of the dynamical stage of the nuclear reaction, the QMD simulation yields many fragments, which are normally in highly excited states. As the next stage of the reaction, the decay process of these excited fragments is taken place. This stage is well separated from dynamical one with their time scales, and dominated by quantum phenomena. As mentioned above, the QMD method is a semi-classical approach and lacks an ability to trace the Fermi statistics that is essential to deal the quantum phenomena. On account of this, QMD simulation is switched to SDM simulation in typical nuclear reaction times; 100 fm/c.

The SDM<sup>4)</sup> is one of the statistical models based on the Weisskopf-Ewing's formulation to describe the light particle emission from the excited nucleus. The decay probability is derived from Fermi gas model. The emitting particles considered in the SDM model are neutron, proton, deuteron, triton, <sup>3</sup>He nucleus, and alpha particle.

#### 4. Comparisons with Experimental Data and Calculation by Another

The calculation results of SCINFUL-QMD<sup>5)</sup> have been compared with the experimental data<sup>12,19-24)</sup> and the results of the Monte Carlo based computer program CECIL<sup>2)</sup>, which have been widely used to estimate the response of liquid organic scintillators.

This report is devoted to a instruction of SCINFUL-QMD, so the detailed discussion about the physical aspects is detached to the references<sup>5,22)</sup>

##### 4.1 Response Function

The response functions calculated by SCINFUL-QMD were compared with the experimental data.<sup>12,19-22)</sup> In Figures 13, 14 and 15, the detector is an NE213-type liquid organic scintillator with 12.7 cm in diameter and 12.7 cm in thickness. In Figures 16 and 17, the diameter and the thickness of the NE213-type scintillator are 12.4 cm and 12.7 cm, respectively.

SCINFUL-QMD reproduces the experimental data well. Small discrepancies are caused by the poor resolution of detection system in the experiment. The calculation results must be smeared with the consideration of the experimental resolution. The marks depicted in Figures 16 and 17 are obtained from our experiment<sup>22)</sup> performed at the Heavy Ion Medical Accelerator in Chiba (HIMAC) of the National Institute of Radiological Sciences, Japan. By these comparisons, the accuracy of response function calculated by SCINFUL-QMD is verified up to 800 MeV.

##### 4.2 Detection Efficiency

The neutron detection efficiencies calculated by SCINFUL-QMD are shown in Figure 18 along with the experimental data<sup>12,20,23,24)</sup> and the calculation results of CECIL<sup>2)</sup>. Figure 18 includes two size of scintillator, (A) a 12.7 cm in diameter by 17.78 cm in thickness NE213-type liquid organic scintillator at 0.45 MeV<sub>ee</sub> bias setting and (B) a 12.7 cm in diameter by 12.7 cm in thickness one at 4.33 MeV<sub>ee</sub> bias setting.

For both (A) and (B) cases, the results of SCINFUL-QMD agree with the experimental data better than those of CECIL. The CECIL code gives larger values in the whole energy region. This can be explained that the CECIL employs the large cross sections for  $C(n, x\alpha)$  reaction. On the other hand, the SCINFUL-QMD code employs the reliable cross-section data, and represents the production of charged particles, which are directly connected with the light output yields. Hence, the detection efficiencies calculated by SCINFUL-QMD are more reliable than those by CECIL.

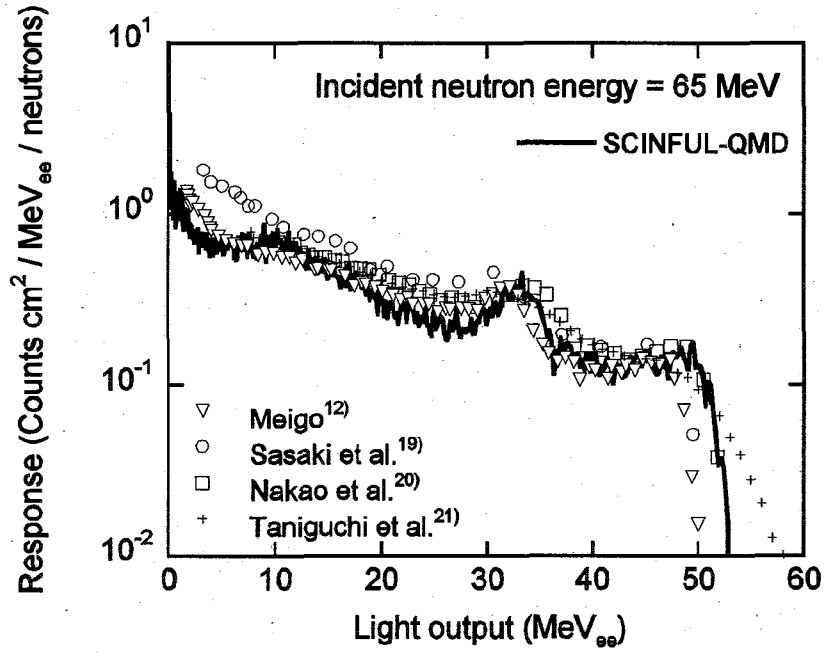


Figure 13. Response functions of the NE213 (12.7 cm in diameter and 12.7 cm in thickness).  
Incident neutron energy is set at 65 MeV

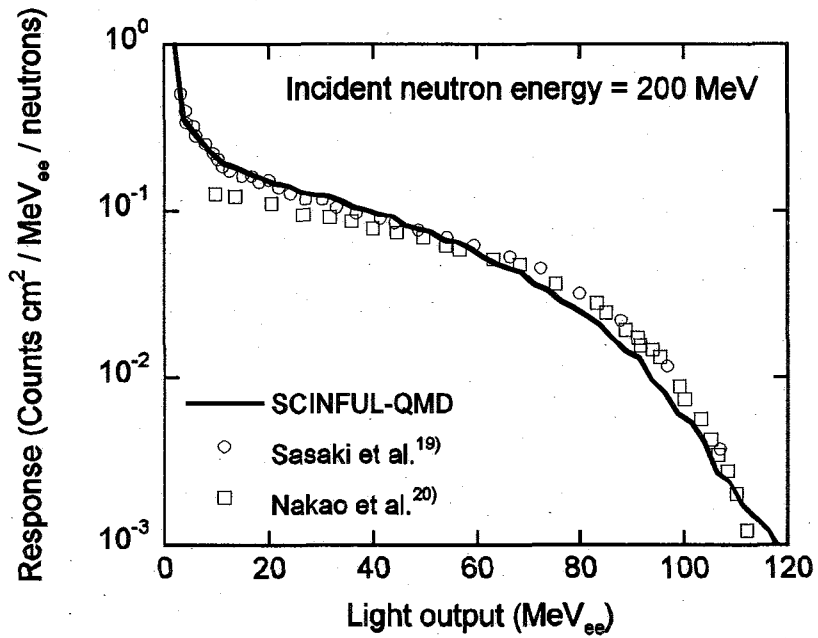


Figure 14. Response functions of the NE213 (12.7 cm in diameter and 12.7 cm in thickness).  
Incident neutron energy is set at 200 MeV



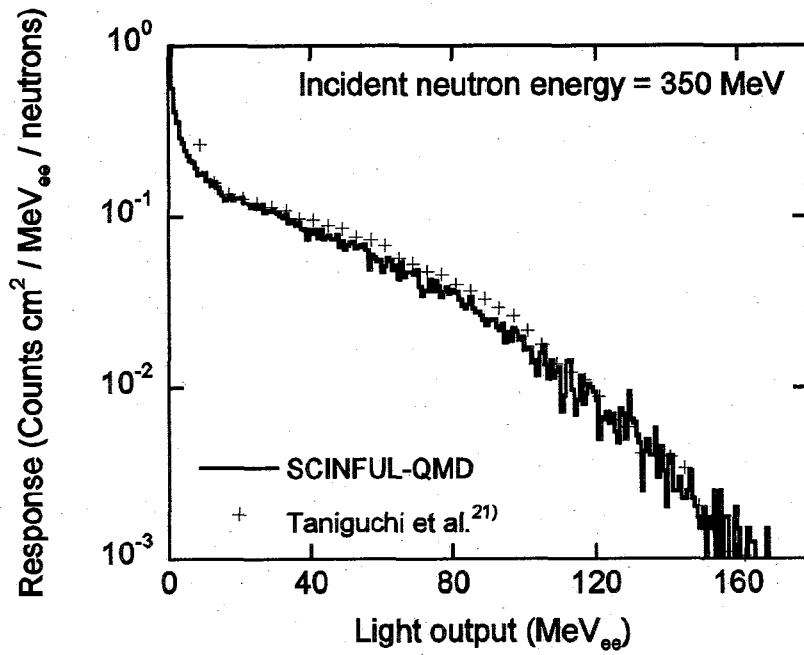


Figure 15. Response functions of the NE213 (12.7 cm in diameter and 12.7 cm in thickness).  
Incident neutron energy is set at 350 MeV

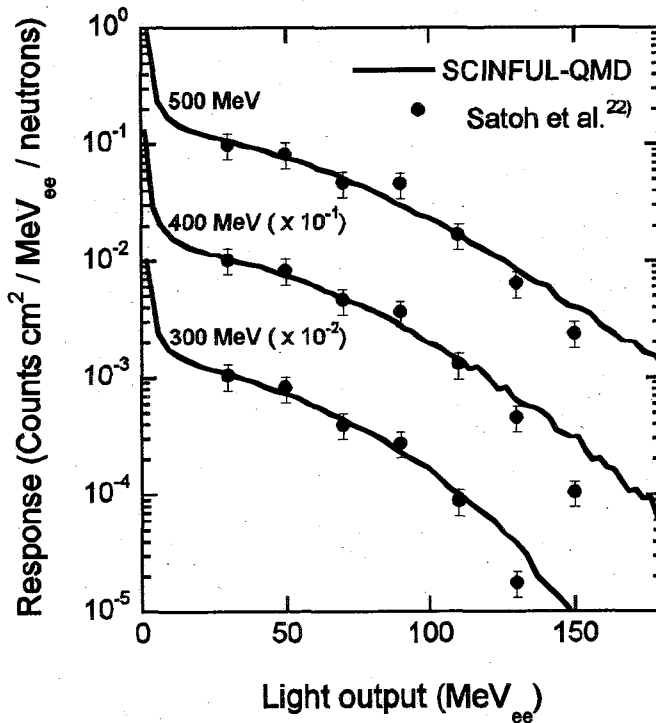


Figure 16. Response functions of the NE213 (12.4 cm in diameter and 12.7 cm in thickness).  
Incident neutron energies are set at 300, 400, and 500 MeV

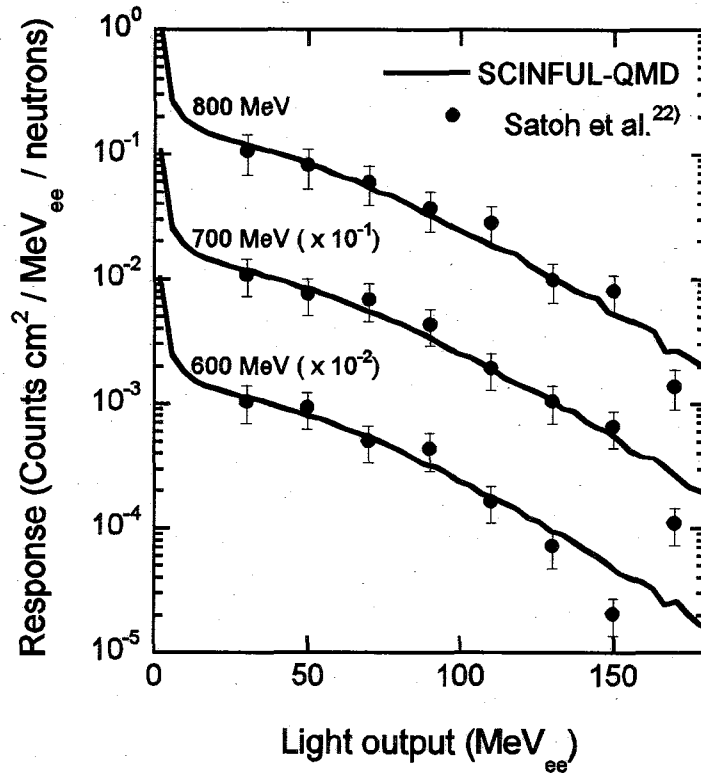


Figure 17. Response functions of the NE213 (12.4 cm in diameter and 12.7 cm in thickness). Incident neutron energies are set at 600, 700, and 800 MeV

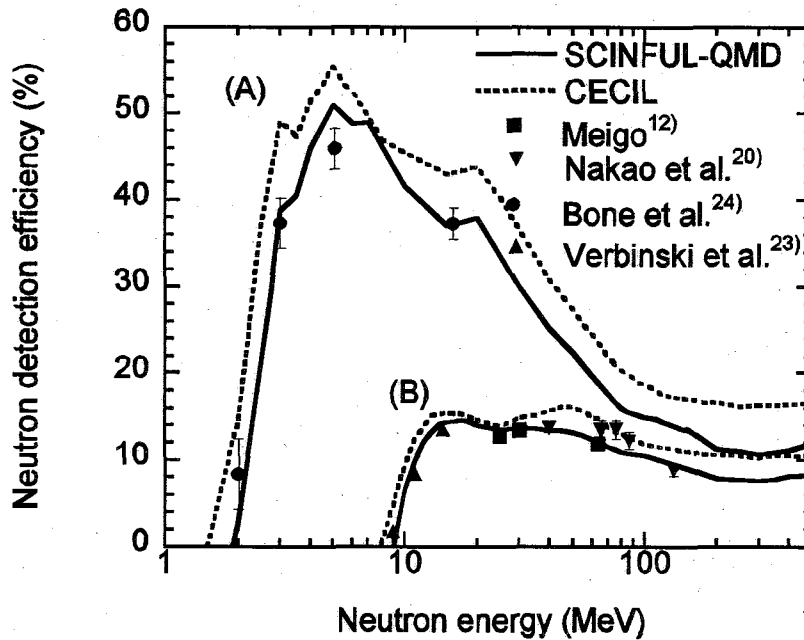


Figure 18. Neutron detection efficiencies. (A) NE213 (12.7 cm in diameter and 17.78 cm in thickness) at 0.45 MeV<sub>ee</sub> bias setting. (B) NE213 (12.7 cm in diameter and 12.7 cm in thickness) at 4.33 MeV<sub>ee</sub> bias setting

## 5. User Guide to SCINFUL-QMD

### 5.1 Installation

The program of SCINFUL-QMD is designed for the computers of Pentium (Intel), Alpha (DEC), and SPARC (Sun Microsystems) systems with a Fortran90 compiler. The SCINFUL-QMD code has been tested on a DEC workstation, Sun workstation, and Pentium personal computer with Windows.

#### 5.1.1 Source and Include Files

In order to compile the SCINFUL-QMD code (current version is 5.00), the following source files and include files are required.

<b>List 5-1 ● Source and include files</b>
--

banker 41.f	gamma.f	mdp.f	s2j.f
choos.f	ground.f	mfield00.f	scin.f
coll00.f	input6.f	param01.inc	sdml.f
conv.f	interact.n.f	param02.inc	sigma3.f
decay4.f	interact2.f	phitsdump4.f	sigma4.f
dedx2.f	jqmd00.f	qmdflt.f	trans2.f
omega.f	kinema4.f	qmdinit.f	ut00.f
effn2.f	legendre.f	qmdout1.f	
energetic.f	main51.f	qmdout2.f	
etol4.f	make file	random.f	

#### 5.1.2 Makefile

An example of the makefile script to build the executable is given below. "make" command on UNIX system may be available. With this script, compiling the source and linking the objects are performed automatically, and an executable file is generated in the same directory.

<b>List 5-2 ● Makefile</b>
----------------------------

```

#/bin/sh
#-----
#   Makefile for SCINFUL -QMD
#-----
FC      = f90
OPT     = -O
LIBES   =
INCLUD ES =
TERGET  = ./scinful-qmd.exe

OBJS = ¥
      main51.o s2j.o qmd init.o jqmd 00.o coll00.o ¥
      mdp.o ground.o mfield00.o qmdd fit.o ¥
      qmd out1.o qmd out2.o sdm1.o utd00.o conv.o ¥
      trans2.o scin.o interact.n.o sigma3.o choos.o ¥
      dedx2.o banker41.o etol4.o kinema4.o effn2.o ¥
      gamma.o decay4.o energetic.o legendre.o ¥
      omega.o input6.o interact2.o phitsdum p4.o random.o

.f.o :
      $(FC) $(OPT) $(INCLUD ES) -c $<

all :$(OBJS)
      $(FC) -o $(TERGET) $(OPT) $(OBJS) $(LIBES)

clean :
      rm -f $(OBJS)

```

### 5.1.3 Execution Line

The execution line of SCINFUL-QMD has the following form,

<b>List 5-3 ● Command line to execute SCINFUL-QMD</b>
---

**scinful-qmd.exe**

where "scinful-qmd.exe" is the executable file of SCINFUL-QMD.

The name of input file is fixed to be "Input.data". The files "Input.data", "scin\_bias.data", "NEW.pch", and "NEW.lpt" are must be in the same directory with the "scinful-qmd.exe".

### 5.2 Format of Input File

The input parameters are prepared in the file labeled "Input.data" in a semi-free-form format.

Numerical values are separated by commas. A sample data set is as follows.

<b>List 5-4 ● Sample of input file</b>
--

```

Card 1:  *Sample input data* SCINFUL-QMD NE213(5"x5")
2:      100000, -213., 0.0080
3:      80.0,0.,0.,0.0 1
4:      12344325
5:      0.0,0.0, -400.0
6:      6.350,12.70,6.350
7:      2, 1, 1, 1
  
```

Interpretation of the parameters in the 7 cards of the input is given below.

#### CARD 1: Title

A title of the calculation is defined. The maximum size is 80 characters. The title is shown on the top of the standard output files.

#### CARD 2: Nhist, Sctyp, Grho

**Nhist** is the number of histories to be traced. The maximum value is set at 1,000,000 (one million). If **Nhist** is greater than the maximum value, the program terminates the calculation. **Sctyp** exhibits a scintillator type with the value of either 110. or 213. for NE110 or NE213, respectively. When the value of -213. is given for **Sctyp**, software Pulse Shape Discrimination (PSD) is executed. In this case, if the photon production event occurs, and the program determines the photon subsequently interacts in the scintillator, the complete history for that neutron is discarded. **Grho** means a light attenuation factor in unit  $\text{cm}^{-1}$  for the light attenuation inside the scintillation material expressed with following equation,

$$Light' = Light * \exp(-Grho * Dist)$$

where *Light'* and *Light* indicate corrected and original light output, respectively. *Dist* is the distance from the interaction spot to the surface of PMT.

#### CARD 3: Esourc, E1, T, Ecutoff

Neutron source energy information is defined in this card. If T equals zero, **Esourc** means the energy of monoenergetic neutron source. If T is negative, the neutron energies are chosen from a uniform distribution between **E1** and **Esourc**. If T is positive, T means the Maxwellian temperature used for choosing the neutron energies between **E1** and **Esourc** from a Maxwellian distribution. **Ecutoff** is the

low-energy bound for the colliding neutron in the scintillator. The unit of all parameter in this card is mega-electron volt (MeV).

**CARD 4: Irx**

**Irx** is used as a seed for the pseudo-random-number generator. Multiplicative congruence method is employed in SICNFUL-QMD. If the same random seed is used, the calculation represents completely the same results.

**CARD 5: Xsourc, Ysourc, Zsourc**

This card defines the source position in Cartesian coordinate. The unit is centimeter (cm). Incident neutrons are assumed to be emitted from a point source. In addition, the coordinate of the source may occupy any position with respect to the scintillator, even inside it. The only forbidden area is just behind the scintillator. This is a reason of a light pipe and photomultiplier tube usually attached there, and the interactions with them are not considered in the code. Therefore, if a source placed behind the scintillator, it is moved to an equivalent position in front of the detector.

**CARD 6: Radius, Height, Rcolim**

This card gives a geometry configuration. The shape of scintillator is just a right circular cylinder. Complex geometries are not embodied in SCINFUL-QMD. Figure 19 shows the geometry of cylindrical scintillator together with the specific delineation of the Cartesian coordinate axes. The origin of the Cartesian coordinate for the geometry description is the center of the front face of the cylinder.

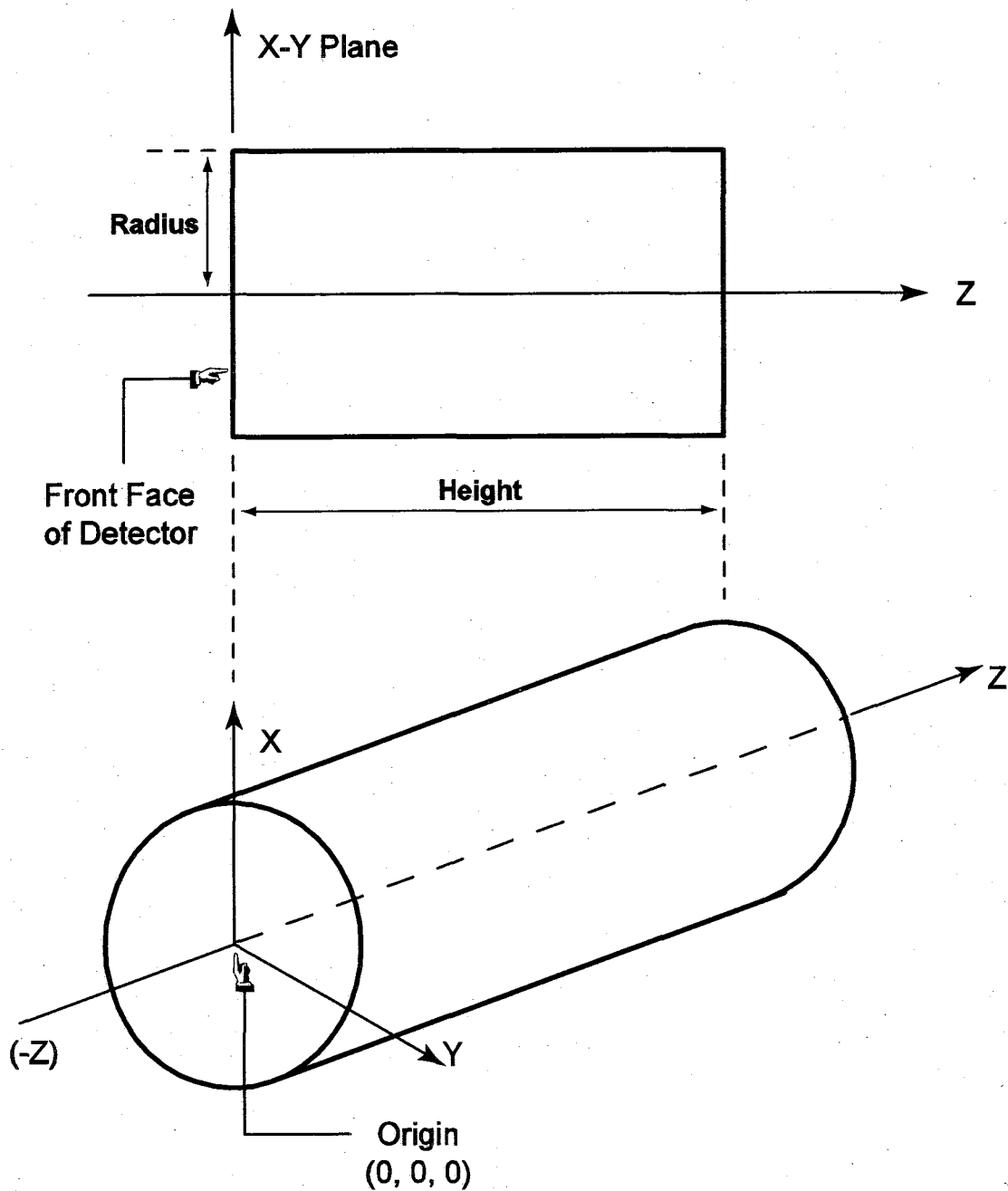
**Radius** means the scintillator radius. **Height** is the length of scintillator along the z-axis. **Rcolim** is the radius of a collimator for the front face of the scintillator. The collimator defined here has the features of infinitely absorbing and zero thickness, and may also be used to mask the curved surface of the scintillator from a neutron source.

**CARD 7: Iswt, Icont, Iesc, Ilight**

This card gives special parameters for the SCINFUL-QMD calculation. **Iswt** is a switching option for "efficiency mode" or "response mode". If **Iswt** equals 1, SCINFUL-QMD outputs only the neutron detection efficiencies corresponding to each bias. If **Iswt** is 2, both the efficiency and the response function are written in files.

**Icont** makes a continuous calculation of SCINFUL-QMD possible. If **Icont** is 1, the calculation finishes once in one incident neutron energy. If **Icont** is 2, the continuous calculations will be executed in different neutron energies. In this mode, the source neutron energies are not read from the "Input.data". An

## Detector Geometry



**Figure 19.** Geometry of a cylindrical scintillator exhibiting the specific delineation of the Cartesian coordinate axes. The origin is defined as the center of the front face of the detector; the photomultiplier tube of intervening light pipe is attached to the back face of the cylinder, at  $z = +\text{Height}$ .

This figure is cited from Ref. 1

additional input file named "energy.inp" is required. Then the energies for each calculation are read from this file. A sample data set of "energy.inp" is as follows.

<b>List 5-5 ● Sample data set of "energy.inp"</b>
---

```
60.0
75.0
80.0
```

This sample means that the calculation is performed three times in the neutron energies of 60.0, 75.0 and 80.0 MeV. Only monoenergetic neutron source is selectable in this mode.

**Iesc** is an option for the treatment of escaping protons. In PSD analysis for experimental data, the events of high-energy proton that escapes from the scintillator wall are eliminated because it is difficult to distinguish them from the gamma-ray events. In that case, the escaping proton events must be discarded in the calculation for consistency. If **Iesc** equals 2, the elimination mode is activated, and 1 means inactivation.

**Ilight** designates the conversion method of the kinetic energy into the light output as follows. The values of the light outputs are discussed in Section 2.

- Ilight* = 1; Light output database employed in the original SCINFUL code<sup>1)</sup>.
- = 2; Light output function proposed by Nakao *et al.*<sup>11)</sup>.
- = 3; Light output function proposed by Satoh *et al.*<sup>10)</sup>

The interpretation of the sample input exhibited in List 5-4 is as follows: the case is a single calculation of 80 MeV neutrons incident to the face of a 12.7 cm diameter by 12.7 cm long NE213 scintillator. To represent a parallel beam of neutrons, the source is positioned on the z-axis, and 4.0 m upstream from the front face of a scintillator. The minus sign with the 213 entry (second card) indicates requesting the software PSD to exclude the events which resulted in gamma-ray emission and subsequent detection. The source is monoenergetic with a low-energy cutoff of 10 keV. The light attenuation factor is set at  $8 \times 10^{-3} \text{ cm}^{-1}$ . Both the detection efficiency and the response function are written in files as a result. The light outputs of the escaping proton events are not eliminated from the response.

### 5.3 Bias for Detection Efficiency

Detection efficiency is obtained by integrating the response function above a bias. In SCINFUL-QMD, five biases are defined at once in the file named "scin\_bias.data" using the unit of electron-equivalent energy ( $\text{MeV}_{ee}$ ). An example of "scin\_bias.data" is shown in List 5-6.



List 5-6 ● Sample data set of "scin_bias.data"
--

0.0 0.493 1.07 4.33 8.66

Numerical values are separated by spaces.

#### 5.4. Output Data

SCINFUL-QMD writes the output data in a file labeled "scinful-qmd.out". An output data corresponding to the sample input presented in List 5-4 is given below.

List 5-7 ● Sample of output file
----------------------------------

```

1:  c -----
2:  *Sample input data* SCINFUL-QMD NE213(5**5")
3:  Energy = 80.00
4:  Source Pos = 0.00 0.00 -400.00
5:  c -----
6:  No. of Neutrons traced = 1000000
7:  No. of Neutrons used = 3399696
8:  Zero-bias efficiency = 0.294144
9:  Subtended Solid angle = 7.91581E-04 sr
10: c -----
11: Bias =====> 0.000 0.493 1.070 4.330 8.660
12: Efficiency ==> 0.290356 0.128196 0.124552 0.108899 0.092262
13: c -----

```

The interpretation of this output data is as follows: the 1st, 5th, 10th and 13th lines are divider line. The 2nd line is the title echo of the calculation. The following two lines give the energy and the position information of the neutron source. The lines from 6th to 9th are the result of the first part of calculation. They are interpreted as follows.

*No. of Neutron traced* = Number of neutrons to occur the initial interactions inside the scintillator (NHIST).

*No. of Neutron used* = Number of neutrons from the source to store the events with the number of NHIST (NHITS).

*Zero-bias efficiency* = Ratio into which NHIST is divided by NHITS.

*Subtended Solid angle* = Monte Carlo determined solid angle of the exposed surface of the scintillator with respect to the source position.

Last part from 11th to 12th line is the final result of the calculation. *Bias* is defined in the file "scin\_bias.data" and *Efficiency* is the results for each biases.

If the "response mode" is on; *i.e.* *iswt* = 2, an additional output file "res.out" is generated to give the information of the response function. Sample data set of "res.out" for the problem discussed above is shown in List 5-8. The first two columns give the light range for rows of the table; the bin widths are defined in a source file "effn.f". The next column tabulates the response normalized by the light bin width and the number of incident neutrons. The last column estimates the Monte Carlo errors in the form of one sigma.

"NEW.lpt" and "NEW.pch" are default output files of the original SCINFUL. SCINFUL-QMD also generates these files, but they are not supported in the neutron energies above 80 MeV.

List 5-8 ● Sample data set of response function

--- RESPONSE FUNCTION ---

```

+++++
Incident neutron energy = 80.00 MeV
Nhits = 339084
Nhist = 100000
+++++
LO_low(MeVee), LO_up(MeVee), Response/(MeVee/n), Error/(MeVee/n)
8.665E-03 1.739E-02 1.107E+01 6.116E-02
1.739E-02 2.617E-02 2.640E+00 2.977E-02
2.617E-02 3.502E-02 1.472E+00 2.215E-02
3.502E-02 4.393E-02 8.665E-01 1.694E-02
4.393E-02 5.290E-02 5.455E-01 1.339E-02
5.290E-02 6.193E-02 3.994E-01 1.142E-02
6.193E-02 7.102E-02 2.708E-01 9.371E-03
7.102E-02 8.018E-02 1.684E-01 7.365E-03
8.018E-02 8.940E-02 1.052E-01 5.802E-03
8.940E-02 9.868E-02 7.179E-02 4.775E-03
9.868E-02 1.080E-01 6.562E-02 4.550E-03
1.080E-01 1.174E-01 6.830E-02 4.626E-03
1.174E-01 1.269E-01 7.623E-02 4.870E-03
1.269E-01 1.365E-01 7.385E-02 4.777E-03
1.365E-01 1.461E-01 7.211E-02 4.704E-03
1.461E-01 1.558E-01 5.333E-02 4.031E-03
1.558E-01 1.655E-01 2.996E-02 3.011E-03
1.655E-01 1.753E-01 2.314E-02 2.637E-03
1.753E-01 1.852E-01 1.821E-02 2.331E-03
1.852E-01 1.951E-01 1.601E-02 2.178E-03
1.951E-01 2.052E-01 1.178E-02 1.862E-03
2.052E-01 2.152E-01 8.187E-03 1.547E-03
2.152E-01 2.254E-01 6.969E-03 1.422E-03
2.254E-01 2.356E-01 1.298E-02 1.934E-03
2.356E-01 2.459E-01 7.732E-03 1.488E-03
2.459E-01 2.563E-01 9.954E-03 1.683E-03
2.563E-01 2.667E-01 9.886E-03 1.671E-03
2.667E-01 2.772E-01 5.610E-03 1.254E-03
2.772E-01 2.878E-01 6.964E-03 1.393E-03
2.878E-01 2.985E-01 6.916E-03 1.383E-03
2.985E-01 3.092E-01 1.017E-02 1.671E-03
3.092E-01 3.200E-01 6.003E-03 1.280E-03
3.200E-01 3.419E-01 7.859E-03 1.459E-03
3.419E-01 3.529E-01 7.859E-03 1.459E-03
3.529E-01 3.640E-01 7.697E-03 1.420E-03
5.858E+01 5.899E+01 6.116E-04 6.595E-05
5.899E+01 5.941E+01 7.133E-04 7.097E-05
5.941E+01 5.983E+01 5.541E-04 6.234E-05
5.983E+01 6.025E+01 5.990E-04 6.459E-05
6.025E+01 6.068E+01 5.880E-04 6.378E-05
6.068E+01 6.111E+01 6.870E-04 6.870E-05
6.111E+01 6.154E+01 7.095E-04 6.958E-05
6.154E+01 6.198E+01 7.589E-04 7.171E-05
6.198E+01 6.242E+01 6.527E-04 6.627E-05
6.242E+01 6.286E+01 6.014E-04 6.340E-05
6.286E+01 6.330E+01 6.968E-04 6.800E-05
6.330E+01 6.375E+01 5.602E-04 6.076E-05
6.375E+01 6.420E+01 4.320E-04 5.318E-05
6.420E+01 6.465E+01 4.160E-04 5.200E-05
6.465E+01 6.511E+01 2.389E-04 3.927E-05
6.511E+01 6.557E+01 2.565E-04 4.055E-05
6.557E+01 6.603E+01 1.719E-04 3.308E-05
6.603E+01 6.650E+01 1.012E-04 2.529E-05
6.650E+01 6.697E+01 1.884E-05 1.088E-05

```

## 6. Summary

We have developed a Monte Carlo based computer code SCINFUL-QMD<sup>5)</sup>, which is a modified version of SCINFUL<sup>1)</sup>, to calculate response function and detection efficiency for a liquid organic scintillator. We have introduced a new physical model, quantum molecular dynamics model incorporated with statistical decay model (QMD+SDM<sup>4)</sup>), into SCINFUL. These additional routines can extend the applicable energy range of the code in principle up to 3 GeV.

According to the increase of the applicable energy, we have upgraded the total cross-section data for hydrogen and carbon nuclei, which are the components of the organic scintillator. Furthermore, the extra-nuclear cascade of secondary particles is also considered in the code. These modifications play important roles to reproduce the particle behavior inside the scintillator for the high-energy-neutron incidence.

As verification of the code accuracy, we have compared the data calculated by SCINFUL-QMD with several experimental data<sup>12,19-24)</sup> and the predictions of computational code CECIL<sup>2)</sup>. The results of SCINFUL-QMD showed better agreement with the experimental data than those of CECIL.

By the improvements of the code described in this report, SCINFUL-QMD enables us to estimate the reliable scintillator response in the incident neutron energy from 0.1 MeV to 3 GeV.

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## Appendix. Program List of SCINFUL-QMD code

A program list of the SCINFUL-QMD code is provided. It is divided to three components; MAIN STEERING, SCINFUL, and QMD+SDM. The names of these routines and brief descriptions of purposes are as follows.

### MAIN STEERING Part

*Program MAIN:*

To control whole computation of SCINFUL-QMD.

*Entries in BANKR:*

To do bookkeeping, updates collision counters, increments light-unit-bin counters. The entries are named BANKR0, BANKR1, BANKR2, BANKR3, and BANKR4.

*Subroutine CMTRAN:*

Relativistic transformation from laboratory-reference frame to the center-of-mass frame.

*Subroutine DEDXL:*

To calculate energy deposition on basis of the Bethe formula.

*Subroutine DIRCOS:*

To determine direction cosines from velocity vectors.

*Function DOMEGA:*

To determine and record coordinates and direction cosines of initial interactions inside scintillator for NHIST events, and deduce the subtended solid angle.

*Subroutine EFFN:*

To define width of light-unit bins, and initialize light-unit-bin counters.

*Subroutine EFFT:*

To construct light-output distribution (response function), and deduce the detection efficiency.

*Function EFROMV:*

To compute particle energy from velocity with relativistic correction.

*Function ETOL:*

Conversion between light output and kinetic energy of charged particles.

*Function EXTERP:*

To provide interpolation from tabular data.

*Function IBOX:*

To determine by random number whether a neutron interaction took place along the path, and if so the type of the interaction.

*Function IBOX2:*

To determine by random number whether a neutron interaction took place along the path, and if so the type of target nucleus for QMD+SDM simulation.

*Subroutine INPUT:*

To read input data file, and set up computation.

*Subroutine INTERACT:*

To determine by random number whether a first collision took place inside scintillator.

*Subroutine JQMD:*

Entry of QMD+SDM simulation.

*Subroutine LABTRAN:*

Relativistic transformation from center-of-mass reference-frame to the laboratory frame.

*Subroutine PHITSDUMP:*

To connect the calculation results of PHITS code. This option has not been supported officially.

*Function PLNGTH:*

To compute length of a vector with direction cosine from the interaction spot to the surface of scintillator.

*Subroutine RAND:*

To generate random number.

*Subroutine RANGEAL:*

To compute range of particles on basis of dE/dx calculation.



*Function RCKE:*

To correct center-of-mass energy relativistically.

*Subroutine RVECT:*

To obtain random unit vector.

*Subroutine SCIN:*

Entry of SCINFUL simulation.

*Function SIGCELAS:*

To return a cross section for elastic  $n + {}^{12}\text{C}$  collision in barn.

*Function SIGCINEL:*

To return a cross section for inelastic  $n + {}^{12}\text{C}$  excitation of the first-excited state in  ${}^{12}\text{C}$ .

*Function SIGCN2N:*

To return a cross section for  ${}^{12}\text{C}(n, 2n)$  reaction.

*Function SIGCN3HE:*

To return a cross section for  ${}^{12}\text{C}(n, {}^3\text{He})$  reaction.

*Function SIGCNAL:*

To return a cross section for  ${}^{12}\text{C}(n, \alpha){}^9\text{Be}$  ground-state reaction.

*Function SIGCND:*

To return a cross section for  ${}^{12}\text{C}(n, d)$  reaction.

*Function SIGCNN3A:*

To return a cross section for  ${}^{12}\text{C}(n, n')3\alpha$  reaction.

*Function SIGCNP:*

To return a cross section for  ${}^{12}\text{C}(n, p){}^{12}\text{B}$  bound-state reaction.

*Function SIGCNPN:*

To return a cross section for  ${}^{12}\text{C}(n, p){}^{12}\text{B}$  unbound-state reaction.

*Function SIGCNT:*

To return a cross section for  ${}^{12}\text{C}(n, t)$  reaction.

*Function SIGHYD:*

To return a cross section for n + p scattering below 150 MeV.

*Function SIGHYD2:*

To return a cross section for n + p scattering above 150 MeV.

*Function SIGTOT:*

To return a total cross section for carbon nucleus.

*Function TOTALX:*

To determine total attenuation cross section and fractional cross sections for each major reaction channel below 150 MeV.

*Function TOTALX2:*

To determine total attenuation cross section and fractional cross sections for each major reaction channel above 150 MeV.

*Subroutine TRANSVEC:*

Vector transformation from one coordinate system to another.

*Subroutine TRANSP:*

To compute particle transport for multiple collision.

*Function VELOCITY:*

To compute velocity from kinetic energy.

**SCINFUL Part**

*Subroutine ALFAPD:*

Energetics for  ${}^7\text{Li} \rightarrow \text{d} + \alpha$  decay.

*Subroutine ALFAPT:*

Energetics for  ${}^7\text{Li} \rightarrow \text{t} + \alpha$  decay.

*Subroutine AP7L: I*

Energetics for  ${}^{11}\text{B} \rightarrow {}^7\text{Li} + \alpha$  decay, including any subsequent decay of excited  ${}^7\text{Li}$  ion.

*Function BETARG:*

To compute electron range from kinetic energy.

*Function CHOOSA:*

To choose alpha particle energy for the  $^{12}\text{C} \rightarrow 3\alpha$  three-body breakup reaction.

*Function CHOOSL:*

To choose an azimuthal angle from a distribution described by Legendre polynomial expansion.

*Function CHOOSM:*

To choose a neutron energy from a Maxwellian distribution.

*Function CHOOSN:*

To choose a neutron energy from a distribution approximating the continuum of  $^{12}\text{C}$  excitations.

*Function CHOOSP:*

To choose a proton energy from a similarly estimated proton continuum energy distribution.

*Subroutine COMDCS:*

To compute polar scattering angles for electron and photon following a Compton scattering event.

*Function COMPSIG:*

To return a cross section for gamma-ray scattering.

*Subroutine COMPTN:*

To compute electron energy from a photon energy initiating a Compton scattering.

*Subroutine CSCAT:*

Finish up  $n + ^{12}\text{C}$  elastic or inelastic scattering.

*Subroutine DPLI7:*

Energetics for  $^9\text{Be} \rightarrow d + ^7\text{Li}$

*Subroutine ELI8DK:*

Energetics for  $^8\text{Li} \rightarrow n + ^7\text{Li}$  decay, including any subsequent decay of excited  $^7\text{Li}$  ion.

*Function EX8LI:*

To determine excitation energy of residual  ${}^8\text{Li}$  ion for alpha decay of highly excited  ${}^{12}\text{B}$  ion.

*Function EXLI8:*

To determine excitation energy of residual  ${}^8\text{Li}$  ion for proton decay of highly excited  ${}^9\text{Be}$  ion.

*Subroutine HYDROG:*

Kinematics for  $n + p$  collisions.

*Subroutine INELAS:*

Kinematics for inelastic neutron scattering exciting the first-excited state (at 4.43 MeV) in  ${}^{12}\text{C}$

*Block data LEGNDR:*

To return Legendre coefficients for  $n + {}^{12}\text{C}$  elastic scattering angular distributions.

*Subroutine N2N:*

Kinematics for  $n + {}^{12}\text{C} \rightarrow 2n + {}^{11}\text{C}$  reactions.

*Subroutine N3HE:*

Kinematics for  $n + {}^{12}\text{C} \rightarrow {}^3\text{He} + {}^{10}\text{Be}$  reactions.

*Subroutine NALPHA:*

Kinematics for  $n + {}^{12}\text{C} \rightarrow \alpha + {}^9\text{Be}$  ground-state reactions.

*Subroutine ND:*

Kinematics for  $n + {}^{12}\text{C} \rightarrow d + {}^{11}\text{B}$  reactions.

*Subroutine NN3ALF:*

Kinematics for  $n + {}^{12}\text{C} \rightarrow n' + 3\alpha$  reactions;  
also includes minor reactions  $n + {}^{12}\text{C} \rightarrow \alpha + p + \dots$

*Subroutine NP:*

Kinematics for  $n + {}^{12}\text{C} \rightarrow p + {}^{12}\text{B}$  bound-state reactions.

*Subroutine NPX:*

Kinematics for  $n + {}^{12}\text{C} \rightarrow p + {}^{12}\text{B}$  unbound-state reactions, and subsequent decay of excited  ${}^{12}\text{B}$  ion.

*Subroutine NT:*

Kinematics for  $n + {}^{12}\text{C} \rightarrow t + {}^{10}\text{B}$  reactions.

*Subroutine P3ALPH:*

To choose reaction path for  $n + {}^{12}\text{C} \rightarrow n' + 3\alpha$  reaction.

*Subroutine PHOTON:*

To follow gamma-ray scattering.

*Subroutine PP8LI:*

Energetics for  ${}^9\text{Be} \rightarrow p + {}^8\text{Li}$  decay, including any subsequent decay of excited  ${}^8\text{Li}$  ion.

*Block data PROTN:*

Tabular range-energy data for protons in NE213.

*Subroutine PSCAT:*

Kinematics for elastic neutron scattering by  ${}^{12}\text{C}$ .

*Subroutine TENBDK:*

Energetics for decay of highly excited  ${}^{10}\text{B}$  ion.

**QMD+SDM Part**

*Subroutine JQMD00:*

To control total QMD+SDM simulation.

*Subroutine QMDEVENT:*

To simulate one event by QMD.

*Subroutine FINSUMRY:*

To summarize the overall events in QMD+SDM.

*Subroutine QMDJUDGE:*

To determine the weight of one event of QMD and judge the elastic or inelastic reaction type.

*Subroutine QMDSUM:*

To summarize one event of QMD.

*Subroutine SDMSUM:*

To summarize one event of SDM.

*Subroutine READCFG:*

To obtain the input parameters for QMD+SDM nuclear reaction simulation.

*Subroutine QMDINT:*

To initialize the QMD part.

*Subroutine KCOMP:*

To determine the parameters of the interactions.

*Subroutine IDNAME:*

To identify the particle or nucleus.

*Subroutine GROUND:*

To make the ground state.

*Subroutine PACKQMD:*

To make the ground state by random packing method.

*Subroutine GCMANG:*

To kill cm motion and angular momentum of the nucleus.

*Subroutine RBOOST:*

To boost the ground state.

*Subroutine BCOUL:*

To determine the initial position and momentum according to Coulomb trajectory.

*Subroutine CALDISA:*

To calculate the two-body quantities for all particles.

*Subroutine CALDIS2:*

To calculate the two-body quantities for i1 and i2

*Subroutine GRADU:*

To calculate the graduate of equation of motion for Runge-Kutta-Gill (RKG)

*Subroutine RK12:*

To propagate particles by 2nd order RKG.

*Subroutine RKG4:*

To propagate particles by 4th order RKG.

*Subroutine PAULI:*

To calculate the Pauli blocking factor.

*Subroutine EPOTALL:*

To calculate total potential energy.

*Subroutine ETOTAL:*

To calculate total energy of cluster.

*Subroutine PCMCL:*

To calculate energy and angular momentum of cluster.

*Subroutine CLDIST:*

To determine nuclear cluster.

*Subroutine RELCOL:*

To calculate the kinematics between two particles.

*Subroutine CROSW:*

To determine collision channel and final state.

*Subroutine PIONEM:*

To calculate the decay of  $\Delta$  or  $N^*$ .

*Subroutine PIONAB:*

To calculate pion absorption.

*Subroutine FPIDECAY:*

To calculate final decay of the responses.

*Subroutine RESMAS:*

To calculate the mass and width of  $\Delta$  or  $N^*$ .

*Function PIDENO:*

To calculate the correction factor of inverse cross section.

*Function SOO:*

To calculate  $\Delta$  and  $N^*$  cross section.

*Subroutine SDMENT:*

Entry of SDM from QMD results.

*Subroutine SDMINT:*

To initialize SDM.

*Subroutine SDMEEXEC:*

To execute statistical particle decay or fission.

*SubroutineSDMWID0:*

To calculate decay width and decay products without angular momentum.

*Subroutine SDMWID1:*

To calculate decay width and decay products with angular momentum.

*Function SDMLEV:*

To calculate level density.

*Subroutine SDJSUM:*

To sum up angular momentum.

*Subroutine SDMFISW:*

To calculate fission width.

*Subroutine SDMFISS:*

To determine the mass and charge of fission fragment.



***Function SDMFISB:***

To determine the fission barrier.

***Subroutine SDMLIST:***

To list event record and particle data.

***Function BNDENG:***

To give binding energy per baryon (MeV).

***Function ELIQ:***

To calculate liquid drop binding energy (MeV).

***Subroutine SDMTABLE:***

To read mass table from block data.

***Block QMDDATA:***

To give default values for switches and parameters for QMD simulation.

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# 国際単位系 (SI)

表1. SI 基本単位

基本量	SI 基本単位	
	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質の量	モル	mol
光度	カンデラ	cd

表2. 基本単位を用いて表されるSI組立単位の例

組立量	SI 基本単位	
	名称	記号
面積	平方メートル	m <sup>2</sup>
体積	立方メートル	m <sup>3</sup>
速度	メートル毎秒	m/s
加速度	メートル毎秒毎秒	m/s <sup>2</sup>
波数	メートル <sup>-1</sup>	m <sup>-1</sup>
密度 (質量密度)	キログラム毎立方メートル	kg/m <sup>3</sup>
質量体積 (比体積)	立方メートル毎キログラム	m <sup>3</sup> /kg
電流密度	アンペア毎平方メートル	A/m <sup>2</sup>
磁界の強さ (物質量の) 濃度	アンペア毎メートル	A/m
輝度	カンデラ毎平方メートル	cd/m <sup>2</sup>
屈折率	(数の) 1	1

表5. SI 接頭語

乗数	接頭語	記号	乗数	接頭語	記号
10 <sup>24</sup>	ヨタ	Y	10 <sup>-1</sup>	デシ	d
10 <sup>21</sup>	ゼタ	Z	10 <sup>-2</sup>	センチ	c
10 <sup>18</sup>	エクサ	E	10 <sup>-3</sup>	ミリ	m
10 <sup>15</sup>	ペタ	P	10 <sup>-6</sup>	マイクロ	μ
10 <sup>12</sup>	テラ	T	10 <sup>-9</sup>	ナノ	n
10 <sup>9</sup>	ギガ	G	10 <sup>-12</sup>	ピコ	p
10 <sup>6</sup>	メガ	M	10 <sup>-15</sup>	フェムト	f
10 <sup>3</sup>	キロ	k	10 <sup>-18</sup>	アト	a
10 <sup>2</sup>	ヘクト	h	10 <sup>-21</sup>	ゼプト	z
10 <sup>1</sup>	デカ	da	10 <sup>-24</sup>	エクト	y

表3. 固有の名称とその独自の記号で表されるSI組立単位

組立量	SI 組立単位		他のSI単位による表し方	SI基本単位による表し方
	名称	記号		
平面角	ラジアン <sup>(a)</sup>	rad		m <sup>-1</sup> ・m <sup>1</sup> =1 <sup>(b)</sup>
立体角	ステラジアン <sup>(a)</sup>	sr <sup>(c)</sup>		m <sup>2</sup> ・m <sup>-2</sup> =1 <sup>(b)</sup>
周波数	ヘルツ	Hz		s <sup>-1</sup>
力	ニュートン	N		m <sup>1</sup> ・kg <sup>1</sup> ・s <sup>-2</sup>
圧力, 応力	パスカル	Pa	N/m <sup>2</sup>	m <sup>-1</sup> ・kg <sup>1</sup> ・s <sup>-2</sup>
エネルギー, 仕事, 熱量	ジュール	J	N・m	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-2</sup>
工率, 放射束	ワット	W	J/s	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-3</sup>
電荷, 電気量	クーロン	C		s <sup>1</sup> ・A
電位差 (電圧), 起電力	ヴォルト	V	W/A	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-3</sup> ・A <sup>-1</sup>
静電容量	ファラド	F	C/V	m <sup>-2</sup> ・kg <sup>-1</sup> ・s <sup>4</sup> ・A <sup>2</sup>
電気抵抗	オーム	Ω	V/A	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-3</sup> ・A <sup>-2</sup>
コンダクタンス	ジーメン	S	A/V	m <sup>-2</sup> ・kg <sup>-1</sup> ・s <sup>3</sup> ・A <sup>2</sup>
磁束密度	ウェーバ	Wb	V・s	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-2</sup> ・A <sup>-1</sup>
磁束	テスラ	T	Wb/m <sup>2</sup>	kg <sup>1</sup> ・s <sup>-2</sup> ・A <sup>-1</sup>
インダクタンス	ヘンリー	H	Wb/A	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-2</sup> ・A <sup>-2</sup>
セルシウス温度	セルシウス度 <sup>(d)</sup>	°C		K
光照射度	ルーメン	lm	cd・sr <sup>(c)</sup>	m <sup>2</sup> ・m <sup>-2</sup> ・cd=cd
(放射線核種の) 放射能	ベクレル	Bq	lm/m <sup>2</sup>	m <sup>2</sup> ・m <sup>-1</sup> ・cd・m <sup>-2</sup> ・cd
吸収線量, 質量エネルギー	グレイ	Gy	J/kg	s <sup>-1</sup>
線量当量, 周辺線量当量, 方向性線量当量, 個人線量当量, 組織線量当量	シーベルト	Sv	J/kg	m <sup>2</sup> ・s <sup>-2</sup>

- (a) ラジアン及びステラジアンの使用は、同じ次元であっても異なった性質をもった量を区別するときの組立単位の表し方として利点がある。組立単位を形作る際のいくつかの用例は表4に示されている。
- (b) 実際には、使用する際には記号rad及びsrが用いられるが、習慣として組立単位としての記号“1.”は明示されない。
- (c) 測光学では、ステラジアンの名称と記号srを単位の表し方の中にそのまま維持している。
- (d) この単位は、例としてミリセルシウス度m°CのようにSI接頭語を伴って用いても良い。

表4. 単位の中に固有の名称とその独自の記号を含むSI組立単位の例

組立量	SI 組立単位		SI 基本単位による表し方
	名称	記号	
粘着力	パスカル秒	Pa・s	m <sup>-1</sup> ・kg <sup>1</sup> ・s <sup>-1</sup>
面の張力	ニュートンメートル	N・m	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-2</sup>
角速度	ニュートン毎メートル	N/m	kg <sup>1</sup> ・s <sup>-2</sup>
角加速度	ラジアン毎秒	rad/s	m <sup>-1</sup> ・s <sup>-1</sup> =s <sup>-1</sup>
熱流密度, 放射照度	ラジアン毎平方秒	rad/s <sup>2</sup>	m <sup>-1</sup> ・m <sup>-1</sup> ・s <sup>-2</sup> =s <sup>-2</sup>
熱容量, エントロピー	ワット毎平方メートル	W/m <sup>2</sup>	kg <sup>1</sup> ・s <sup>-3</sup>
質量熱容量 (比熱容量)	ジュール毎ケルビン	J/K	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-2</sup> ・K <sup>-1</sup>
質量エンタルピー (比エンタルピー)	ジュール毎キログラム	J/(kg・K)	m <sup>2</sup> ・s <sup>-2</sup> ・K <sup>-1</sup>
熱伝導率	ジュール毎キログラム	J/kg	m <sup>2</sup> ・s <sup>-2</sup> ・K <sup>-1</sup>
体積エネルギー	ワット毎メートル毎ケルビン	W/(m・K)	m <sup>1</sup> ・kg <sup>1</sup> ・s <sup>-3</sup> ・K <sup>-1</sup>
電界の強さ	ジュール毎立方メートル	J/m <sup>3</sup>	m <sup>-1</sup> ・kg <sup>1</sup> ・s <sup>-2</sup>
体積電荷	ボルト毎メートル	V/m	m <sup>1</sup> ・kg <sup>1</sup> ・s <sup>-3</sup> ・A <sup>-1</sup>
電気変位	クーロン毎立方メートル	C/m <sup>3</sup>	m <sup>-3</sup> ・s <sup>1</sup> ・A
誘電率	クーロン毎平方メートル	C/m <sup>2</sup>	m <sup>-2</sup> ・s <sup>1</sup> ・A
透磁率	ファラド毎メートル	F/m	m <sup>-5</sup> ・kg <sup>-1</sup> ・s <sup>4</sup> ・A <sup>2</sup>
モルエンタルピー	ヘンリー毎メートル	H/m	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-2</sup> ・A <sup>-2</sup>
モルエンタルピー	ジュール毎モル	J/mol	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-2</sup> ・mol <sup>-1</sup>
モル熱容量	ジュール毎モル毎ケルビン	J/(mol・K)	m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-2</sup> ・K <sup>-1</sup> ・mol <sup>-1</sup>
照射線量 (X線及びγ線)	クーロン毎キログラム	C/kg	kg <sup>-1</sup> ・s <sup>1</sup> ・A
放射線強度	グレイ毎秒	Gy/s	m <sup>2</sup> ・s <sup>-3</sup>
放射輝度	ワット毎ステラジアン	W/sr	m <sup>4</sup> ・m <sup>-2</sup> ・kg <sup>1</sup> ・s <sup>-3</sup> =m <sup>2</sup> ・kg <sup>1</sup> ・s <sup>-3</sup>
	ワット毎平方メートル毎ステラジアン	W/(m <sup>2</sup> ・sr)	m <sup>2</sup> ・m <sup>-2</sup> ・kg <sup>1</sup> ・s <sup>-3</sup> =kg <sup>1</sup> ・s <sup>-3</sup>

表6. 国際単位系と併用されるが国際単位系に属さない単位

名称	記号	SI 単位による値
分	min	1 min=60s
時	h	1h=60 min=3600 s
日	d	1 d=24 h=86400 s
度	°	1°=(π/180) rad
分	′	1′=(1/60)°=(π/10800) rad
秒	″	1″=(1/60)′=(π/648000) rad
リットル	l, L	1l=1 dm <sup>3</sup> =10 <sup>-3</sup> m <sup>3</sup>
トン	t	1t=10 <sup>3</sup> kg
ネーパ	Np	1Np=1
ベル	B	1B=(1/2)ln10(Np)

表7. 国際単位系と併用されこれに属さない単位でSI単位で表される数値が実験的に得られるもの

名称	記号	SI 単位であらわされる数値
電子ボルト	eV	1eV=1.60217733(49)×10 <sup>-19</sup> J
統一原子質量単位	u	1u=1.6605402(10)×10 <sup>-27</sup> kg
天文単位	ua	1ua=1.49597870691(30)×10 <sup>11</sup> m

表8. 国際単位系に属さないが国際単位系と併用されるその他の単位

名称	記号	SI 単位であらわされる数値
海里	海里	1海里=1852m
ノット	ノット	1ノット=1海里毎時=(1852/3600)m/s
アール	a	1a=1 dam <sup>2</sup> =10 <sup>2</sup> m <sup>2</sup>
ヘクタール	ha	1ha=1 hm <sup>2</sup> =10 <sup>4</sup> m <sup>2</sup>
バール	bar	1bar=0.1MPa=100kPa=1000hPa=10 <sup>5</sup> Pa
オングストローム	Å	1Å=0.1nm=10 <sup>-10</sup> m
バイン	b	1b=100fm=10 <sup>-28</sup> m <sup>2</sup>

表9. 固有の名称を含むCGS組立単位

名称	記号	SI 単位であらわされる数値
エルグ	erg	1 erg=10 <sup>-7</sup> J
ダイン	dyn	1 dyn=10 <sup>-5</sup> N
ポアズ	P	1 P=1 dyn・s/cm <sup>2</sup> =0.1Pa・s
ストークス	St	1 St =1cm <sup>2</sup> /s=10 <sup>-4</sup> m <sup>2</sup> /s
ガウス	G	1 G =10 <sup>4</sup> T
エルステッド	Oe	1 Oe = (1000/4π) A/m
マクスウェル	Mx	1 Mx =10 <sup>-8</sup> Wb
マクスウェル	sb	1 sb =1cd/cm <sup>2</sup> =10 <sup>4</sup> cd/m <sup>2</sup>
ホバ	ph	1 ph=10 <sup>4</sup> lx
ガリ	Gal	1 Gal =1cm/s <sup>2</sup> =10 <sup>-2</sup> m/s <sup>2</sup>

表10. 国際単位に属さないその他の単位の例

名称	記号	SI 単位であらわされる数値
キュリー	Ci	1 Ci=3.7×10 <sup>10</sup> Bq
レントゲン	R	1 R = 2.58×10 <sup>-4</sup> C/kg
ラド	rad	1 rad=1cGy=10 <sup>-2</sup> Gy
レム	rem	1 rem=1 cSv=10 <sup>-2</sup> Sv
X線単位	1X unit	1X unit=1.002×10 <sup>-4</sup> nm
ガンマ	γ	1γ=1 nT=10 <sup>-9</sup> T
ジャンスキー	Jy	1 Jy=10 <sup>-26</sup> W・m <sup>-2</sup> ・Hz <sup>-1</sup>
フェルミ	fm	1 fermi=1 fm=10 <sup>-16</sup> m
メートル系カラット	metric carat	1 metric carat = 200 mg = 2×10 <sup>-4</sup> kg
トル	Torr	1 Torr = (101 325/760) Pa
標準大気圧	atm	1 atm = 101 325 Pa
カロリ	cal	
マイクロン	μ	1 μ =1μm=10 <sup>-6</sup> m