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Development of a reaction ejectile sampling algorithm to recover kinematic correlations from inclusive cross-section data in Monte-Carlo particle transport simulations

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ABSTRACT

A new phenomenological approach is developed to reproduce the stochastic distributions of secondary particle energy and angle with conservation of momentum and energy in reactions ejecting more than one ejectiles using inclusive cross-section data. The summation of energy and momentum in each reaction is generally not conserved in Monte-Carlo particle transport simulation based on the inclusive cross-sections because the particle correlations are lost in the inclusive cross-section data. However, the energy and angular distributions are successfully reproduced by randomly generating numerous sets of secondary particle configurations which are compliant with the conservation laws, and sampling one set considering their likelihood. This developed approach was applied to simulation of (n,*x*n) reactions ($x \geq 2$) of various targets and to other reactions such as (n,np) and (n,2nα). The calculated secondary particle energy and angular distributions were compared with those of the original inclusive cross-section data to validate the algorithm. The calculated distributions reproduce the trend of original cross-section data considerably well especially in case of heavy targets. The developed algorithm is beneficial to improve the accuracy of event-by-event analysis in particle transport simulation.

1. Introduction

An event-by-event analysis of interactions between radiation and materials using particle transport simulation codes is essential for detector performance prediction, soft error analyses, dosimetry studies, etc. In general-purpose Monte-Carlo radiation transport codes [1–5], the interactions of particles (except for neutrons below 20 MeV) are usually simulated by using event generators to predict particle trajectories and energy deposition events with conservation of energy and momentum. On the other hand, the transport of neutrons below 20 MeV is simulated based on the cross-section data libraries. In the transport calculations based on cross-section data without explicit consideration of the conservation laws, energy and momentum in the reaction final state do not always agree with those in the reaction initial state. This problem is attributed to the fact that the kinematic correlations between particles are not specified in the inclusive cross-section data. Therefore, some particle transport simulation codes employ supplementary algorithms to perform transport calculations based on the cross-section data with conservation of energy and momentum (referred to as the event generator mode, EGM hereafter).

A good example is the EGM of PHITS (Particle and Heavy Ion Transport code System) [6], which samples the secondary neutron emission angles and energies based on the cross-section data and accordingly balances the energy and momentum through the excitation and recoiling of the residue. However, for reactions emitting more than one secondary particle, the evaporation model was used to sample the second and the subsequent outgoing neutrons in EGM. With this approach, the simulated energy and angular distributions do not agree with the cross-section data owing to the application of the evaporation model.

Particularly, in the nuclear cross-section data libraries intended for high-energy ($\geq$ 20 MeV) particle transport, such as LA150 [7] and JENDL (Japanese Evaluated Nuclear Data Library)/HE-2007 [8], the secondary particle multiplicity is often greater than 1, and the secondary particle energy distributions deviate from the evaporation spectrum; therefore, EGM algorithms compatible with high-multiplicity reactions are essential for event-by-event analyses of energetic particle transport simulations.

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In principle, it is impossible to reproduce kinematic correlations between particles if the particle transport is calculated based on inclusive cross-section data. In this study, we develop a method to simulate the particle transport with event-by-event energy and momentum conservation based on the inclusive cross-section data without distorting the secondary particle energy and angular distribution. In this method, the energy and momentum of all the

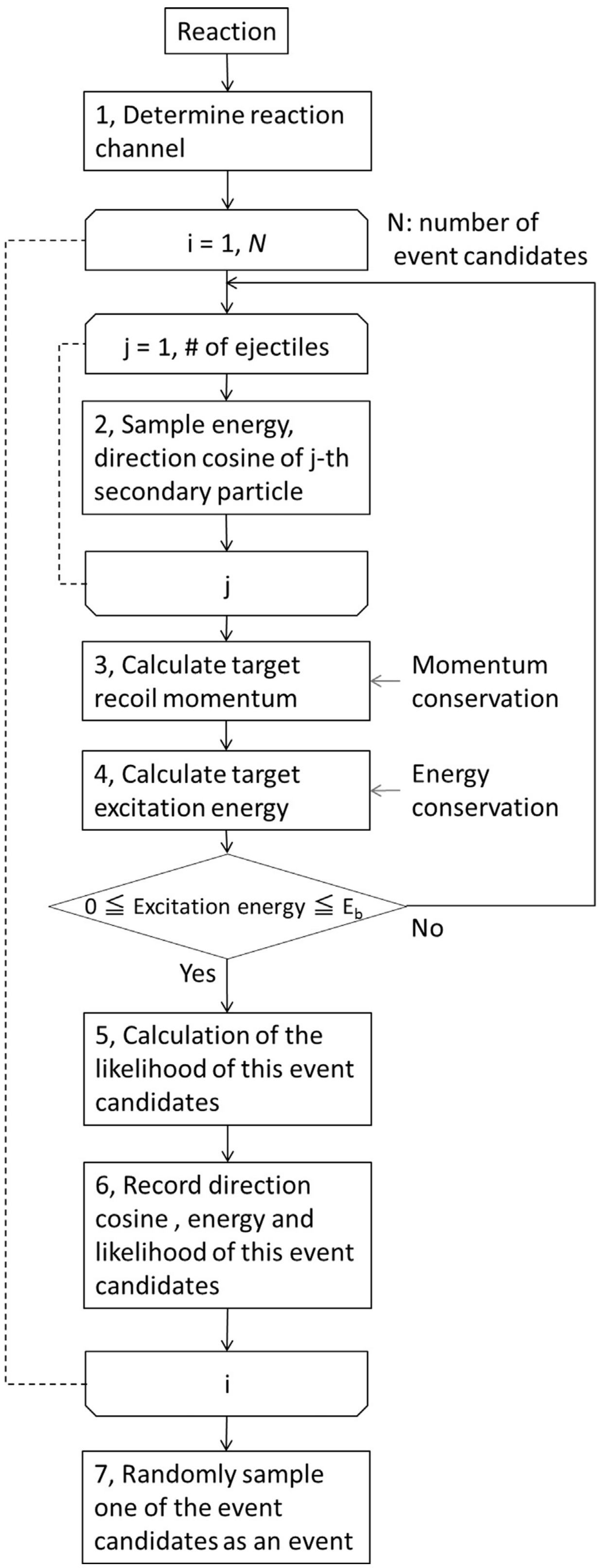

Fig. 1. Calculation flowchart of RAKIC.

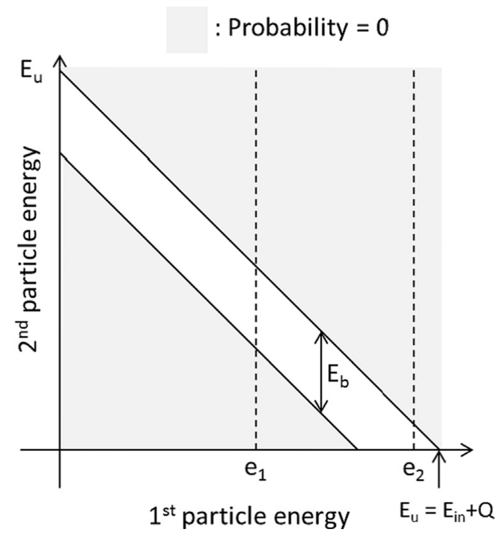

Fig. 2. Example of the probability space for the (n,2n) reaction (excitation and recoil kinetic energy are disregarded). The event candidates within the gray areas are not sampled owing to the restriction of energy conservation or nucleon binding in the residual nucleus. In the white region, the length of the right dashed line (i.e., the probability that secondary particle energy is e_2) is shorter than that of the left dashed line (i.e., the probability that secondary particle energy is e_1). To compensate for this difference, the likelihood of event candidates on the right dashed line is biased using the function f_i described in Eq. (3).

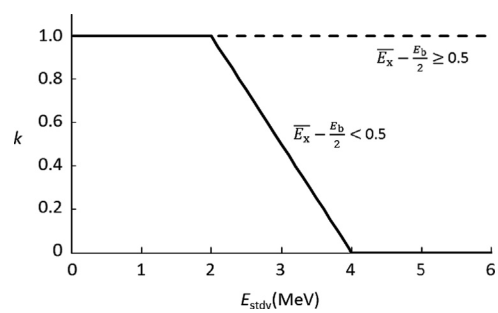

Fig. 3. The dependence of k factor on E_{stdv}.

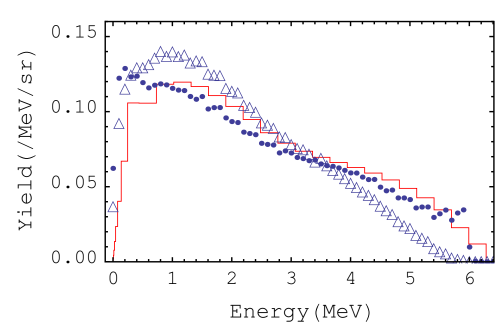

Fig. 4. Secondary neutron energy spectra of ^{54}Fe(n,2n) reactions taken from JENDL4.0 (histogram), calculation with the sampling bias factor f (full circles) and calculation without sampling bias factor f (open triangles). Angular bin: $-0.05 \leq \cos(\theta) \leq 0.05$.