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Exclusive data-based modeling of neutron-nuclear reactions below 20 MeV

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Abstract. We are developing CHIPS-TPT physics library for exclusive simulation of neutron-nuclear reactions below 20 MeV. Exclusive modeling reproduces each separate scattering and thus requires conservation of energy, momentum and quantum numbers in each reaction. Inclusive modeling reproduces only selected values while averaging over the others and imposes no such constraints. Therefore the exclusive modeling allows to simulate additional quantities like secondary particle correlations and gamma-lines broadening and avoid artificial fluctuations. CHIPS-TPT is based on the formerly included in Geant4 CHIPS library, which follows the exclusive approach, and extends it to incident neutrons with the energy below 20 MeV. The NeutronHP model for neutrons below 20 MeV included in Geant4 follows the inclusive approach like the well known MCNP code. Unfortunately, the available data in this energy region is mostly presented in ENDF-6 format and semi-inclusive. Imposing additional constraints on secondary particles complicates modeling but also allows to detect inconsistencies in the input data and to avoid errors that may remain unnoticed in inclusive modeling.

1. Introduction

CHIPS-TPT [1,2] is the successor of CHIPS [3] physics package formerly included in Geant4 [4,5] package. Starting from the Geant-4.10 release, CHIPS is no longer supported by the Geant4 Collaboration. The main goals of the CHIPS-TPT project are further maintenance of the universal CHIPS algorithms and the development of exclusive TPT (Toolkit for Particle Transport) algorithms of nuclear reactions at low energies for neutrons and light charged nuclear fragments. The exclusive TPT model can be a replacement for the inclusive NeutronHP model [6] currently used in the Geant4 framework for neutrons below 20 MeV. Exclusive modeling also reproduces kinematic effects such as secondary particle correlations and Doppler broadening of spectral lines and allows to avoid the fluctuations in the simulated detector response due to energy non-conservation in an inclusive approach.

The main features of CHIPS-TPT are:

- charge and baryon number conservation.
- energy and momentum conservation in each nuclear interaction.
- full isotope coverage.
- full neutron-nuclear reactions coverage below 20 MeV.

While CHIPS-TPT targets a broad range of isotopes, its exclusive nature and consistency with physical laws allow for a rigorous investigation of the reactions of interest. One of such reactions is nonelastic neutron scattering on ^{12}C, an important moderator and scintillator material.

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2. Energy and momentum conservation

Figure 1 shows the measure of energy and momentum non-conservation in nonelastic scattering processes of NeutronHP and CHIPS-TPT. The incident energy was typical 14 MeV, with a ^{12}C nucleus as the target. The non-conservation in neutronHP is due to the inclusive approach and can reach the incident particle energy. The non-conservation in TPT is due to rounding error and is limited to 10^{-5} eV for the energy and 10^{-2} eV/c for the momentum. Because of the Lorentz invariance of the energy-momentum four-vector, the conservation in TPT is preserved in any system of reference.

3. Neutron scattering on ^{12}C

3.1. Secondary neutron energy distribution

In ENDF-6 format energy-angular secondary distributions of each particle is given independently. Usually it is represented either as a linear interpolated table, Legendre polynomial expansion or Kalbach-Mann representation [7]. In inclusive modeling each secondary is sampled independently, while in exclusive modeling the secondaries are correlated. As an example of an non-elastic scattering process we chose $^{12}C(n, n3\alpha)$ reaction, because of multiple secondary particle emission. In the ENDF/B-VII.1 database [8], which is usually used in calculations, it is recorded as a $^{12}C(n, n')^{12}C$ reaction with a residual breakup flag indicating that the excited ^{12}C disintegrates into 3α. Figure 2 shows energy distribution of nonelastically scattered neutrons on ^{12}C at 14.1 MeV. The narrow peaks correspond to the excitation of discrete levels, the most energetic one stems from

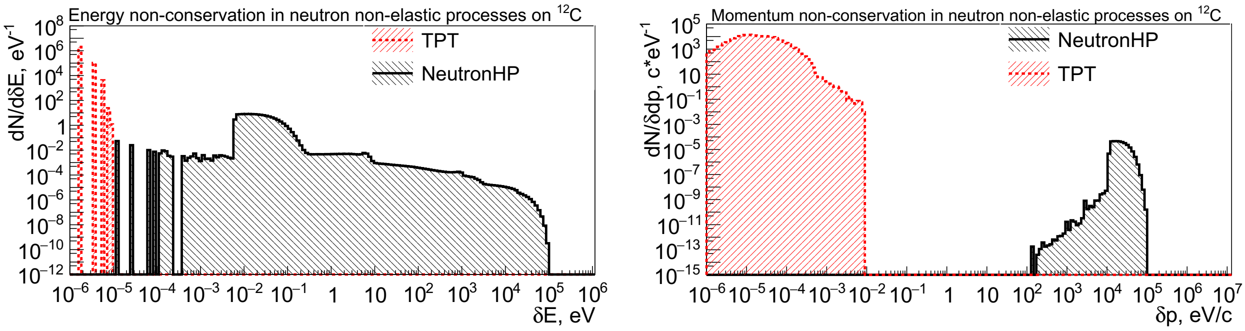

Figure 1. Energy (left) and momentum (right) non-conservation in NeutronHP (black solid line) and CHIPS-TPT (red dashed line).

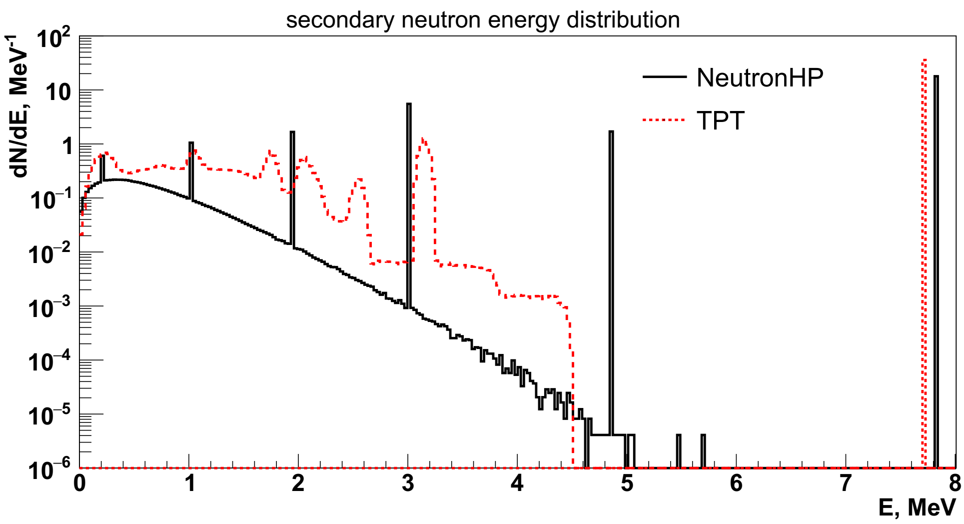

Figure 2. Energy distribution of nonelastically scattered neutrons on ^{12}C in the center of mass system of reference. The incident neutron energy is 14.1 MeV in the laboratory system. Black solid line - NeutronHP, red dashed line - TPT.

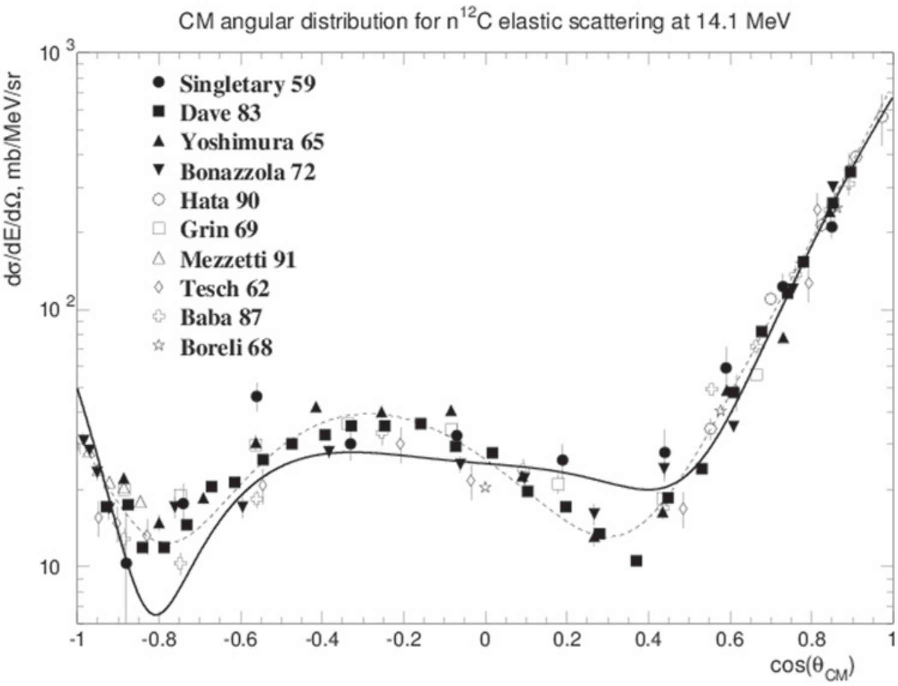

Figure 3. Angular distribution of elastically scattered neutrons on ^{12}C at 14.1 MeV. Black solid line – ENDF/B-VII.1 evaluation, dashed line – approximation accounting for newer data.

the $^{12}C(n, n'\gamma)^{12}C$ reaction. NeutronHP includes also a Maxwellian-like continuous contribution. But $^{12}C(n, n3\alpha)$ reaction also incorporates other intermediate channels like $^{12}C(n, n\alpha)^{8}Be^{*}$ and $^{12}C(n, \alpha)^{9}Be^{*}$ [9], where $^{9}Be^{*}$ indicates the excited states of ^{9}Be, and $^{8}Be^{*}$ indicates the $\alpha - \alpha$ resonances. It leads to a more complex neutron spectrum. This behavior is reflected in the CENDL-3.1 library [10], which thus became the choice for TPT.

3.2. Elastic neutron angular distribution

The ENDF/B-VII.1 evaluation is also outdated in the angular distribution file. Figure 3 shows angular distribution of elastically scattered neutrons on 12 C at 14.1 MeV. Points represent experimental data taken from EXFOR database [11]. The solid line is the ENDF/B-VII.1 evaluation. It follows older experimental data [12]. Other evaluated libraries, including CENDL, use the same evaluation. The dashed line is a fit of newer data with an exponential polynomial function of Mandelstam variables. The angular distribution determines the neutron energy distribution because the elastic scattering is a binary reaction. Thus the angular distribution influences the calculated flux in any carbon loaded material, including moderators and neutron detectors.

4. Conclusion

The exclusive CHIPS-TPT code reproduces the results of simulations with inclusive Monte-Carlo codes, being capable to simulate quantities obtainable with exclusive codes only. CHIPS-TPT also strictly complies the energy and momentum conservation requirements inherited from CHIPS. It allows to check the input data for consistency. One of the input ENDF/B-VII.1 files that needs updating is for ^{12}C, which is an important moderator and scintillator material.

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