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MCNP6 Fission Cross Section Calculations at Intermediate and High Energies

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MCNP6 has been Validated and Verified (V&V) against intermediate- and high-energy fission-cross-section experimental data. An error in the calculation of fission cross sections of ^{181}Ta and a few nearby target nuclei by the CEM03.03 event generator in MCNP6 and a “bug” in the calculation of fission cross sections with the GENXS option of MCNP6 while using the LAQGSM03.03 event generator were detected during our V&V work. After fixing both problems, we find that MCNP6 using CEM03.03 and LAQGSM03.03 calculates fission cross sections in good agreement with available experimental data for reactions induced by nucleons, pions, and photons on both subactinide and actinide nuclei at incident energies from several tens of MeV to about 1 TeV.

I. INTRODUCTION

MCNP6 [1] is used in various applications involving fission reactions at low, but also at intermediate and high energies. It is critical that it describes such reactions as well as possible, therefore it is often validated and verified against available experimental data and calculations by other models (see, e.g., [1, 2] and references therein). However, for nuclear reactions involving fission, generally the transport codes are only tested for how well they describe the fission-fragment yields, and the emission of particles from them (spectra and multiplicities, both “prompt” and “delayed”). Calculation of fission cross sections, σ_f , themselves by the transport codes is usually not tested, as it is assumed that data libraries used at energies below 150 MeV must provide reliable σ_f , as should the event generators used at higher energies. Our recent work [3] shows that this assumption is too optimistic, as some event generators have problems describing well some fission cross sections. In such cases, all the characteristics of the corresponding fission reactions calculated by the transport codes, like the yields of fission fragments, spectra and multiplicities of neutrons and other particles, both “prompt” and “delayed” would also not be reliable. To assess this situation, we test how MCNP6 calculates σ_f using the Cascade-Exciton Model (CEM) and the Los Alamos version of the Quark-Gluon String Model (LAQGSM) as realized in the event generators CEM03.03 and LAQGSM03.03, respectively, for reactions induced by nucleons, pions, and photons at incident energies from several tens of MeV to ~ 1 TeV.

A comprehensive description of the CEM03.03 and LAQGSM03.03 event generators can be found in Ref. [4]. Therefore, we present only a brief summary of how CEM03.03 and LAQGSM03.03 calculate fission cross sections, needed to better understand our results.

II. σ_f CALCULATION BY CEM AND LAQGSM

CEM03.03 and LAQGSM03.03 calculate the fission cross sections (and the yields of fission products and evaporation of particles from them) using a modification of the Generalized-Evaporation-Model code GEM2 by Furihata [5]. GEM2, in its turn, is based on a modification of the older RAL fission-model code by Atchison (see [6] and references therein). For fissioning nuclei with $Z_j \leq 88$, GEM2 uses the original Atchison calculation of the neutron emission width Γ_n and fission width Γ_f to estimate the fission probability as

$$P_f = \frac{\Gamma_f}{\Gamma_f + \Gamma_n} = \frac{1}{1 + \Gamma_n/\Gamma_f}. \quad (1)$$

Atchison uses [6] the Weisskopf and Ewing statistical model [7]. All details on the RAL and GEM2 codes and all formulas used by them to calculate σ_f can be found in Refs. [5, 6]. Let us mention here only that in the case of subactinide nuclei, the main parameter that determines the fission cross sections calculated by GEM2 is the level-density parameter in the fission channel, a_f (or more exactly, the ratio a_f/a_n), where a_n is the level-density parameter for neutron evaporation. GEM2 uses for it the following approximation:

$$a_f = a_n \left(1.08926 + 0.01098(\chi - 31.08551)^2 \right), \quad (2)$$

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with $\chi = Z^2/A$.

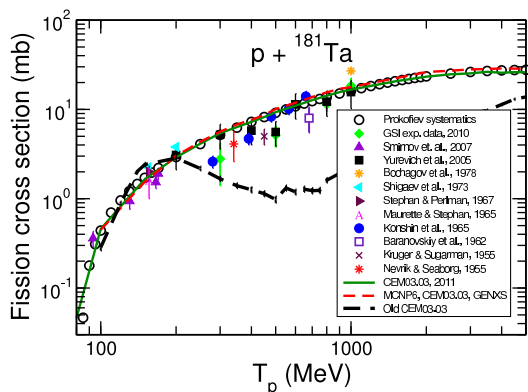


FIG. 1. Prokofiev systematics [10] (open circles) and experimental proton-induced fission cross sections of ^{181}Ta (symbols, see detailed references in [3]) compared with our old MCNP6 calculations (black dashed lines) using the CEM03.03 event generator before we fixed the error, with the corrected CEM03.03 results (green line), and with calculations by the updated MCNP6 using the corrected CEM03.03 event generator (red dashed line), as indicated.

Furihata obtained Eq. (2) as the best approximation for the ratio a_f/a_n while calculating σ_f with GEM2 used after the Bertini IntraNuclear Cascade (INC) model [8], without taking into account possible preequilibrium emission of particles after the INC. The INC's of CEM and LAQGSM are different from the Bertini version [8], and both models account for preequilibrium emission of particles. Hence, for any particular reaction, the mean mass, $\langle A \rangle$, and charge, $\langle Z \rangle$, numbers of compound nuclei that may fission, as well as their mean excitation energy, $\langle E \rangle$, calculated by CEM and LAQGSM differ from the ones provided by the Bertini INC. As a result, the best approximation provided by Eq. (2) for the Bertini INC is not the best for CEM and LAQGSM. In Ref. [9], we performed our own fitting of the ratio a_f/a_n which works the best for CEM and LAQGSM, using as “experimental” proton-induced σ_f the systematics by Prokofiev [10]. After this adjustment for proton-induced reactions, CEM and LAQGSM were tested on reactions induced by neutrons, photons, and pions, and were found to calculate well σ_f for these types of reactions (see details in [9]).

III. RESULTS

Kowing from [9] that both CEM and LAQGSM describe well σ_f for various reactions, we did not check until very recently how well MCNP6 and its precursor, MCNPX, using CEM and LAQGSM, calculated fission cross sections. The first attempt to calculate σ_f with MCNP6 using CEM03.03 for $p + ^{181}\text{Ta}$ found some very bad results at proton energies above ~ 200 MeV (see the black dashed line in Fig. 1). We verified that these

MCNP6 results were not a problem of the incorporation of CEM03.03 into MCNP6, but were a result of an error inadvertently introduced into CEM03.03 in 2005 during a major upgrade of the code [11].

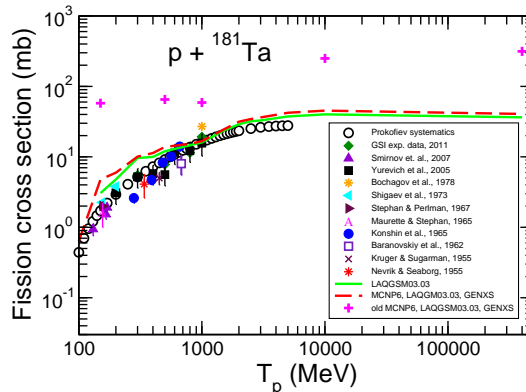


FIG. 2. Prokofiev systematics [10] (open circles) and experimental proton-induced fission cross sections of ^{181}Ta (symbols, see detailed references in [3]) compared with our results by the updated MCNP6 using the LAQGSM03.03 event generator with the GENXS option (red dashed lines) and with calculations by LAQGSM03.03 used as a stand alone code (green lines), as indicated. For comparison, wrong initial results by an older version of MCNP6 (called “Beta 1”), before the “bug” in the calculation of the fission cross section with the GENXS option while using LAQGSM03.03 was fixed, are shown as well with several magenta crosses.

To fix this problem, we have refitted in [3] the values of a_f/a_n in GEM2 for ^{181}Ta . Our new CEM03.03 results for ^{181}Ta are shown in Fig. 1 with a green line. We have replaced in MCNP6 the initial defective CEM03.03 module with the corrected version with the correct values of a_f/a_n in GEM2. Results from the updated MCNP6 are also shown in Fig. 1 by a red dashed line.

Having discovered this 2005 error and knowing how it affects the CEM results, we can understand now why in a recent work [12] it was found that CEM03.02 (which has practically the same physics as the version CEM03.03 used here) provided such a poor agreement with the measured yields of the nuclides produced in proton interactions with ^{181}Ta and nearby target nuclei for energies above 250 MeV.

Unfortunately, we also discovered [3] that σ_f printed in the output files of MCNP6 while using the GENXS option with LAQGSM03.03 were not correct; we present an example of such erroneous results in Fig. 2, shown in the plot with magenta crosses. MCNP6 provides correct results for fission-fragment yields and for particle spectra in its output file. However, an unobserved error in counting the number of fissioning nuclei in the GENXS portion of MCNP6 when using the LAQGSM03.03 event generator was present in the initial Beta 1, version of MCNP6 [1]. We have fixed that error. The current version of MCNP6 is free of that error and provides in its output files correct values for σ_f (see the red dashed line in Fig. 2).

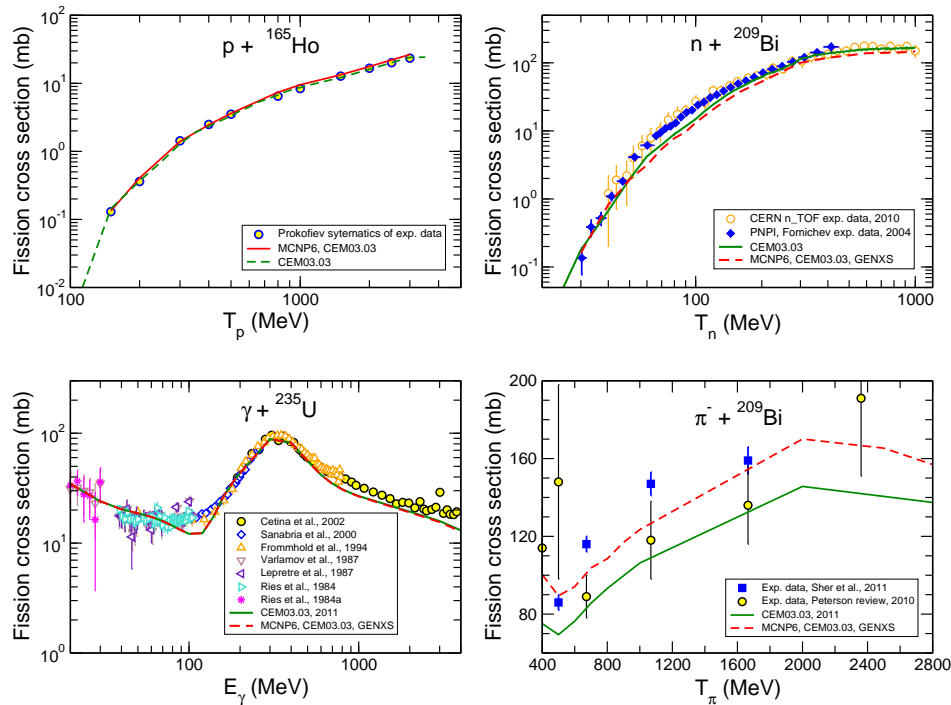


FIG. 3. Examples of σ_f for reactions induced by p , n , γ , and π^- . Detailed references to measured data (symbols) can be found in [3]. Differences in the absolute values of σ_f calculated with CEM03.03 used as a stand-alone code and with MCNP6 using CEM are related to different total reaction cross sections calculated by CEM and used by MCNP6 for these reactions.

After fixing both these problems, we find [3] that MCNP6 using CEM03.03 and LAQGSM03.03 calculates σ_f in good agreement with available data for reactions induced by p , n , γ , and π^- on both subactinide and actinide nuclei, at incident energies from several tens of MeV up to ~ 1 TeV (see an example in Fig. 3 and more details in Ref. [3]).

IV. CONCLUSIONS

MCNP6 has been validated and verified against intermediate- and high-energy fission-cross-section exper-

imental data. An error in the calculation of fission cross sections of ^{181}Ta and other nearby target nuclei by the CEM03.03 event generator of MCNP6 and a “bug” in the calculation of fission cross sections with the GENXS option of MCNP6 while using the LAQGSM03.03 event generator were detected during our current V&V work. After fixing both these problems, we find that MCNP6 using CEM03.03 and LAQGSM03.03 event generators calculates σ_f in a good agreement with available experimental data for reactions induced by nucleons, pions, and photons on both subactinide and actinide nuclei (from ^{165}Ho to ^{239}Pu) at incident energies from several tens of MeV to about 1 TeV.

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