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MCNP6 updated proton-induced fission cross section calculations at intermediate energies

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Abstract. MCNP6 has been Validated and Verified against intermediate- and high-energy fission cross-section experimental data. Recent improvements contained in CEM03.03F and MCNP6-F to consider precompound emission of heavy clusters up to ^{28}Mg has necessitated a re-calculation of fission cross sections. With our re-calculation, we find that CEM03.03F, which is used in MCNP6-F, predicts fission cross sections in good agreement with available experimental data for reactions induced by protons on both subactinide and actinide nuclei at incident energies from several tens of MeV to several GeV.

1. Introduction

The Monte Carlo Methods, Codes, and Applications group within the Computational Physics Division at Los Alamos National Laboratory has led the development of the transport code MCNP6 (Monte Carlo N-Particle transport code, version 6) [1]. MCNP6 is a general-purpose, continuous-energy, generalized-geometry, time-dependent, Monte-Carlo radiation-transport code designed to track many particle types over broad ranges of energies. It is used around the world in applications ranging from radiation protection and dosimetry, nuclear-reactor design, nuclear criticality safety, detector design and analysis, decontamination and decommissioning, accelerator applications, medical physics, space research, and beyond. At lower energies, the code uses tables of evaluated nuclear data, while for higher energies ($>$ 150 MeV), MCNP6 uses the cascade-exciton model, version 03.03 (CEM03.03) [2,3], and the Los Alamos quark-gluon string model, version 03.03 (LAQGSM03.03) [3,4] to model nuclear reactions.

Several significant improvements in CEM03.03 have been made recently, leading to expanded capability to produce energetic heavy clusters heavier than ^{4}He [5,6]. These improvements include expansion of the preequilibrium model to include emission of light fragments up to ^{28}Mg, expansion of the coalescence model to coalesce fragments up to ^{7}Be, and implementation of the Tripathi, et al., inverse cross section model within the preequilibrium stage, among others [7]. These changes have been implemented within a working version of MCNP6, which we call MCNP6-F. Figure 1 illustrates the improved production of heavy clusters obtainable with MCNP6-F. In this figure, MCNP6 with only the GENXS expansion contains none of the heavy cluster upgrades in CEM03.03F; MCNP6 with `npreqtyp=6` contains the cross section and γ_j upgrades but not the preequilibrium or coalescence expansions; and MCNP6 with `npreqtyp=66` contains all four CEM03.03F heavy cluster upgrades.

These improvements in the precompound stages of our codes lead to changes in the distributions of Z, A, and E* at the beginning of the equilibrium decay phase, and thus mandated a refitting of the fission parameters. This paper addresses these new fission cross section calculations.

2. Calculation of fission cross sections

CEM03.03 utilizes the Generalized Evaporation Model as implemented in the code GEM2 by Furihata [9] to calculate fission cross sections. A comprehensive description of GEM2 was published by Furihata [9], therefore we recall here only how fission cross sections are calculated by GEM2, to show how we modify them here. The fission model used in GEM2 is based on Atchison's model [10], often referred in the literature as the Rutherford Appleton Laboratory (RAL) model, which is where Atchison developed it. There are two choices of parameters for the fission model: one of them is the original parameter set by Atchison as implemented in LAHET [11], and the other is a parameter set evaluated by Furihata [9], used here as a default of GEM2.

The Atchison fission model is designed to only describe fission of nuclei with $Z \geq 70$ (we extended it in our codes down to $Z \geq 65$). It assumes that fission competes only with neutron emission, i.e., from the widths Γ_j of n, p, d, t, ^{3}He, and ^{4}He, the RAL code calculates the probability of evaporation of any particle. When a charged particle is selected to be evaporated, no fission competition is taken into account. When a neutron is selected to be evaporated, the code does not actually simulate its evaporation, instead it considers that fission may compete, and chooses either fission or evaporation of a neutron according to the fission probability P_f. This quantity is treated by the RAL code differently for the elements above and below $Z = 89$.

1) $65 \leq Z_j \leq 88$. For fissioning nuclei with $Z_j \leq 88$, GEM2 uses the original Atchison calculation of the

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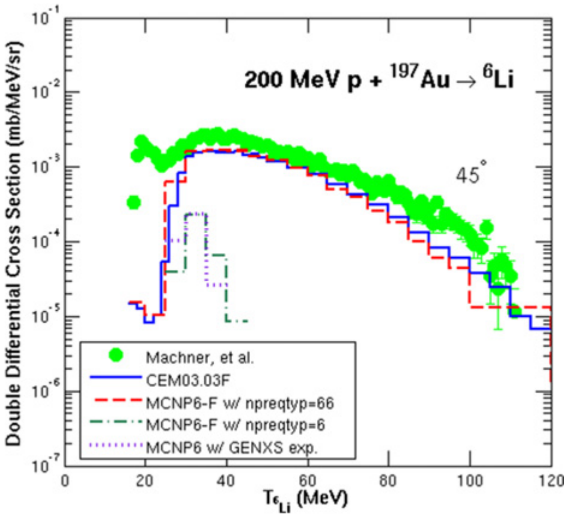

Figure 1. Comparison of experimental data for 200 MeV p + ^{197}Au → ^{6}Li at 45°, measured by Machner, et al. [8] (green circles) to calculations from CEM03.03F (blue solid lines), MCNP6-F with npreqtyp=66 (red dashed lines), MCNP6-F with npreqtyp = 6 (green dash- dotted lines), and MCNP6 with the GENXS extension only (purple dotted lines).

neutron emission width Γ_n and fission width Γ_f to estimate the fission probability as

$$P_f = \frac{\Gamma_f}{\Gamma_f + \Gamma_n} = \frac{1}{1 + \Gamma_n/\Gamma_f}. \tag{1}$$

Atchison uses the Weisskopf and Ewing statistical model [12] with an energy-independent pre-exponential factor for the level density and Dostrovsky's [13] inverse cross section for neutrons and estimates the neutron width Γ_n as

$$\Gamma_n = 0.352(1.68 J_0 + 1.93 A_i^{1/3} J_1 + A_i^{2/3}(0.76 J_1 - 0.05 J_0)) \tag{2}$$

where J_0 and J_1 are functions of the level density parameter a_n and $s_n = 2\sqrt{a_n(E - Q_n - \delta)}$ as

$$J_0 = \frac{(s_n - 1)e^{s_n} + 1}{2a_n}, \tag{3}$$

$$J_1 = \frac{(2\,s_n^2 - 6s_n + 6)e^{s_n} + s_n^2 - 6}{8a_n^2}. \tag{4}$$

The RAL model uses a fixed value for the level density parameter a_n, namely

$$a_n = (A_i - 1)/8. \tag{5}$$

The fission width for nuclei with $Z_j \leq 88$ is calculated in the RAL model and in GEM2 as

$$\Gamma_f = \frac{(s_f - 1)e^{s_f} + 1}{a_f} \tag{6}$$

where $s_f = 2\sqrt{a_f(E - B_f - \delta)}$ and the level density parameter in the fission mode a_f is fitted by Atchison to describe the measured Γ_f/Γ_n as

$$a_f = a_n(1.08926 + 0.01098(\chi - 31.08551)^2) \tag{7}$$

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

2) $Z_j \geq 89$. For heavy fissioning nuclei with $Z_j \geq 89$ GEM2 follows the RAL model and does not calculate at all the fission width Γ_f and does not use Eq. (1) to estimate the fission probability P_f. Instead, the following semi-empirical expression obtained by Atchison by approximating the experimental values of Γ_n/Γ_F published by Vandenbosch and Huizenga [14] is used to calculate the fission probability:

$$\log(\Gamma_n/\Gamma_f) = C(Z_i)(A_i - A_0(Z_i)), \tag{8}$$

where $C(Z)$ and $A_0(Z)$ are constants dependent on the nuclear charge Z only. The values of these constants are those used in the current version of LAHET [11].

When we modified the GEM2 parameters in Refs. [15,16] so that it describes well proton-induced fission cross sections in our CEM and LAQGSM codes, we chose not to use the experimental fission cross sections directly as they are published in the literature. For intermediate- and high-energy reactions, where our codes are intended to be used, the experimental data on proton-induced fission cross sections are sparse and not as precise as for low-energy reactions measured for reactor applications. Fission cross sections measured at such energies in different experiments differ so significantly from each other that it is difficult to use such data in development and validation of models and codes, without a special analysis of all details of every measurement. Fortunately, this has been done by Prokofiev [17] so we use his results. At our energies, we consider Prokofiev's systematics as the most reliable "experimental" fission cross sections and prefer to use them to develop and test our codes instead of using experimental values published in original publications by different authors.

The main parameters that determine the fission cross sections calculated by GEM2 are the level-density parameter in the fission channel, a_f (or more exactly, the ratio a_f/a_n as calculated by Eq. (7)) for preactinides, and parameter $C(Z)$ in Eq. (8) for actinides. The sensitivity of results to these parameters is much higher than to fission barriers used in calculation or other parameters of the model.

In Refs. [15,16] we chose to adjust only these two parameters in our merged CEM+GEM2 and LAQGSM+GEM2 codes. We did not change the form of systematics (7) and (8) derived by Atchison. We only introduced additional coefficients both to a_f and $C(Z)$, replacing $a_f \rightarrow C_a * a_f$ in Eq. (7) and $C(Z_i) \rightarrow C_c * C(Z_i)$ in Eq. (8) and fitted C_a and C_c separately for the CEM+GEM2 and LAQGSM+GEM2 codes for all nuclei and incident proton energies where Prokofiev's systematics apply. The other parameters in GEM2 were unchanged. For preactinides, we fit only C_a; these values are close to one and change smoothly with the proton energy and the charge or mass number of the target. This gives us confidence in our procedure, and allows us to interpolate or extrapolate the values of C_a for nearby nuclei and incident proton energies not covered by Prokofiev's systematics. For actinides, we fit both C_a and C_c. The values of C_a we found are also very close to one, while the values of C_c are more varied, but both of them change smoothly with the proton energy and Z and A of the target, again allowing us to interpolate and extrapolate them for nuclei and energies outside Prokofiev's systematics.

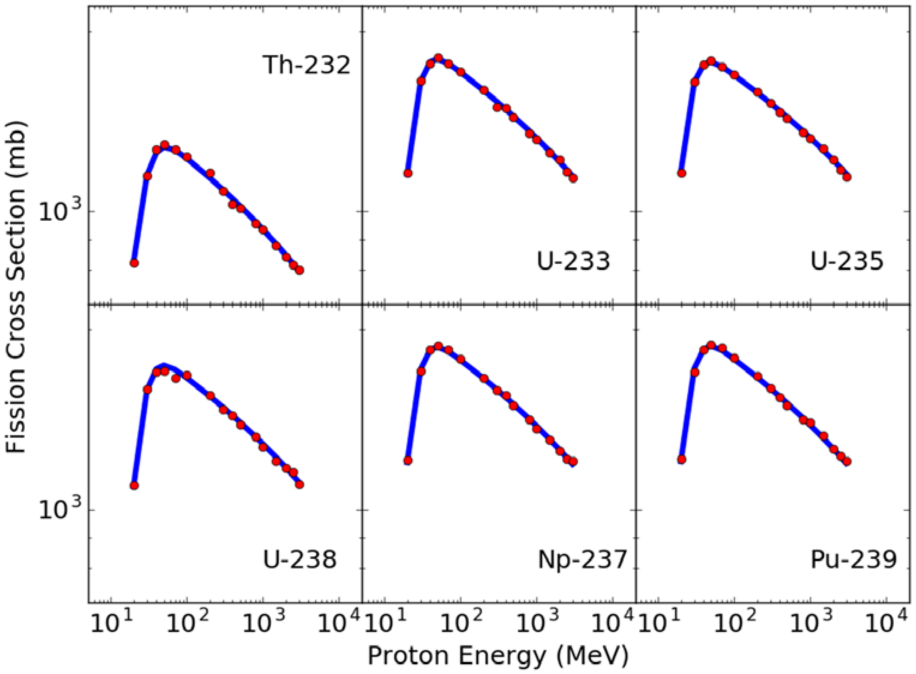

Figure 2. Comparison of Prokofiev's systematics [17] of experimental (p,f) cross sections of ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{237}Np, and ^{239}Pu nuclei (lines) with our CEM03.03F calculations (circles).

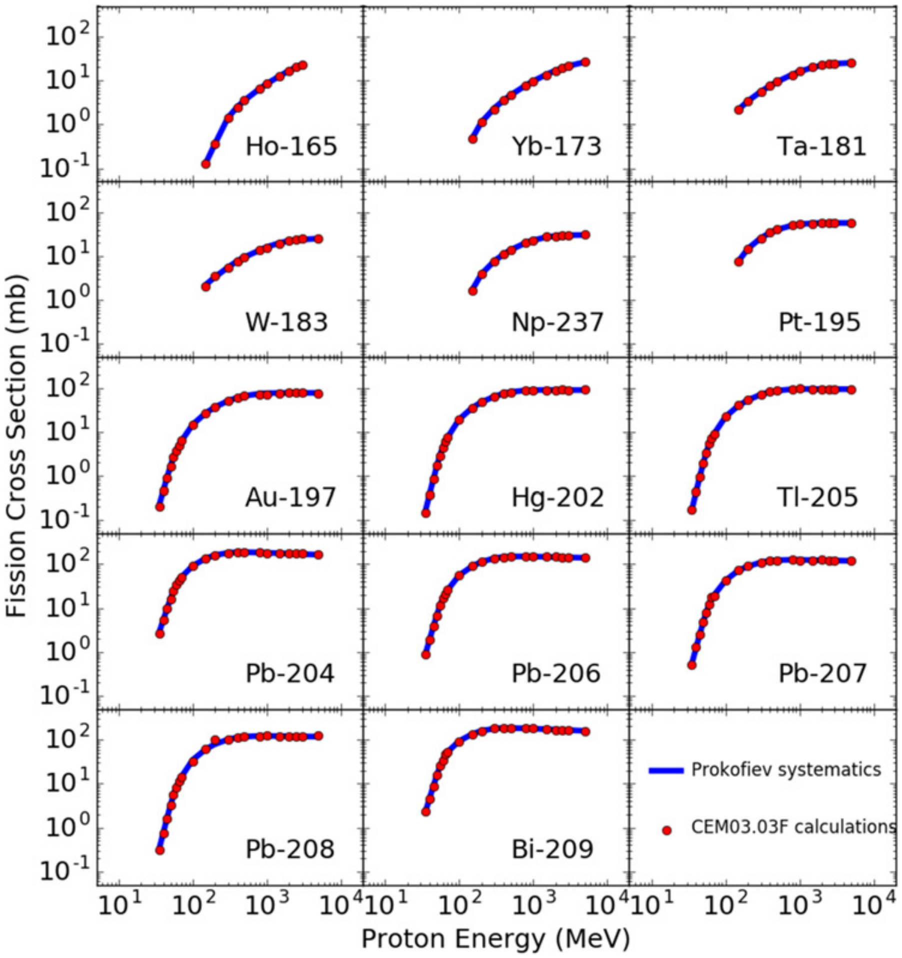

Figure 3. Comparison of Prokofiev's systematics [17] of experimental (p,f) cross sections of ^{165}Ho, ^{173}Yb, ^{181}Ta, ^{183}W, ^{186}Re, ^{195}Pt, ^{197}Au, ^{202}Hg, ^{205}Tl, ^{204}Pb, ^{206}Pb, ^{207}Pb, ^{208}Pb, and ^{209}Bi nuclei (lines) with our CEM03.03F calculations (circles).

3. Results

By fitting each of Prokofiev's systematics and employing interpolation routines, we found the results shown in Figs. 2 and 3 for CEM03.03F. These updated fission cross sections are currently being incorporated into MCNP6-F and we expect all heavy cluster upgrades and fission re-calculations to be part of the next MCNP6 release.

We regret to inform the reader that one of our co-authors, Stepan Mashnik, passed away shortly before ND2016. We miss him dearly.

References

[1] T. Goorley, M. James, T. Booth, F. Brown, J. Bull, L. Cox, J. Durkee, J. Elson, M. Fensin, R. Forster et al., Nuclear Technology **180**, 298 (2012)

[2] K. Gudima, S. Mashnik, V. Toneev, Nuclear Physics A **401**, 329 (1983)

[3] S. Mashnik, K. Gudima, R. Prael, A. Sierk, M. Baznat, N. Mokhov, *CEM03.03 and LAQGSM03.03 event generators for the MCNP6, MCNPX, and MARS15 transport codes*, Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions. Trieste, Italy (2008), LANL Report LA-UR-08-2931, arXiv:0812.1820

[4] K. Gudima, S. Mashnik, A. Sierk (2001), LANL Report LA-UR-01-6804; `http://lib-www.lanl.gov/lapubs/00818645.pdf`

[5] L. Kerby, S. Mashnik, K. Gudima, A. Sierk, J. Bull, M. James, Transactions of the American Nuclear Society **114**, 647 (2016)

[6] S. Mashnik, L. Kerby, K. Gudima, A. Sierk, J. Bull, M. James, *Production of energetic light fragments in CEM, LAQGSM, and MCNP6*, to be published in Physical Review C

[7] R. Tripathi, F. Cucinotta, J. Wilson, Nuclear Instruments and Methods in Physics Research B **117**, 347 (1996)

[8] H. Machner, D. Aschman, K. Baruth-Ram, J. Carter, A. Cowley, F. Goldenbaum, B. Nangu, J. Pilcher, E. Sideras-Haddad, J. Sellschop et al., Physical Review C **73**, 044606 (2006)

[9] S. Furihata, K. Nita, S. Meigo, Y. Ikeda, F. Maekawa, *GEM code – a simulation program for the evaporation and the fission process of an excited nucleus*, Japan Atomic Energy Research Institute (2001), JAERI-Data/Code 2001–015

[10] F. Atchison, *Spallation and fission in heavy metal nuclei under medium energy proton bombardment*, Proc. Meeting on Targets for Neutron Beam Spallation Source (1979)

[11] R. Prael, H. Lichtenstein, *User guide to LCS: the LAHET code system*, LANL Report LA-UR-89-3014 (1989)

[12] V. Weisskopf, D. Ewing, Physical Review **57**, 472 (1940)

[13] I. Dostrovsky, Z. Fraenkel, G. Friedlander, Physical Review **116**, 683 (1959)

[14] R. Vandenbosch, J. Huizenga, *Nuclear Fission* (Academic Press, 1973)

[15] M. Baznat, K. Gudima, S. Mashnik, *Proton-induced fission cross section calculation with the LANL codes CEM2k+GEM2 and LAQGSM+GEM2*, American Nuclear Society Annual Meeting, AccApp'03 Embedded Topical Meeting, San Diego, California (2003), LANL Report LA-UR-03-3750, `arXiv:nucl-th/0307014`

[16] S. Mashnik, A. Sierk, R. Prael, *MCNP6 fission cross section calculations at intermediate and high energies*, LANL Report LA-UR-12-00228 (2012)

[17] A. Prokofiev, Nuclear Instruments and Methods A **463**, 557 (2001)