

Complex particle production by CEM03.03

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Abstract

The coalescence, preequilibrium, evaporation, fission, and Fermi breakup models used by the last versions of our Cascade-Exciton Model event generator CEM03.03 have been extended recently to improve description of complex particles production from nuclear reactions. Here, we test how CEM03.03 describes complex particle spectra and yields from all reactions included in the Mandatory List of the International Benchmark of models organized in 2008 under the auspices IAEA and discussed in details at the Satellite Meeting "Nuclear Spallation Reactions", as well as from many other reactions not covered by the Mandatory List. On the whole, CEM03.03 describes reasonably well many measured data on production of d, t, He3, and He4 from various reactions. However, we identified several problems to be solved for a better description of complex particles emission from some reactions, and we see a necessity to extend the preequilibrium emission for fragments heavier than He4, currently neglected by CEM03.03.

This work was partially supported by the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396

The **INC** of **CEM03.03** is based on the “standard”(non-time-dependent) version of the Dubna cascade model [1,2], improved and developed further at LANL during recent years [3-7]:

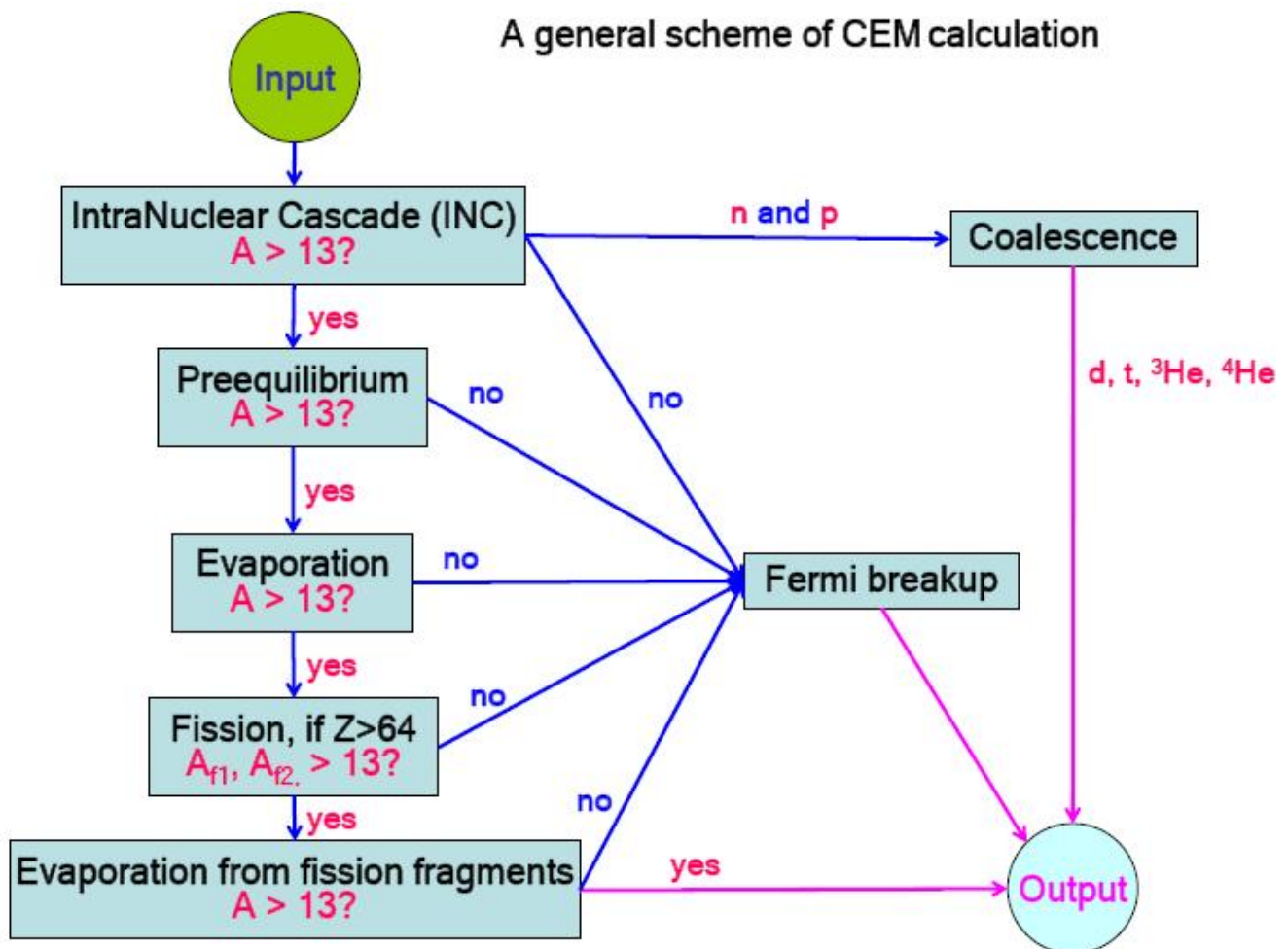
The **CEM03.03** code calculates nuclear reactions induced by nucleons, pions, and photons. It assumes that reactions occur generally in three stages. The first stage is the **IntraNuclear Cascade (INC)**, in which primary particles can re-scattered and produce secondary particles several times prior to absorption by, or escape from the nucleus. Then the cascade stage of a reaction is completed, CEM03.03 uses the **coalescence** model to “create” high energy d, t, ^3He , and ^4He by final-state interactions among emitted cascade nucleons, already outside of the target. The emission of the cascade particles determines the particle-hole configuration, Z,A, and excitation energy that is the starting point for the second, **preequilibrium** stage of the reaction. The subsequent relaxation of the nuclear excitation is treated in terms of an improved version of the modified exciton model of preequilibrium decay followed by the **equilibrium evaporation/fission** stage of the reaction. But if the residual nuclei after INC have mass numbers with $A \leq 12$, CEM03.03 uses the **Fermi breakup** model to calculate their further desintegration instead of using the preequilibrium and evaporation models. Generally, all four components may contribute to experimentally measured particle spectra and other distributions:

$$\sigma(\mathbf{p})d\mathbf{p} = \sigma_{\text{in}}[N^{\text{cas}}(\mathbf{p}) + N^{\text{prq}}(\mathbf{p}) + N^{\text{eq}}(\mathbf{p})]d\mathbf{p}.$$

$$N^{\text{cas}}(\mathbf{p})d\mathbf{p} = \frac{1}{\sigma_{\text{in}}} \int_0^R d^2b \int_{r>R} d\mathbf{r} \int_0^{t_{\text{cas}}} dt f_b^{\text{cas}}(\mathbf{r}, \mathbf{p}, t)d\mathbf{p},$$

$$N^{\text{p.eq.}}(\mathbf{p})d\mathbf{p} = \int_{t_{\text{cas}}}^{t_{\text{eq}}} \sum_n \lambda_c^j(n, E, T)P(E, n, t) \frac{\partial(p, \Omega)}{\partial(T, \Omega)} F(\Omega)dT d\Omega.$$

$$N^{\text{eq}}(\mathbf{p})d\mathbf{p} = \int_{t_{\text{eq}}}^{\infty} dt \sum_n \lambda_c^j(n, E, T)P(E, n, t) \frac{\partial(p, \Omega)}{\partial(T, \Omega)} F(\Omega)dT d\Omega,$$



In comparison with the initial version [1,2] of INC, in CEM03.03 we have:

- 1) Developed better approximations for the total elementary cross sections;
- 2) Developed new approximations to describe more accurately experimental elementary energy and angular distributions of secondary particles from hadron-hadron and photon-hadron interactions;
- 3) Normalized photonuclear reactions to detailed systematics developed by M. Kossov and nucleon-induced reactions, to NASA and Kalbach systematics;
- 4) The condition for transition from the INC stage of a reaction to preequilibrium was changed; on the whole, the INC stage in CEM03.03 is longer while the preequilibrium stage is shorter in comparison with previous versions;
- 5) Incorporation of real binding energies for nucleons in the cascade instead of the approximation of a constant separation energy of 7 MeV used in the initial versions of the CEM; imposing momentum-energy conservation for each simulated event (provided only “on the average” by

the initial versions);

6) The algorithms of many INC routines were changed and almost all INC routines were rewritten, which speeded up the code significantly;

7) Some preexisting bugs in the INC were fixed.

An **important ingredient** of the CEM is the criterion for transition from the intranuclear cascade to the preequilibrium model. In conventional cascade-evaporation models (like the Bertini INC used in MCNPX [8]), fast particles are traced down to some minimal energy, the cutoff energy T_{cutt} (or one compares the duration of the cascade stage of a reaction with a cutoff time, in “time-like” INC models, such as the Liege INC [9]). This cutoff is usually less than ≈ 10 MeV above Fermi energy, below which particles are considered to be absorbed by the nucleus. The CEM uses a different criterion to decide when a primary particle is considered to have left the cascade.

An effective local optical absorptive potential $W_{\text{opt.mod.}}(\mathbf{r})$ is defined from the local interaction cross section of the particle, including Pauli-blocking effects. This imaginary potential is compared to one defined by a phenomenological global optical model $W_{\text{opt.exp.}}(\mathbf{r})$. We characterize the degree of similarity or difference of these imaginary potentials by the parameter

$$C = |(W_{\text{opt.mod.}} - W_{\text{opt.exp.}}) / W_{\text{opt.exp.}}|$$

When C increases above an empirically chosen value, the particle leaves the cascade, and is then considered to be an exciton. From a physical point of view, such a smooth transition from the cascade stage of the reaction seems to be more attractive than the “sharp cutoff” method. CEM03.03 uses a fixed value $P = 0.3$.

The Coalescence Model

When the cascade stage of a reaction is completed, CEM03.03 use the coalescence model proposed for heavy ion collisions to “create” high-energy d, t, ^3He , and ^4He by final-state interactions among emitted cascade nucleons, already outside of the target nucleus. We assume that all the cascade nucleons having differences in their momenta smaller than p_c and the correct isotopic content form an appropriate composite particle. This means that the formation probability for, e.g. a deuteron is

$$W_d(\mathbf{p}, b) = \int \int d^3\mathbf{p}_p d^3\mathbf{p}_n \rho^C(\mathbf{p}_p, b) \rho^C(\mathbf{p}_n, b) \delta(\mathbf{p}_p + \mathbf{p}_n - \mathbf{p}) \Theta(p_c - |\mathbf{p}_p - \mathbf{p}_n|),$$

where the particle density in momentum space is related to the one-particle distribution function f^C by

$$\rho^C(\mathbf{p}, b) = \int d^3\mathbf{r} f^C(\mathbf{r}, \mathbf{p}, b)$$

and values of coalescence parameters

$$p_c = 150, 175, 175, 175 \text{ MeV}/c \text{ for } d, t, {}^3\text{He} \text{ and } {}^4\text{He}.$$

Preequilibrium Reactions

The subsequent preequilibrium interaction stage of nuclear reactions is considered by our current CEM in the framework of the latest version of the Modified Exciton Model (MEM) [10,11] as implemented in CEM03.01 [12]. At the preequilibrium stage of a reaction we take into account all possible nuclear transitions changing the number of excitons n with $\Delta n = +2, -2$, and 0 , as well as possible multiple subsequent emissions of $n, p, d, t, {}^3\text{He}$, and ${}^4\text{He}$. The corresponding system of master equations describing the behavior of a nucleus at the preequilibrium stage is solved by the Monte-Carlo technique [13,14].

Evaporation/Fission

CEM03.03 use an extension of the Generalized Evaporation Model (GEM) code GEM2 by Furihata [15] after the preequilibrium stage of reactions to describe evaporation of nucleons, complex particles, and light fragments heavier than ${}^4\text{He}$ (up to ${}^{28}\text{Mg}$) from excited compound nuclei and to describe their fission, if the compound nuclei are heavy enough to fission ($Z \geq 65$). The GEM2 includes up to 66 types of particles and fragments that can be evaporated from an excited nucleus.

The Fermi Breakup Model

After calculating the coalescence stage of a reaction, CEM03.03 move to the description of the last slow stages of the interaction, namely preequilibrium decay and evaporation, with a possible competition of

fission. But if the residual nuclei have atomic numbers with $A < 13$ CEM03.03 use the Fermi breakup model [16] to calculate their further disintegration instead of using the preequilibrium and evaporation models. The newer versions of our codes use the Fermi breakup model also during the preequilibrium and/or evaporation stages of reactions, when the residual nucleus has an atomic number $A < 13$. Finally, the latest 03.03 versions of our codes use the Fermi breakup model also to disintegrate the unstable fission fragments with $A < 13$ that can be produced in very rare cases of very asymmetric fission.

Results

The results of benchmarking of CEM03.03 for composite particles production in different nuclear reactions are presented on the figures 1-10 and compared with the experimental data. Generally there is a good description of the data.

Summary

CEM03.03 versions describe the production of composite particles (d, t, ^3He , and ^4He) from nuclear reactions in a wide range of incident energies of interest to Spallation Applications better than earlier versions.

As a rule, CEM03.03 describe such reactions not worse than other codes presently available, and are often much faster, which is very important in complex simulations.

The latest versions of our code CEM03.03, have been or are being incorporated into MCNP6, MCNPX, and MARS15, to be available to users from RSICC and NEA/OECD as the Code Package PSR-0532.

References

- 1) V. S. Barashenkov, K. K. Gudima, and V. D. Toneev, JINR Communications P2-4065 and P2-4066, Dubna (1968); P2-4661, Dubna (1969); Acta Physica Polonica 36(1969) 415.
- 2) V. S. Barashenkov and V. D. Toneev, Interaction of High Energy Particle and Nuclei with Atomic Nuclei, Atomizdat, Moscow (1972); V. S. Barashenkov, et al., Sov. Phys. Usp. 16(1973) 31.
- 3) S. G. Mashnik and A. J. Sierk, Proc. SARE-4, Knoxville, TN, Sep. 13-

- 16, 1998, pp. 29-51 (nucl-th/9812069).
- 4) S. G. Mashnik and A. J. Sierk, Proc. AccApp00, Washington, DC, USA, Nov. 12-16,2000, pp. 328-341 (nucl-th/0011064).
- 5) S. G. Mashnik, K. K. Gudima, A. J. Sierk, R. E. Prael, Proc. ND2004, Sep. 26 —Oct. 1, 2004, Santa Fe, NM, AIP Conf. Proc. 769,pp. 1188-1192 (nucl-th/0502019)
- 6) S. G. Mashnik, K. K. Gudima, R. E. Prael, A. J. Sierk, M. I. Baznat, and N.V.Mokhov, J. Nucl. and Radiochem. Sci. 6, (2005) pp. A1-A19 (nucl-th/0503061).
- 7) S. G. Mashnik, K. K. Gudima, , R. E. Prael, A. J. Sierk, M. I. Baznat, and N.V. Mokhov, Lectures presented at the Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, Feb. 4-8, 2008, ICTP, Trieste, Italy, (LANL Report LA-UR-08-2931).
- 8) *MCNPX User's Manual, Version 2.3.0*, L.S.Waters, Ed., LANL Report LA-UR-02-2607 (April, 2002); Web page <http://mcnpx.lanl.gov/>.
- 9) J. Cugnon, C. Volant, and S. Vuiller, Nucl.Phys. A620 (1997) 475-509; A. Boudard *et al.*, Phys.Rev. C66 (2002) 044615; Th.Aoust and J.Cugnon, Eur.Phys.J. A21 (2004) 79-85.
- 10) K.K. Gudima, G.A. Ososkov, and V.D.Toneev, Yad. Fiz. 21 (1975) [Sov. J. Nucl. Phys. 21 (1975) 138-143].
- 11) S.G. Mashnik and V.D. Toneev, JINR Communication P4-8417, Dubna(1974).
- 12) S.G. Mashnik *et al.*, LANL Report LA-UR-05-7321, Los Alamos (2005); RS-ICC Code Package PSR-532; <http://www-rsicc.ornl.gov/codes/psr/psr5/psr532.html>; <http://www.nea.fr/abs/html/psr-532.html>.
- 13) K.K. Gudima, S.G. Mashnik, and V.D. Toneev, JINR Communication P2-80-774 and P2-80-777, Dubna(1980).
- 14) K.K. Gudima, S.G. Mashnik, and V.D. Toneev, Nucl.Phys. A401 (1983) 329-361.
- 15) S. Furihata, Nucl. Instr. Meth. B 171 (2000) 252-258; S. Furihata *et al.*, JAERI – Data/Code 2001-015, JAERI, Japan (2001); S. Furihata and T.Nakamura, J. Nucl. Sci. Technol. Suppl. 2 (2002) 758 – 761.
- 16) E. Fermi, Progr. Theor. Phys. 5 (1950) 570-583.
- 17) J. Franz *et al.*, Nucl. Phys. A510 (1990) 774
- 18) A. Budzanowsky *et al.*, submitted to PRC.

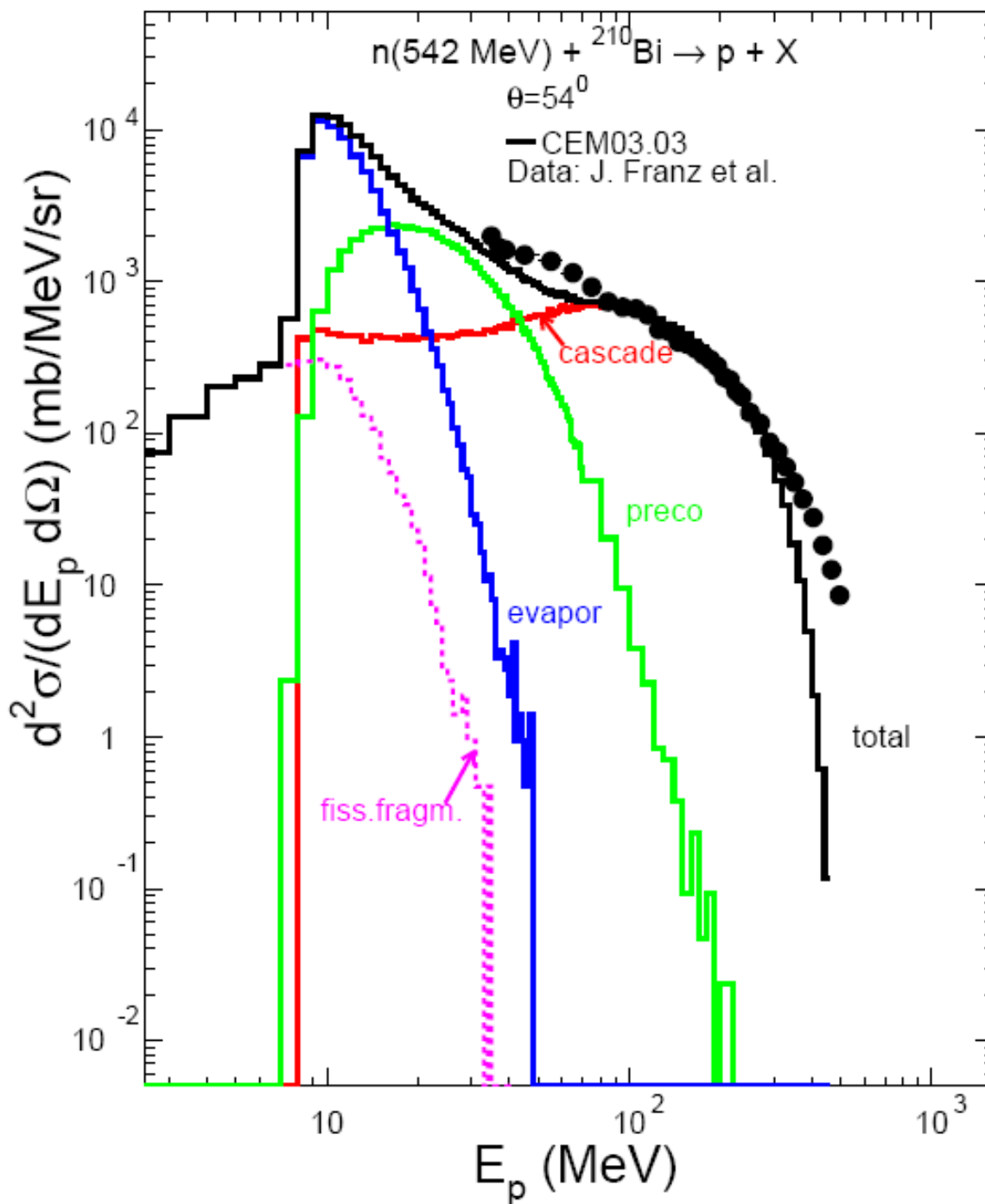


Figure 1. Measured [17] double differential cross sections of protons from interaction of 542 MeV neutrons with ${}^{210}\text{Bi}$ are compared with CEM03.03 calculations. The contributions of different mechanisms to the calculated spectrum are shown: cascade, preequilibrium, evaporation from residual nucleus (evapor) and from fission fragments (fiss.frag.), and sum of all contributions (total) as indicated in corresponding legends of plots.

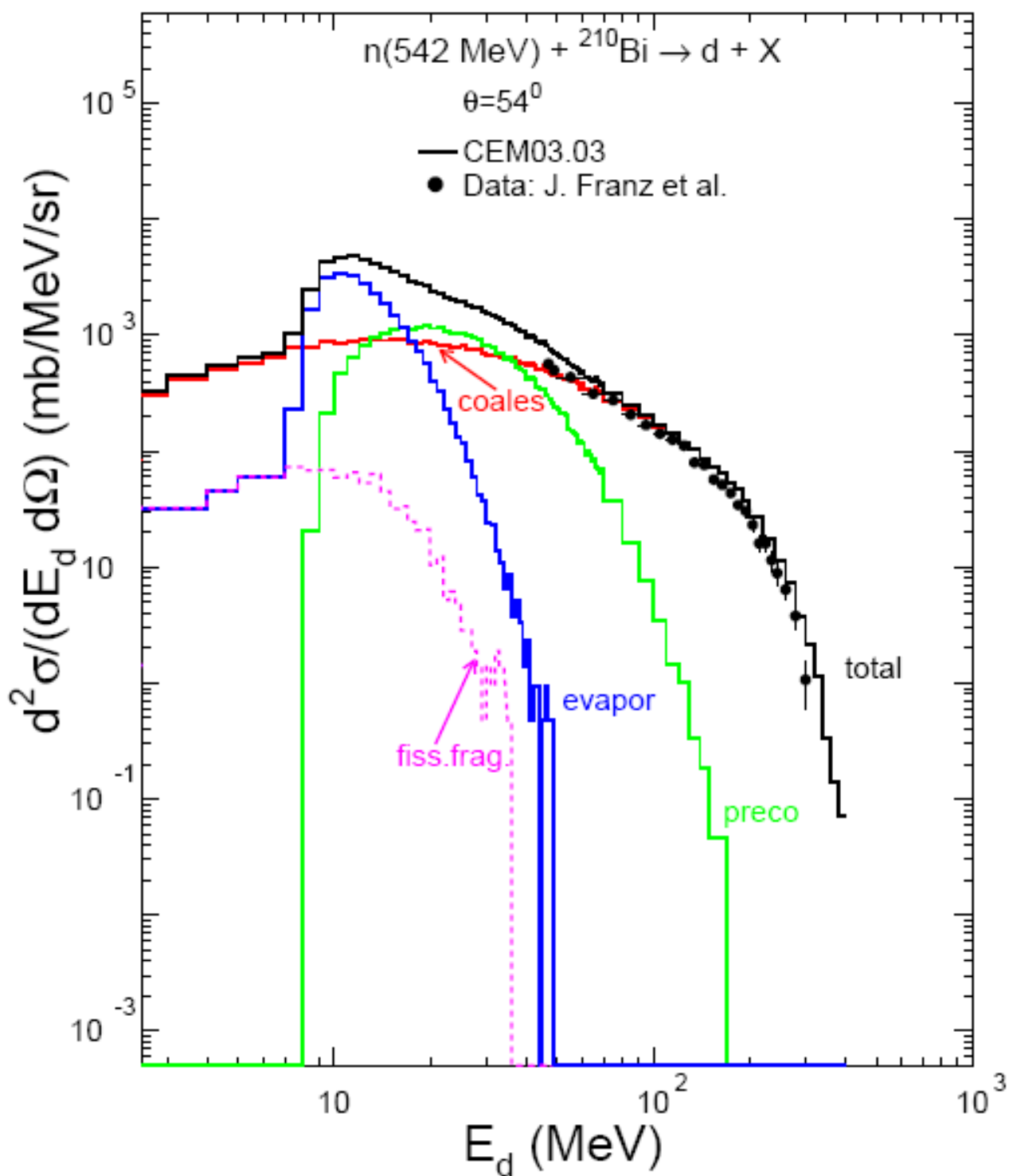


Figure 2. The same as on Figure 1, but for deuterons. Compared with protons here „cascade” component is replaced by coalescence one (coales).

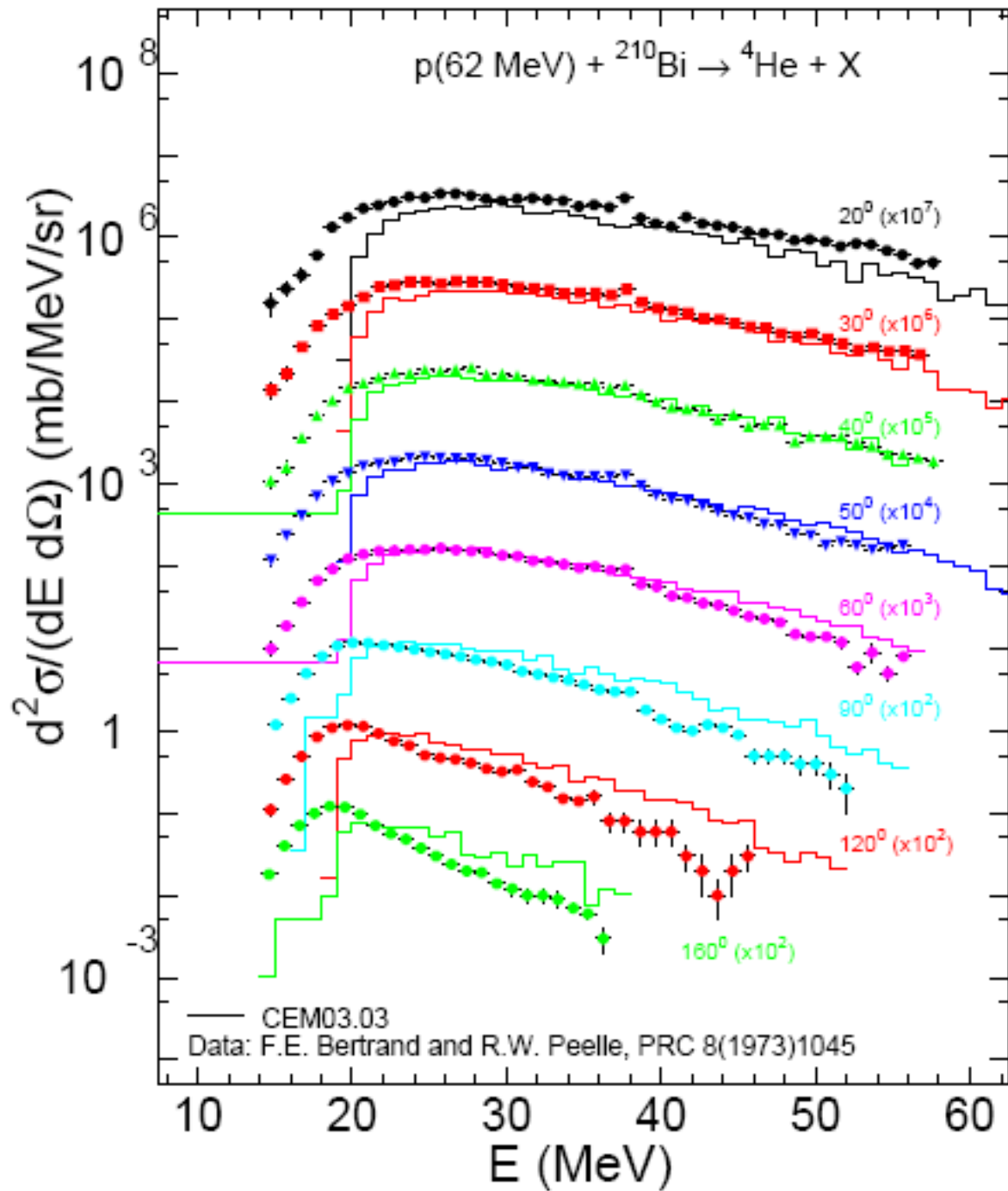


Figure 3. Experimental data for double differential spectra of ${}^4\text{He}$ (points) compared with CEM03.03 calculations (color histograms).

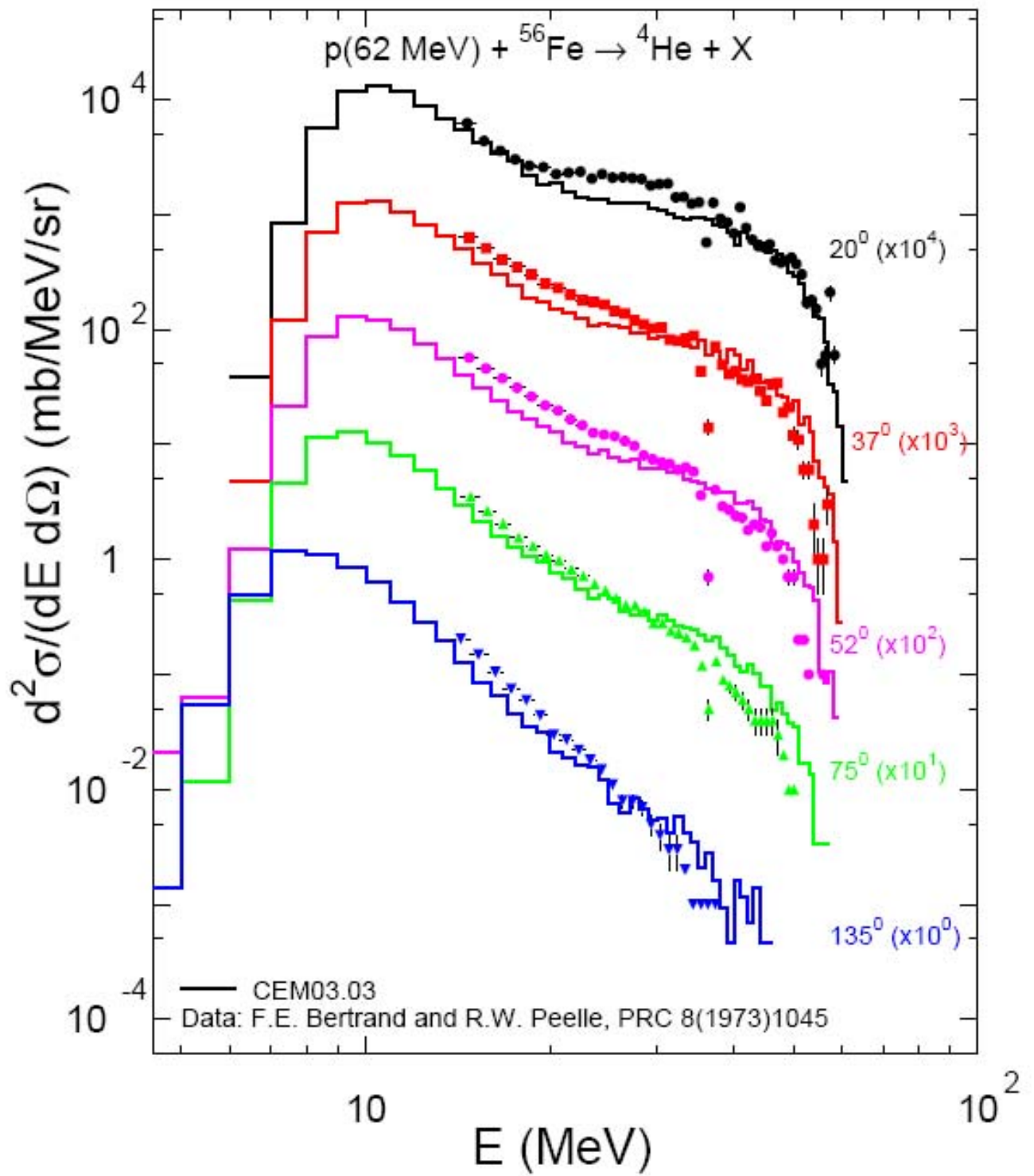


Figure 4. Experimental data for double differential spectra of ${}^4\text{He}$ (points) compared with CEM03.03 calculations (color histograms).

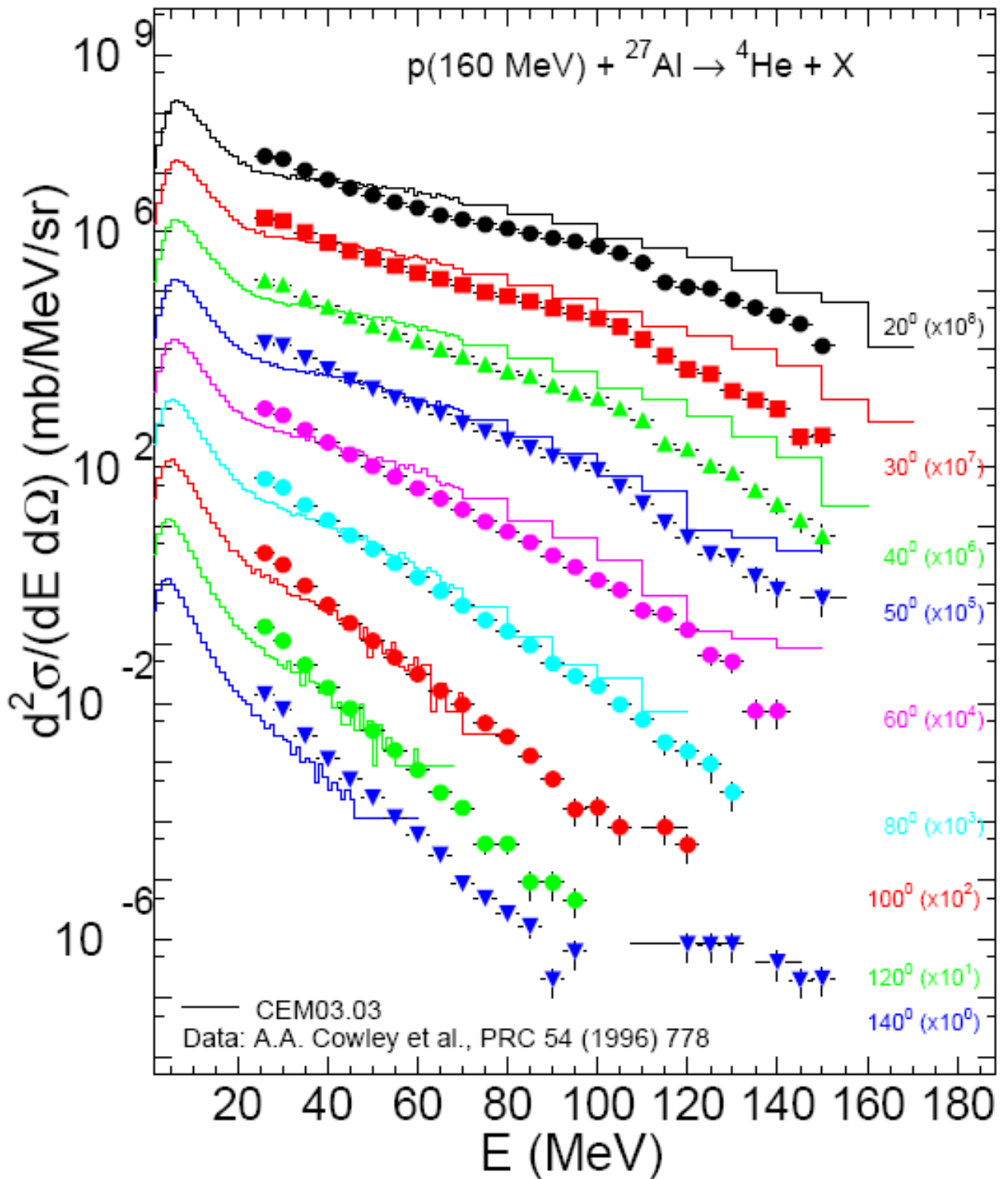


Figure 5. Experimental data for double differential spectra of ${}^4\text{He}$ (points) compared with CEM03.03 calculations (color histograms).

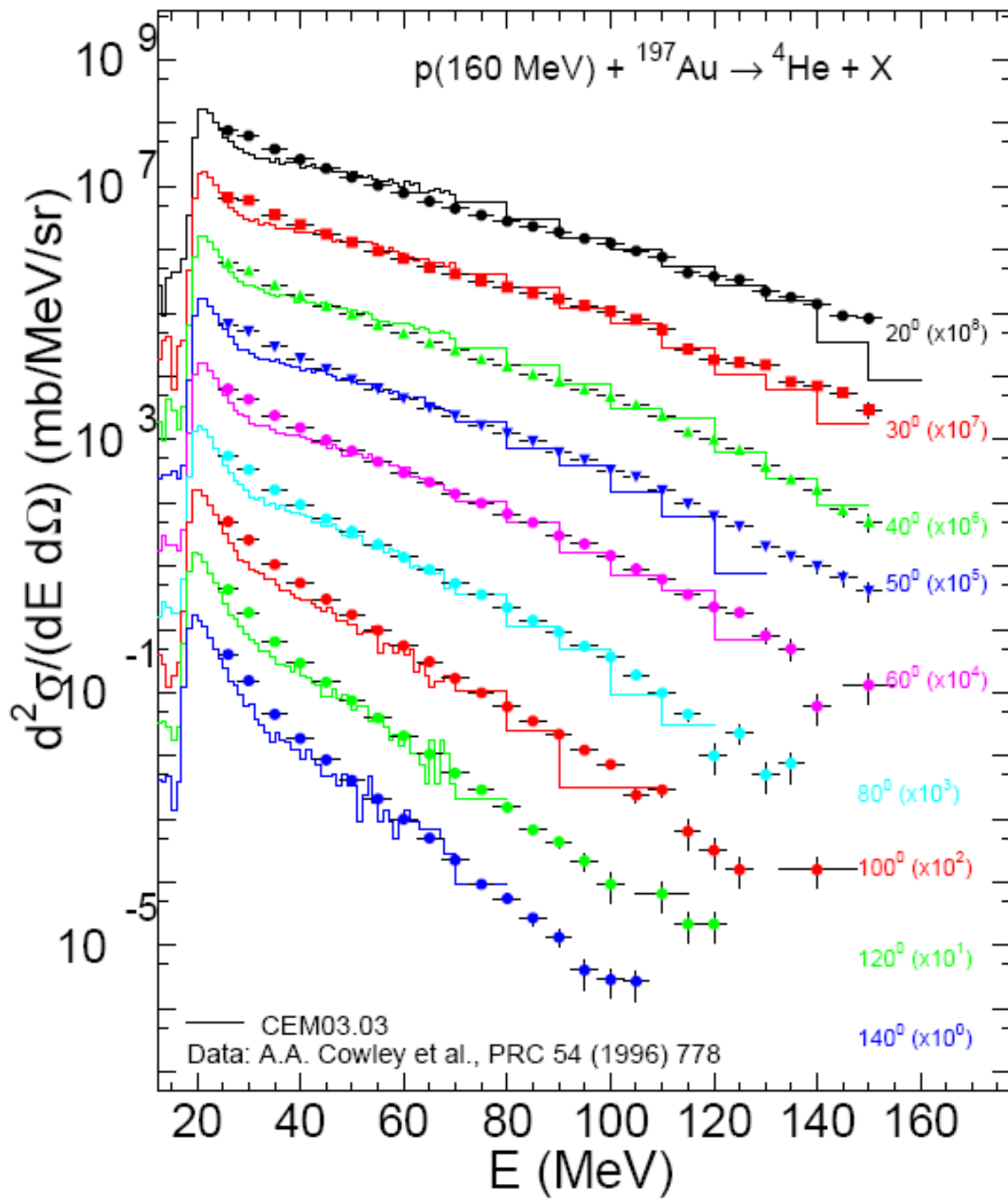


Figure 6. The same as on Figure 5, but for Au target.

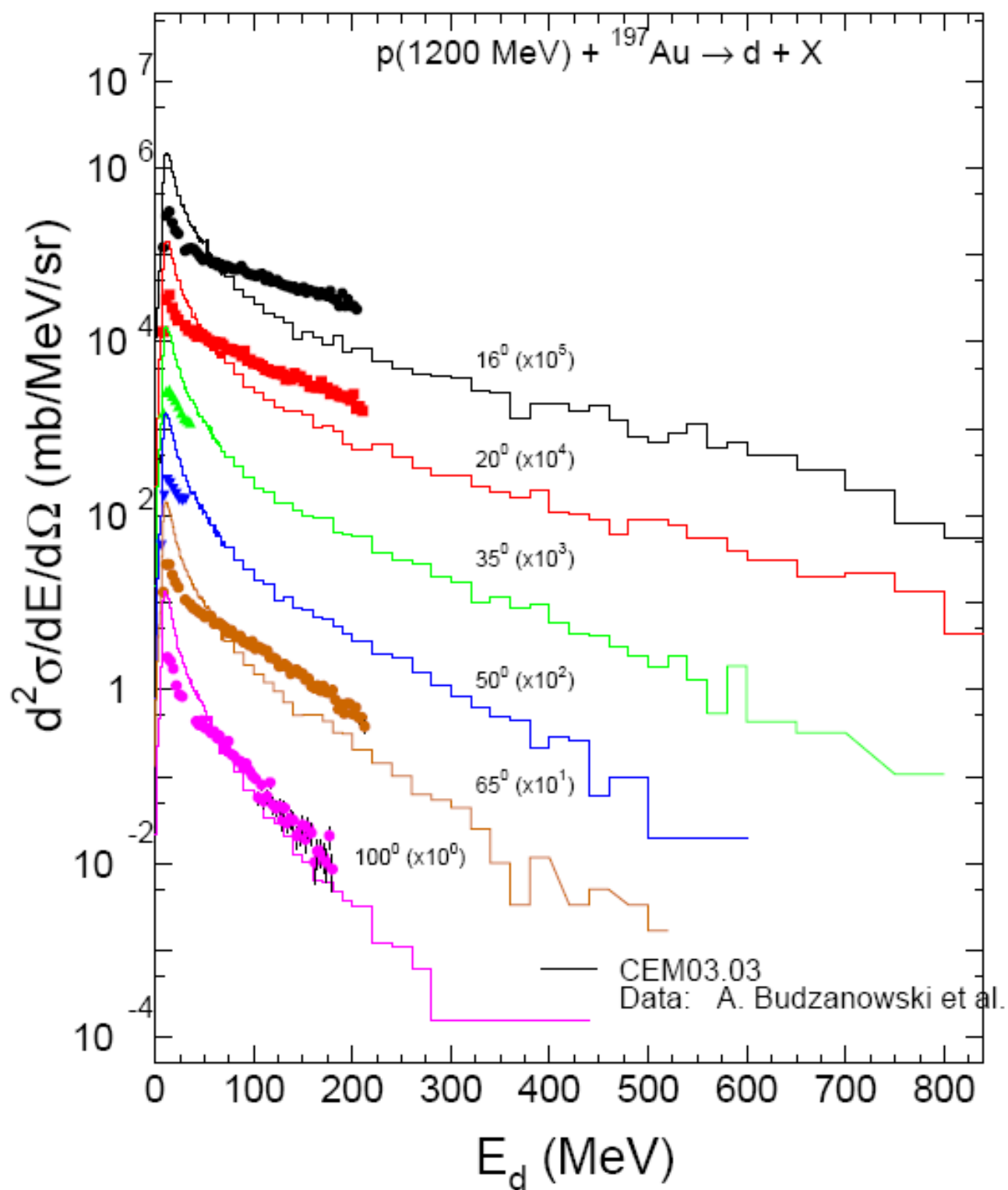


Figure 7. Double differential spectra of deuterons produced in interactions of 1200 MeV protons with ${}^{197}\text{Au}$ target compared with experimental data from [18].

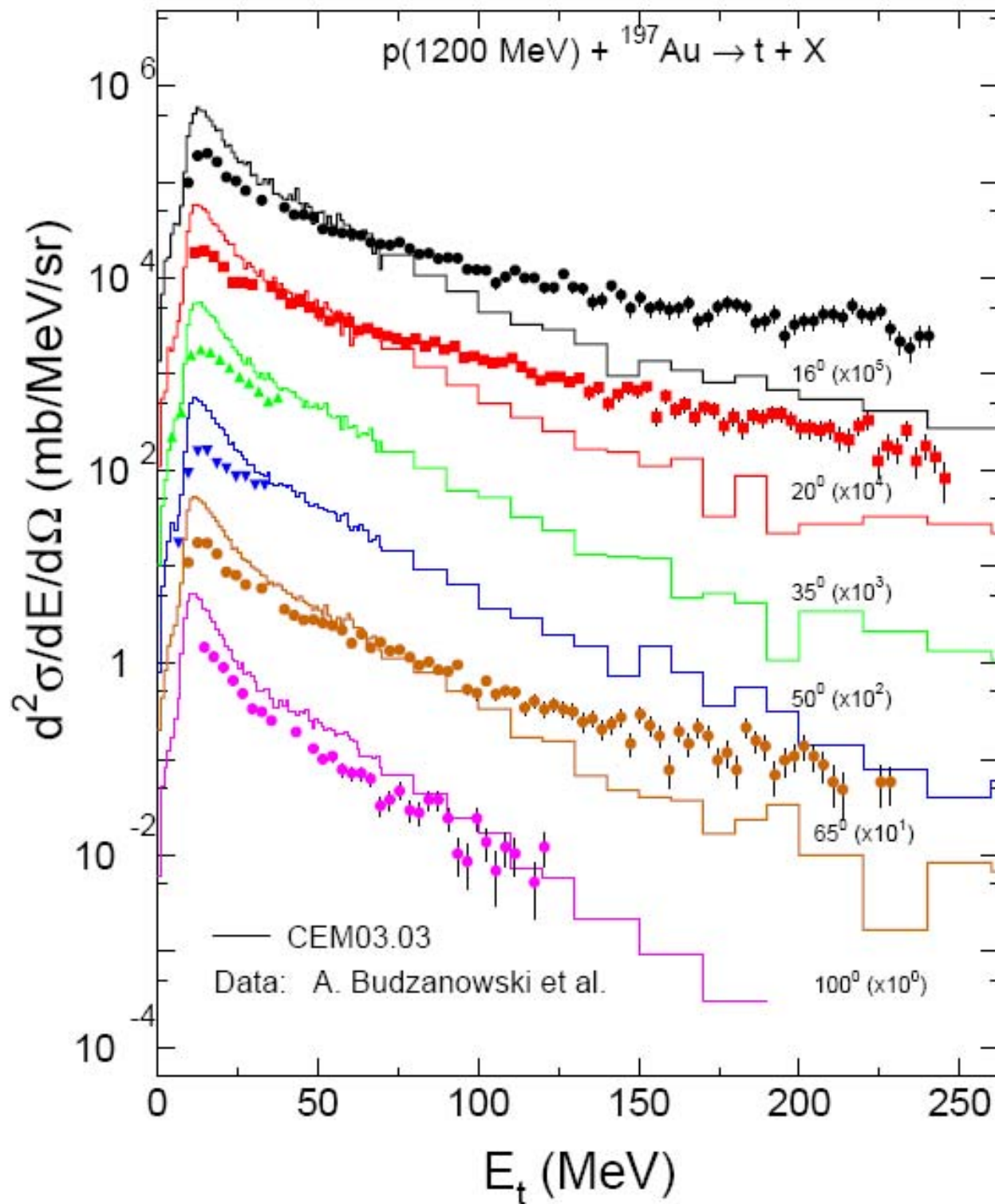


Figure 8. The same as on Figure 7, but for tritium.

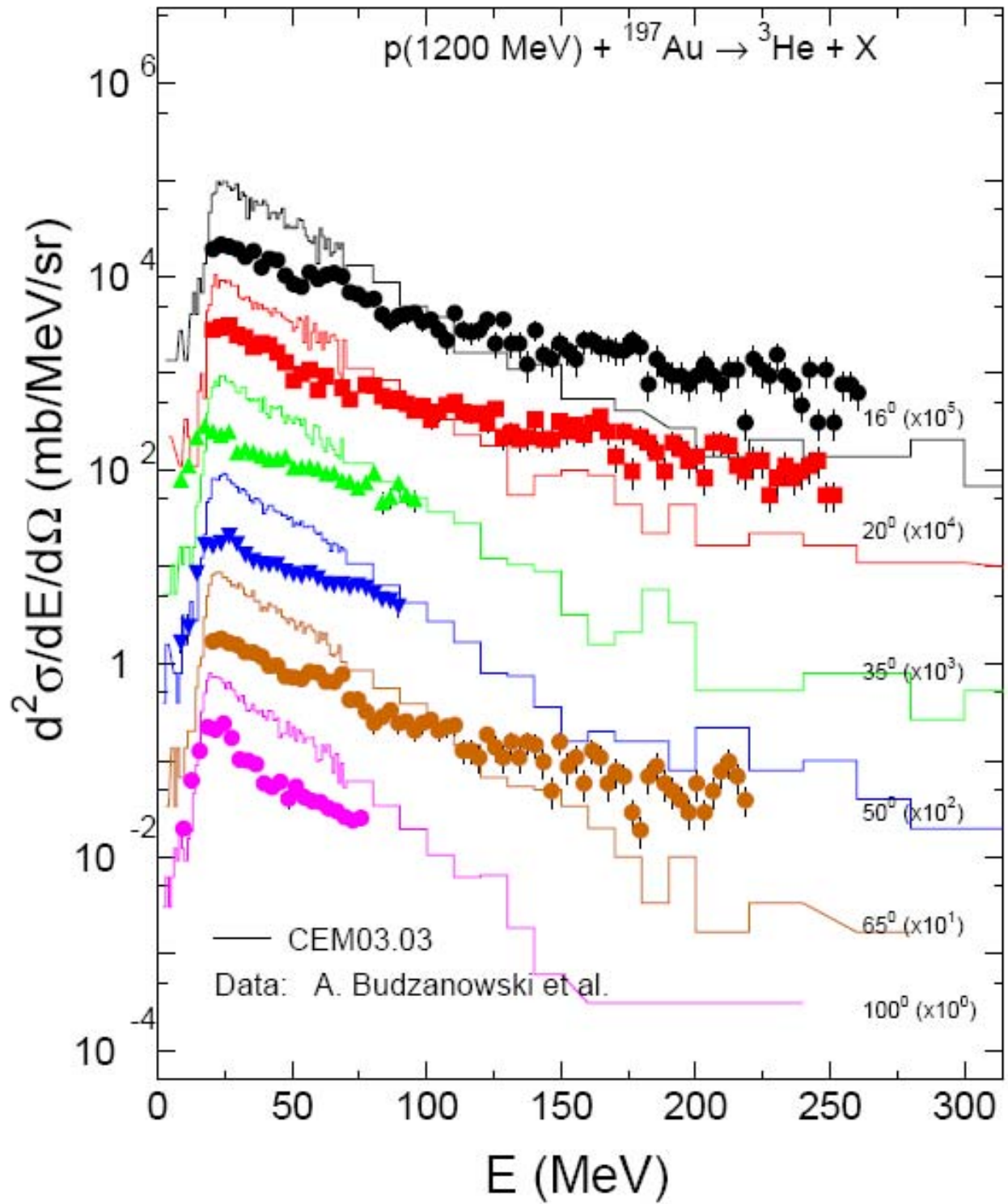


Figure 9. The same as on Figure 7, but for ${}^3\text{He}$.

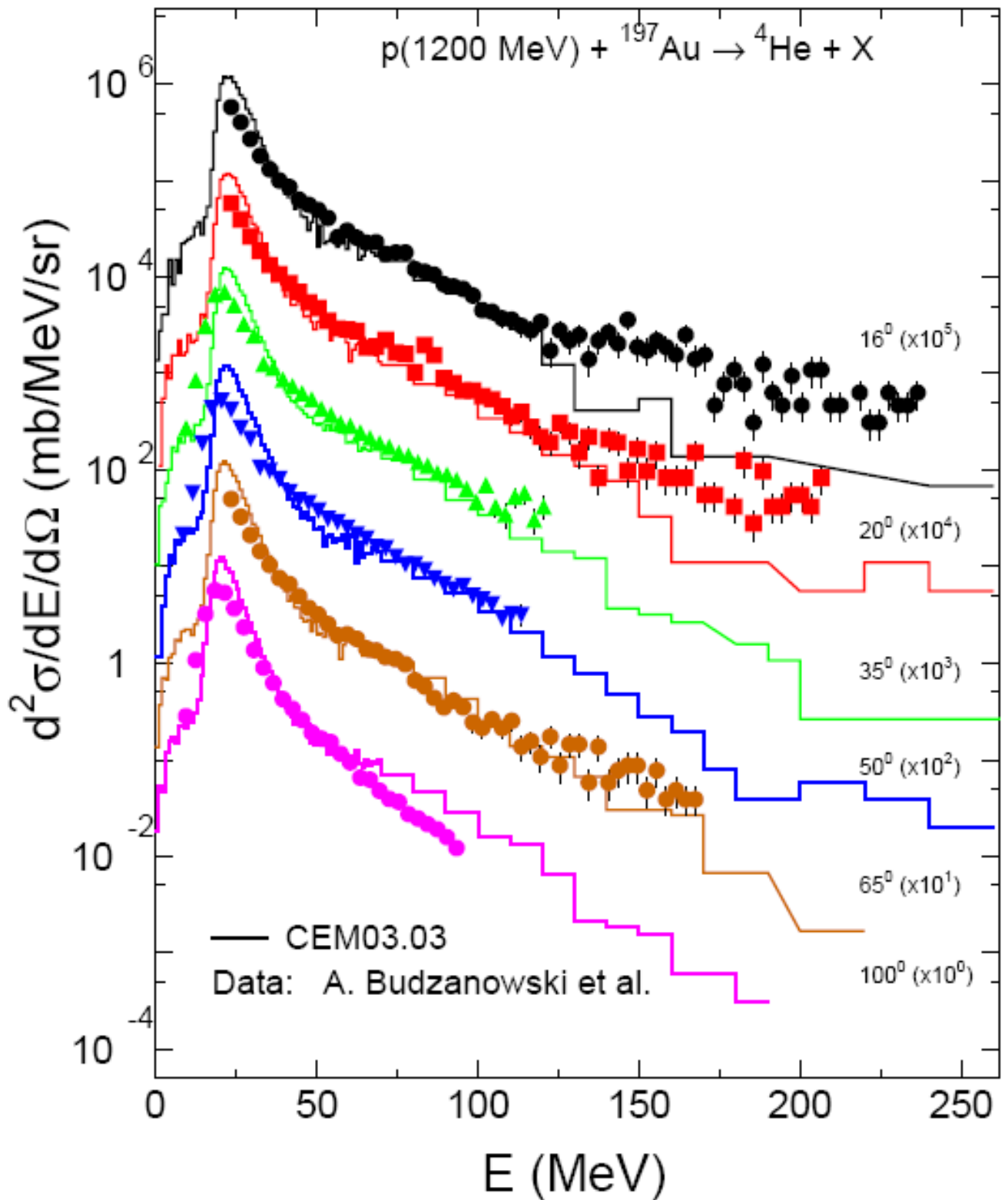


Figure 10. The same as on Figure 7, but for ${}^4\text{He}$.