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Validation and Verification of MCNP6 against High-Energy Experimental Data and Calculations by other Codes. I. The CEM Testing Primer

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Abstract

MCNP6 has been Validated and Verified (V&V) against various recent intermediate- and high-energy measurements as well as against calculations by later versions of MCNPX using different event generators and against results by CEM03.03, LAQGSM03.03/01, INCL+ABLA, INCL4.5+ABLA07, ISABEL+ABLA07, TALYS, ALICE-IPPE, EPAX, ABRABLA, HIPSE, and AMD, used as stand alone codes. New, **/VALIDATION_CEM/** and **/VALIDATION_LAQGSM/** subdirectories in the **/MCNP6/Testing/** directory were created where 18 MCNP6 test-problems that exercise physics of CEM and 18 problems to test MCNP6 with LAQGSM are presented so far together with template files of MCNP6 results, experimental data, and results by other codes. README files that contain short descriptions of every input file, the experiment, the quantity of interest that the experiment measures and its description in the MCNP6 output files, and the publication reference of that experiment are presented for every test-problem. Templates for plotting the corresponding results with **xmgrace** as well as pdf files with figures representing the final results of our V&V efforts are presented. More than a dozen problems or technical "bugs" in MCNP6 and/or in MCNPX discovered during our current V&V of MCNP6 are either fixed already, or are in working process and will be fixed before the next release of MCNP6. Our results show that MCNP6 using our CEM and LAQGSM event generators describes, as a rule, reasonably well different intermediate- and high-energy measured data and agrees very well with similar results obtained with MCNPX and other codes. Here, we describe the V&V of MCNP6 using the CEM event-generator. The test-suite for V&V of MCNP6 using LAQGSM is presented in a separate, second primer of this series. This primer isn't meant to be read from cover to cover. Readers may skip some sections and go directly to a test-problem they are interested in.

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1. Introduction

Following an increased interest in intermediate- and high-energy nuclear reactions in relation to such projects as Accelerator Production of Tritium (APT), Accelerator Transmutation of nuclear Wastes (ATW), Spallation Neutron Source (SNS), Rare Isotope Accelerator (RIA), Proton Radiography (PRAD) as a radiographic probe for the Advanced Hydro-test Facility, NASA needs, and others, the US Department of Energy has supported during the last decade our work on the development of improved versions of the Cascade-Exciton Model (CEM) and of the Los Alamos version of the Quark Gluon String Model (LAQGSM). The latest versions of our codes, CEM03.03 and LAQGSM03.03, have been incorporated recently as event generators in MCNP6 [1, 2], the latest and most advanced LANL Monte Carlo transport code and the principal code product produced by the XCP-3 Group representing a merger of MCNP5 [3] and MCNPX [4]. As multilateral Validation and Verification (V&V) of all our codes is very important and necessary, we decided to V&V specific capabilities of CEM and LAQGSM as event generators in MCNP6.

New, **/VALIDATION_CEM/** and **/VALIDATION_LAQGSM/** subdirectories in the **/MCNP6/Testing/** directory were created where 18 MCNP6 test-problems that exercise physics in CEM and 18 problems to test MCNP6 with LAQGSM are presented so far together with template files of MCNP6 results, experimental data, and results by other codes. README files that contain short descriptions of every input file, the experiment, the quantity of interest that the experiment measures and its description in the MCNP6 output files, and the publication reference of that experiment are presented for every test-problem. Templates for plotting the corresponding results with **xmgrace** as well as pdf files with figures representing the final results of our V&V efforts are presented.

In this primer, we describe the V&V of MCNP6 using the CEM event-generator. The test-suite for V&V of MCNP6 using LAQGSM is presented in a separate, second primer [5] of this series.

To help novice users of MCNP6 and MCNPX, as well as advanced users of MCNP but without sufficient experience in working with our high-energy event generators CEM and LAQGSM, we present here the whole text of all our V&V input files together with a brief description of the corresponding parts of the output files, and provide also extensive comparisons of our MCNP6 results with available experimental data and predictions by other codes.

2. A Brief Survey of CEM and LAQGSM Physics

A detailed description of CEM and LAQGSM may be found in our recent lectures [6] and references therein. Therefore, we present here only a very brief survey of the CEM and LAQGSM physics to help the MCNP6 users chose the proper event generators in their problems as well as a minimum information about the evaporation model used by our codes, needed to better understand several of our current MCNP6 test-problems.

The basic versions of both our CEM and LAQGSM event generators are the so-called "03.01" versions, namely CEM03.01 [7] and LAQGSM03.01 [8]. **The CEM code calculates nuclear reactions induced only by nucleons, pions, and photons, and only at incident energies below $\sim$ 5 GeV.** It assumes that the reactions occur generally in three stages. The first stage is the IntraNuclear Cascade (INC), in which primary particles can be re-scattered and

produce secondary particles several times prior to absorption by, or escape from the nucleus. When the cascade stage of a reaction is completed, CEM03.01 uses the coalescence model to "create" high-energy d, t, ^{3}He, and ^{4}He by final-state interactions among emitted cascade nucleons, already outside of the target (see Fig. 1 below).

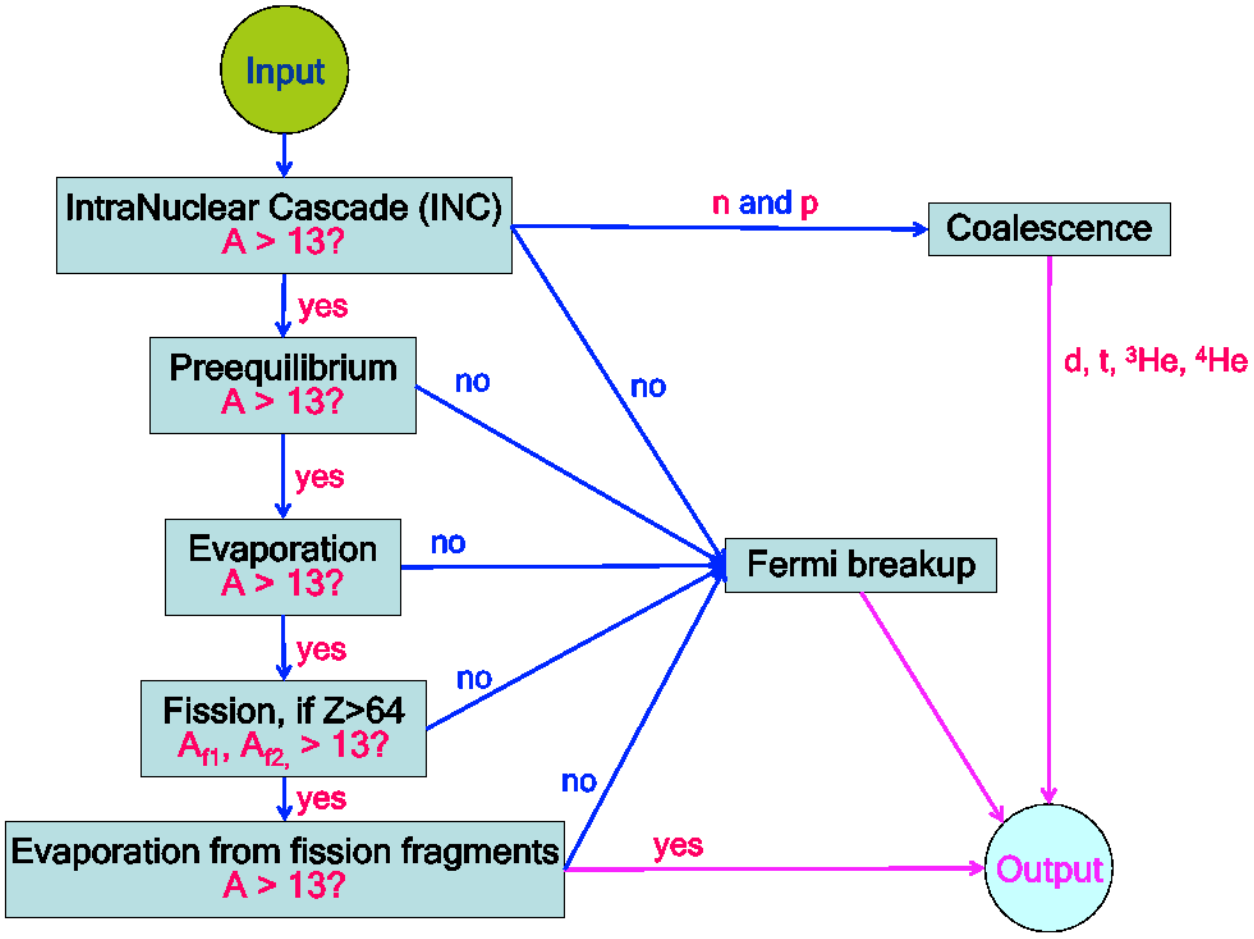

Figure 1: Flow chart of nuclear-reaction calculations by CEM03.03 and LAQGSM03.03.

The emission of the cascade particles determines the particle-hole configuration, Z, A, and the 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. Generally, all four components may contribute to experimentally measured particle spectra and other distributions. But if the residual nuclei after the INC have atomic numbers with $A \leq 12$, CEM03.01 uses the Fermi breakup model to calculate their further disintegration instead of using the preequilibrium and evaporation models. Fermi breakup is much faster to calculate and gives results very similar to the continuation of the more detailed models to much lighter nuclei. LAQGSM03.01 also describes nuclear reactions, generally, as a three-stage process: IntraNuclear Cascade (INC), followed by preequilibrium emission of particles during the equilibration of the excited residual nuclei formed after the INC, followed by evaporation of particles from or fission of the compound nuclei. **LAQGSM was developed with a primary focus on describing reactions induced by nuclei, as well as induced by most elementary particles, at high energies, up to**

about 1 TeV/nucleon. The INC of LAQGSM is completely different from the one in CEM. LAQGSM03.01 also considers Fermi breakup of nuclei with $A \leq 12$ produced after the cascade, and the coalescence model to "produce" high-energy d, t, ^{3}He, and ^{4}He from nucleons emitted during the INC.

The main difference of the following, so-called "03.02" versions of CEM and LAQGSM from the basic "03.01" versions is that the latter use the Fermi breakup model to calculate the disintegration of light nuclei instead of using the preequilibrium and evaporation models only after the INC, when the excited nuclei after the INC have a mass number $A \leq 12$, but do not use the Fermi breakup model at the preequilibrium, evaporation, and fission stages, when, due to emission of preequilibrium particles or due to evaporation or to a very asymmetric fission, we get an excited nucleus or a fission fragment with $A \leq 12$. This problem was solved in the 03.02 versions of CEM and LAQGSM [9], where the Fermi breakup model is used at any stage of a reaction, when we get an excited nucleus with $A \leq 12$.

In addition, the routines that describe the Fermi breakup model in the basic 03.01 version of our codes were written several decades ago in the group of Prof. Barashenkov at JINR, Dubna, Russia, and are far from being perfect, though they are quite reliable and are still used currently without any changes in some transport codes. First, these routines allow in rare cases production of some light unstable fragments like ^{5}He, ^{5}Li, ^{8}Be, ^{9}B, etc., as a result of a breakup of some light excited nuclei. Second, these routines allowed in some very rare cases even production of "neutron stars" (or "proton stars"), i.e., residual "nuclei" produced via Fermi breakup that consist of only neutrons (or only protons). Lastly, in some very rare cases, these routines could even crash the code, due to cases of divide by zero. All these problems of the Fermi breakup model routines are addressed and solved in the 03.02 version of our codes [9]. Several bugs are also fixed in 03.02 in comparison with its predecessor. On the whole, the 03.02 versions describe nuclear reactions on intermediate and light nuclei, and production of fragments heavier than ^{4}He from heavy targets much better than their predecessors, almost do not produce any unstable unphysical final products, and are free of the known bugs.

However, even after solving these problems and after implementing the improved Fermi breakup model into CEM03.02 and LAQGSM03.02 [9], in some very rare cases, our event generators still could produce some unstable products via very asymmetric fission, when the excitation energy of such fragments was below 3 MeV and they were not checked and not disintegrated with the Fermi breakup model (see details in [10]). This problem was addressed in the 03.03 versions of our codes, where we force such unstable products to disintegrate via Fermi breakup independently of their excitation energy. Several more bugs were fixed in the 03.03 version as well. A schematic outline of a nuclear reaction calculation by CEM03.03 or LAQGSM03.03 is shown in Fig. 1. We emphasize that the occurrence of these problems even in the 03.01 versions is quite rare, allowing stand-alone calculations of many nuclear reactions to proceed without problems, but are unacceptable when the event generators are used inside transport codes doing large-scale simulations. Let us note here that the "03.03" version of CEM produced as described above (see more details in [10]) is used at present only in MARS15 [11]. In the latest versions of MCNPX, 2.7.A [12], 2.7.B [13], 2.7.C [14], 2.7.D [15], 2.7.E [16], and 2.7.0 [17] and in MCNP6 [2] (as well as in the Monte Carlo Radiative Energy Deposition (MRED) code developed at Vanderbilt University for single event effect studies [18]) we use now a new modification of CEM03.02 which does not produce any fission fragments with $A < 13$. Therefore, there is no need to use the "standard 03.03" version.

Let us mention that until very recently, we have called the latest version of CEM in MCNP6/X "CEM03.02" (to not confuse it with the version used at FNAL in MARS15) though

its physics corresponds to CEM03.03. We have participated with it in the recent Benchmark of Spallation Models organized at the International Atomic Energy Agency during 2008-2009 [19], and it is referred there as "CEM03.02". As one can see from the numerous and various results presented at the Web-site of that Benchmark [19], the results by "CEM03.02" are practically the same as those by "CEM03.03", just as we expected. The situation with different names of the latest version of CEM in MCNP6/X as "CEM03.02" and as "CEM03.03" in MARS15 was confusing for people outside our Group, as kindly pointed out to us by one of the referees of our recent paper on Validation and Verification of MCNP6 [20]. To address this, we decided to call in Ref. [20] and in all our following publications the latest version of CEM we use at LANL (and in MRED at Vanderbilt University) also as "CEM03.03". This is why we refer here to it as to "CEM03.03".

As several our test-problems address a specific question of the evaporation model used by our CEM and LAQGSM, let us recall here the main assumptions of the evaporation model, without discussing at all the INC, the preequilibrium, the fission, and the coalescence models used by CEM and LAQGSM (we direct readers interested in details of these models to our lectures [6] and references therein).

CEM03.01 and LAQGSM03.01 and their later versions use an extension of the Generalized Evaporation Model (GEM) code GEM2 by Furihata [21]–[23] after the preequilibrium stage of reactions to describe evaporation of nucleons, complex particles, and light fragments heavier than ^{4}He (up to ^{28}Mg) from excited compound nuclei and to describe their fission, if the compound nuclei are heavy enough to fission ($Z \geq 65$). The GEM is an extension by Furihata of the Dostrovsky evaporation model [24] as implemented in LAHET [25] to include up to 66 types of particles and fragments that can be evaporated from an excited compound nucleus plus a modification of the version of Atchison's fission model [26]–[28] used in LAHET. Many of the parameters were adjusted by Furihata for a better description of fission reactions when using it in conjunction with the extended evaporation model.

A very detailed description of the GEM, together with a large amount of results obtained for many reactions using the GEM coupled either with the Bertini or ISABEL INC models in LAHET may be found in [21, 22]. Therefore, we present here only the main features of the GEM, following mainly [22] and using as well useful information obtained in private communications with Dr. Furihata.

Furihata did not change in GEM the general algorithms used in LAHET to simulate evaporation and fission. The decay widths of evaporated particles and fragments are estimated using the classical Weisskopf-Ewing statistical model [29]. In this approach, the decay probability P_j for the emission of a particle j from a parent compound nucleus i with the total kinetic energy in the center-of-mass system between ϵ and $\epsilon + d\epsilon$ is

$$P_j(\epsilon)d\epsilon = g_j \sigma_{inv}(\epsilon) \frac{\rho_d(E - Q - \epsilon)}{\rho_i(E)} \epsilon d\epsilon, \tag{1}$$

where E [MeV] is the excitation energy of the parent nucleus i with mass A_i and charge Z_i, and d denotes a daughter nucleus with mass A_d and charge Z_d produced after the emission of ejectile j with mass A_j and charge Z_j in its ground state. σ_{inv} is the cross section for the inverse reaction, ρ_i and ρ_d are the level densities $[\text{MeV}]^{-1}$ of the parent and the daughter nucleus, respectively. $g_j = (2S_j + 1)m_j/\pi^2\hbar^2$, where S_j is the spin and m_j is the reduced mass of the emitted particle j. The Q-value is calculated using the excess mass $M(A, Z)$ as $Q = M(A_j, Z_j) + M(A_d, Z_d) - M(A_i, Z_i)$. In GEM2, four mass tables are used to calculate Q values, according to the following priorities, where a lower priority table is only used outside

the range of validity of the higher priority one: (1) the Audi-Wapstra mass table [30], (2) theoretical masses calculated by Möller *et al.* [31], (3) theoretical masses calculated by Comay *et al.* [32], (4) the mass excess calculated using the old Cameron formula [33]. As does LAHET, GEM2 uses Dostrovsky's formula [24] to calculate the inverse cross section σ_{inv} for all emitted particles and fragments

$$\sigma_{inv}(\epsilon) = \sigma_g \alpha \left(1 + \frac{\beta}{\epsilon}\right) , \tag{2}$$

which is often written as

$$\sigma_{inv}(\epsilon) = \begin{cases} \sigma_g c_n (1 + b/\epsilon) & \text{for neutrons} \\ \sigma_g c_j (1 - V/\epsilon) & \text{for charged particles} , \end{cases}$$

where $\sigma_g = \pi R_b^2$ [fm^2] is the geometrical cross section, and

$$V = k_j Z_j Z_d e^2 / R_c \tag{3}$$

is the Coulomb barrier in MeV.

One important new ingredient in GEM2 in comparison with LAHET, which considers evaporation of only 6 particles (n, p, d, t, ^{3}He, and ^{4}He), is that Furihata includes the possibility of evaporation of up to 66 types of particles and fragments and incorporates into GEM2 several alternative sets of parameters b, c_j, k_j, R_b, and R_c for each particle type.

The 66 ejectiles considered by GEM2 for evaporation are selected to satisfy the following criteria: (1) isotopes with $Z_j \leq 12$; (2) naturally existing isotopes or isotopes near the stability line; (3) isotopes with half-lives longer than 1 ms. All the 66 ejectiles considered by GEM2 are shown in Table 1.

Table 1. The evaporated particles considered by GEM2

Z_j	Ejectiles						
0	n						
1	p	d	t				
2	^{3}He	^{4}He	^{6}He	^{8}He			
3	^{6}Li	^{7}Li	^{8}Li	^{9}Li			
4	^{7}Be	^{9}Be	^{10}Be	^{11}Be	^{12}Be		
5	^{8}B	^{10}B	^{11}B	^{12}B	^{13}B		
6	^{10}C	^{11}C	^{12}C	^{13}C	^{14}C	^{15}C	^{16}C
7	^{12}N	^{13}N	^{14}N	^{15}N	^{16}N	^{17}N	
8	^{14}O	^{15}O	^{16}O	^{17}O	^{18}O	^{19}O	^{20}O
9	^{17}F	^{18}F	^{19}F	^{20}F	^{21}F		
10	^{18}Ne	^{19}Ne	^{20}Ne	^{21}Ne	^{22}Ne	^{23}Ne	^{24}Ne
11	^{21}Na	^{22}Na	^{23}Na	^{24}Na	^{25}Na		
12	^{22}Mg	^{23}Mg	^{24}Mg	^{25}Mg	^{26}Mg	^{27}Mg	^{28}Mg

Note that when including evaporation of up to 66 particles in GEM2, its running time increases significantly compared to the case when evaporating only 6 particles, up to ^{4}He. The major particles emitted from an excited nucleus are n, p, d, t, ^{3}He, and ^{4}He. For most cases, the total emission probability of particles heavier than α is negligible compared to those for the emission of these light ejectiles. Our detailed study of different reactions (see, *e.g.*, [34]

and references therein) shows that if we study only nucleon and complex-particle spectra or only spallation and fission products and are not interested in light fragments, we can consider evaporation of only 6 types of particles in GEM2 and save much computing time, getting results very close to the ones calculated with the more time consuming "66" option. In CEM03.01 and LAQGSM03.01, we have introduced an input parameter called **nevtype** that defines the number of types of particles to be considered at the evaporation stage. The index of each type of particle that can be evaporated corresponds to the particle arrangement in Table 1, with values, *e.g.*, of 1, 2, 3, 4, 5, and 6 for n, p, d, t, ^{3}He, and ^{4}He, with succeeding values up to 66 for ^{28}Mg. All 66 particles that can possibly evaporate are listed in CEM03.01 and LAQGSM03.01 together with their mass number, charge, and spin values in the **block data bdejc**. For all ten examples of inputs and outputs of CEM03.01 included in Appendices 1 and 2 of the CEM03.01 User Manual [7], whose results are plotted in the figures in Appendix 3 of [7], we have performed calculations taking into account only 6 types of evaporated particles (**nevtype = 6**) as well as with the "66" option (**nevtype = 66**) and we provide the corresponding computing time for these examples in the captions to the appropriate figures shown in Appendix 3 of Ref. [7]. The "6" option can be up to several times faster than the "66" option, providing meanwhile almost the same results. Therefore we recommend that users of CEM and LAQGSM use 66 for the value of the input parameter **nevtype** only when they are interested in all fragments heavier than ^{4}He; otherwise, we recommend the value of 6 for **nevtype**. Alternatively, users may choose intermediate values of **nevtype**, for example 9 if one wants to calculate the production of ^{6}Li, or 14 for modeling the production of ^{9}Be and lighter fragments and nucleons only, while still saving computing time compared to running the code with the maximum value of 66.

3. V&V of MCNP6 using CEM03.03

To help the users of MCNP6, in all the following subsections, we describe the test problems (input/output files, comparisons with experimental data, and results by other models) exactly as they are presented in the **/VALIDATION_CEM/** subdirectory in the basic **/MCNP6/Testing/** directory.

Before presenting our results, let us mention that the easiest way to calculate (in MCNP6) spectra of secondary particles and cross section of products from a thin target is to use either the **noact=-2** option on the **LCA** card of the MCNP6 input file, or the special **GENXS** option of MCNP6. The first option (**noact=-2**) was developed for the MCNPX code and is described in detail in Section 5.4.6.1 of the MCNPX Manual [35]; it migrated later to MCNP6 exactly as implemented in MCNPX [35]. The second option (**GENXS**) was developed by Dr. Richard Prael especially for MCNP6 and is described in detail in Ref. [36]. Both these documents [35, 36] are included in the package to be distributed to MCNP6 users. Below, in test-problems with thin targets, we show examples of using either the first or the second option (or both of them, as shown in Sections 3.6, 3.7, and 3.8).

3.1. Test-problem #1: A) inp01 with inxc02; B) inp01a with inxc79 (for the case with nevtype=66)

The first test problem of this V&V Suite is to check the applicability of MCNP6 using the CEM03.03 event generator for problems of interest for the Defense Threat Reduction Agency

(DTRA) of the US Defense Department and for some other intermediate-energy nuclear applications.

Here, we calculate with MCNP6 the yields of products from a thin ^{238}U target bombarded by 1 GeV protons. Our major interest for this Threat Reduction problem is in the yields of ^{87}Br and ^{88}Br as the main delayed neutron emitters with relatively long half-lives, of 55.60 and 16.29 seconds, respectively. ^{17}N, ^{9}Li, and ^{16}C are also important delayed neutron emitters, though their half-lives are of only 4.173, 0.178, and 0.747 seconds, respectively. ^{136}Te, ^{137}I, and ^{141}Cs with relatively long half-lives of 17.5, 24.3, and 24.94 seconds, respectively, are also delayed neutron emitters, but less important than ^{87}Br and ^{88}Br. Finally, ^{92}Rb, ^{93}Rb, and ^{94}Rb are delayed neutron emitters too, but their contribution can be probably neglected, as significantly less important than ^{87}Br and ^{88}Br.

Several recent GSI measured cross sections of interest for this test problem are published in Refs. [37]-[40]. Production of ^{9}Li, ^{16}C, and ^{17}N by 1 GeV protons from thin targets of natural Uranium was measured 45 years ago by Dostrovsky et al. [41].

As for this test-problem, we need to calculate only the yields (production cross sections) of several nuclides from a thin ^{238}U target bombarded with 1-GeV protons. The easiest way to do this would be to use the GENXS capability [36] of MCNP6. The GENXS option is very useful for such types of problems, as it simulates production cross sections (and spectra of emitted particles) from arbitrary targets, but without particle transport, which would correspond to modeling the interaction of the beam with a very thin target. Note that the GENXS option of MCNP6 requires two input files, the main, standard, MCNP6 input file accompanied by a second, auxiliary **INXC** input file (see details in [36]), specified in the main input file on the **TROPT** card. Both the main MCNP6 input file for this problem called **inp01** and the INXC input file called **inxc01** are shown below:

inp01:

```
MCNP6 test: p + U238 by CEM03.03 at 1 GeV, nevtype=6
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ------------------------------------------------------------

  sdef erg = 1000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 1000
  mode   h
LCA  8j 1    $ use CEM03.03
  tropt genxs inxc01  nreact on  nescat off
c ------------------------------------------------------------
```

```
  print 40 110 95
  nps 1000000
  prdmp 2j -1
```

The INXC Input File **inxc01**:

```
MCNP6 test: p + U238 at 1 GeV for TR applications
1 1 1 /
Cross Section Edit
56 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
1 5 6 7 8 21 22 23 24 /
```

Both the main MCNP6 input file **inp01** and the INXC input file **inxc01** are very simple for this test-problem: In **inp01**, we have a beam of 1000 MeV protons in the direction of the Z-axis defined by the **sdef** card

```
sdef erg = 1000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
```

bombarding the material #1 (^{238}U), defined by the material card

```
m1   92238 1.0
```

which fills a cylinder of a radius $R = 4$ cm on the Z-axis from $Z = -1$ cm to $Z = 1$ cm, as defined by the surface cards

```
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0 .
```

The **LCA** card originating from MCNPX (see, e.g., the MCNPX 2.6.0 User's Manual [35])

```
LCA  8j 1    $ use CEM03.03
```

chooses the CEM03.03 event generator to be used in this calculation.

The only card from the MCNP6 input file **inp01** requiring a little explanation here is the **TROPT** card:

```
tropt genxs inxc01  nreact on  nescat off .
```

It tells us that we use the GENXS option of MCNP6 (the parameter **genxs** on this card, see [36]), and that we use a second input file for this problem, called **inxc01**. It also requires that we calculate only inelastic secondary particle production (NREACT=ON on this card) and we turn off the elastic scattering (NESCAT=OFF on the TROP card).

The INXC input file **inxc01** for this problem is really very simple: The first card is simply a "Problem Title" (see [36]). The 2nd card

```
1 1 1
```

defines the **NCASE**, **KPLOT**, and **L_RES** parameters.

The **NCASE** parameter on this card defines the number of double-differential cross section edits we like to calculate (see [36]). In this particular test-problem we are interested only in cross sections for the production of several delayed-neutron emitters. Therefore, we could use for this parameter the value 0 and to not calculate any particle spectra at all. However, as for this reaction we have already results by CEM03.03 as a stand alone code (presented at the International Benchmark of Spallation Models organized by IAEA during 2008-2009 [19]) for angle integrated energy particle spectra of n, p, d, t, ^{3}He, ^{4}He, π^+, π^0, π^-, and for their multiplicities, we use here NCASE=1, to calculate with MCNP6 also the energy spectra and particle multiplicities — a kind of "extra-results" we could compare later with predictions by CEM03.03.

The second, **KPLOT** parameter on this card is 1, i.e., nonzero, providing cross section edits to the MCTAL file **inp01.m**, needed to plot the results. Note that plotting with MCNP6 is available only with the MCTAL file. The default value of the parameter **KPLOT** is 0.

The third parameter, **L_RES**, is equal to 1, i.e., nonzero, providing a residual nuclei edit (the default is 0; no residual nuclei are calculated).

The 3rd card of the INXC input file **inxc01** is simply a "Case Title".

The 4th card of **inxc01** gives the values of the **NERG**, **NANG**, and **NTYPE** parameters (note, that on this card, we could define three more parameters, but we do not need them here (see details in Ref. [36]). **NERG** is the number of energy bin boundaries; here we use NERG=56. **NANG** is the number of angle bin boundaries (needed when calculating double-differential cross sections). If NANG=0, like here, only angle-integrated energy spectra will be produced. **NTYPE** is the number of particle types we like to tally; here, we use NTYPE=9, as we like to get energy spectra and multiplicities for 9 types of ejectiles: n, p, d, t, ^{3}He, ^{4}He, π^+, π^0, and π^-.

The 5th card of **inxc01** defines the energy bin boundaries. Note, that this "card" is entered here actually on two lines with less than 80 positions; it can be defined on more lines, and the sign of its end is the slash mark "/", just as we have for other cards of the INXC input file. Note, also, that on this card we can enter either all the values of the energy bin boundaries, up to NERG, or a smaller number N $<$ NERG , as we have here; see details in Ref. [36]. In the present problem, we define on this card only the first 21 energy bin boundaries, while the following ones, up to NERG=56, are calculated as $T_i = T_{i-1} + (T_N - T_{N-1})$.

Finally, on the 6th card, we define NTYPE particle types to tally. Actually, we could have one more card (#6) before this one, which would define the angle bin boundaries and would change this card to #7, but here we do not calculate any double-differential spectra (NANG=0), therefore we omit the standard "Card #6" and use directly "Card #7". The complete list of flags defining all particle types in the GENXS option of MCNP6 can be found in Ref. [36]; here, we note only that flags (numbers) 1, 5, 6, 7, 8, 21, 22, 23, and 24 on this card define n, p, d, t, ^{3}He, ^{4}He, π^+, π^0, and π^-, respectively.

Let us recall again that the main aim of this problem is to validate MCNP6 with CEM03.03 against experimental data and calculations by other codes only for the production of the ^{87}Br, ^{88}Br, ^{17}N, ^{9}Li, and ^{16}C delayed neutron emitters.

Note that at the time when this test problem was developed, the default option of MCNP6 was to use **nevtype=6** for CEM03.03 (later on, the default for both CEM and LAQGSM was changed and fixed in MCNP6 as **nevtype=66**; we will return to this point later, with more details and discussion). Results by MCNP6 for the production of all isotopes of Br (Z=35) calculated with the **nevtype=6** option for CEM03.03 using the input files **inp01** and **inxc01**

described above are presented in the output file **inp01.o** and in the MCTAL file **inp01.m** of the **Templates** subdirectory **/VALIDATION_CEM/Templates/LINUX/** and are shown in Fig. 2.

The output file **inp01.o** provided by the GENXS option of MCNP6 is very simple and self-explanatory. Indeed, the cross sections (in barns) for the production of the isotopes we are interested in here are tabulated in the output as:

```
1 Distribution of residual nuclei:

                        Cross Section (b)
     Z =  1  all A     3.74217E+00 0.0011
             A =   2   2.65286E+00 0.0011
             A =   3   1.08930E+00 0.0016
     Z =  2  all A     1.56387E+00 0.0015
             A =   3   2.10229E-01 0.0032
             A =   4   1.35364E+00 0.0016
     Z =  4  all A     2.04483E-06 1.0000
             A =   9   2.04483E-06 1.0000
     Z =  5  all A     6.13449E-06 0.5773
             A =  10   6.13449E-06 0.5773
     Z =  6  all A     5.72552E-05 0.1890
             A =  10   2.04483E-06 1.0000
             A =  11   8.17932E-06 0.5000
             A =  12   3.68069E-05 0.2357
             A =  13   4.08966E-06 0.7071
             A =  14   2.04483E-06 1.0000
             A =  16   4.08966E-06 0.7071
     Z =  7  all A     4.70311E-05 0.2085
             A =  12   2.04483E-06 1.0000
             A =  13   2.04483E-06 1.0000
             A =  14   2.24931E-05 0.3015
             A =  15   1.84035E-05 0.3333
             A =  17   2.04483E-06 1.0000
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     Z = 35  all A     7.20271E-02 0.0052
             A =  73   1.02241E-05 0.4472
             A =  74   3.29217E-04 0.0788
             A =  75   1.26779E-03 0.0401
             A =  76   3.03248E-03 0.0259
             A =  77   5.47196E-03 0.0193
             A =  78   6.13653E-03 0.0182
             A =  79   9.18333E-03 0.0149
             A =  80   7.68038E-03 0.0163
             A =  81   9.02996E-03 0.0150
             A =  82   6.55981E-03 0.0176
             A =  83   7.05466E-03 0.0170
             A =  84   4.54361E-03 0.0212
```

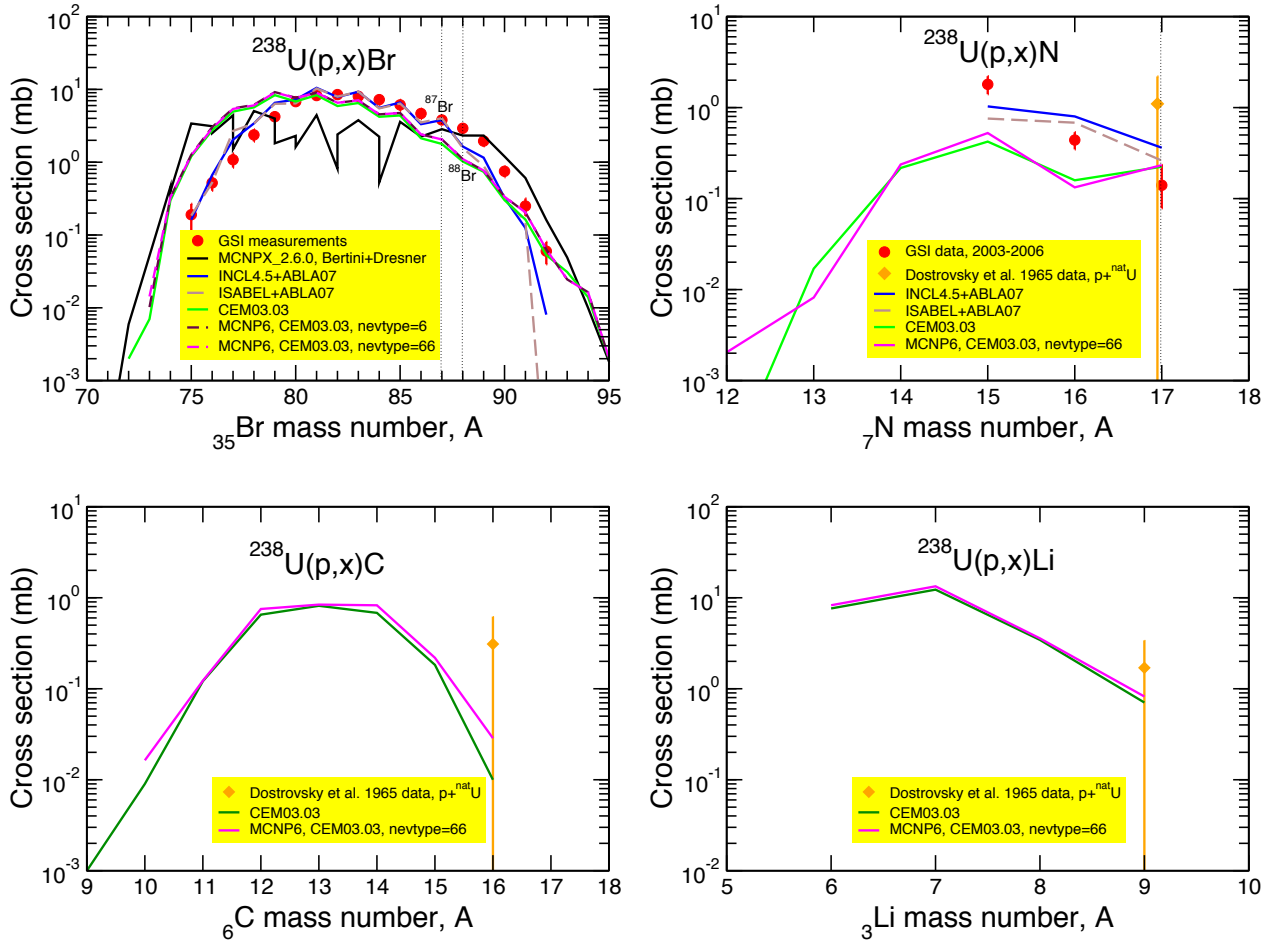

Figure 2: Experimental (symbols) mass distributions [37]-[40], [41] for the yields of Br, N, C, and Li isotopes from ^{238}U thin targets bombarded with a 1 GeV proton beam compared with MCNP6 results using the CEM03.03 event-generator [6] with **nevtype=6** and **nevtype=66**. For comparison, we show also results by CEM03.03 [6] used as a stand alone code, by INCL4.5+ABLA07 [42]-[46], by ISABEL+ABLA07 [47, 45], and by the transport code MCNPX 2.6.0 [35] with default options, i.e., using the Bertini INC [48], Multistage Preequilibrium Model (MPM) [49], Dresner evaporation model [50], and the RAL fission model [26, 27], as presented at the International Benchmark of Spallation Models organized by IAEA during 2008-2009 [19]. Note that while using the option **nevtype=6**, CEM03.03 does not predict any ions of Li from this reaction, and the yields for ^{16}C and ^{17}N are very small, so we do not shown them at all in this figure in the case of **nevtype=6**. The delayed neutron emitters ^{87}Br, ^{87}Br, ^{17}N, ^{16}C, and ^{9}Li, of interest to DTRA are singled out with dotted lines, as indicated.

```
                A =  85   4.74809E-03 0.0207
                A =  86   2.40676E-03 0.0291
                A =  87   2.05710E-03 0.0315
                A =  88   1.10421E-03 0.0430
                A =  89   7.64766E-04 0.0517
                A =  90   3.35352E-04 0.0781
                A =  91   2.04483E-04 0.1000
                A =  92   6.33897E-05 0.1796
                A =  93   2.45379E-05 0.2887
                A =  94   1.63586E-05 0.3536
                A =  95   2.04483E-06 1.0000
      Z = 36  all A     9.23015E-02 0.0046
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

From this portion of the output, we see that the cross sections for the production of ^{87}Br and ^{88}Br are equal to 2.05710E-03 (±3.15%) [b] and 1.10421E-03 (±4.30%) [b], respectively. That agrees quite well with the GSI experimental data [37]-[40] and results by other models, as is shown in Fig. 2.

At the same time, we do not see in the output file **inp01.o** any ions of Li, and so little yields for ^{16}C (4.08966E-06 ±70.71% [b]) and ^{17}N (2.04483E-06 ±100% [b]) that they are below the corresponding lower limits of the Y-axes of Fig. 2, so they are not shown at all in Fig. 2. This confusing situation happens because ^{87}Br, ^{87}Br, ^{17}N, ^{16}C, and ^{9}Li from this reaction are produced via different reaction mechanisms: ^{87}Br and ^{87}Br are produced mainly as fission fragments (with or without possible evaporation of particles from the initial excited fission fragments), while ^{17}N, ^{16}C, and ^{9}Li are too light to be produced with a significant yield via very asymmetric fission or as "spallation products", i.e., via sequential emission of many particles and light fragments from the target. CEM03.03 could produce these light fragments from this reaction via evaporation if we would use the option **nevtype=66**; the option **nevtype=6** does not allow their evaporation at all.

Let us mention that for some historical reasons, in the latest version of MCNP6 used when we have developed this test-problem (September 2010) the default option for the LAQGSM03.03 event-generator was **nevtype=66**. But at the same time, the MCNP6 default for CEM03.03 was to take into account only 6 types of particles (**nevtype=6**) which can be evaporated: n, p, d, t, ^{3}He, and ^{4}He. As mentioned above, this option may be not appropriate for problems where we are interested in the production of fragments heavier than ^{4}He from heavy target-nuclei.

To take into account the possibility of evaporating up to 66 different types of particles, from n to ^{28}Mg, users of MCNP6 had to change the value of **lcaopt(11)** in **subroutine initial_run** of the **module imcn.F90** in subdirectory **/Source/src/** from 6 to 66 and to recompile MCNP6. We performed the calculations for this test-problem just this way; this was the easiest way to address this problem at that time (September, 2010).

Let us mention here that this "historical" situation with the values of **nevtype** was both not self-consistent and not user-friendly: First, the default for **nevtype** was 66 in LAQGSM03.03 and only 6 for CEM03.03. Second, to change the values of **nevtype**, users had to edit the source code and to recompile MCNP6 every time they needed to change **nevtype**; this was not convenient. To address this question, Dr. Grady Hughes recently modified MCNP6 so that it uses now as default the same value of **nevtype = 66** for both CEM and LAQGSM. In addition, the MCNP6 users can now easily change the default values of **nevtype**, the same way

in both CEM and LAQGSM, with a new input parameter of MCNP6 which should be defined on the 11th position of the **LCA** MCNP6 input card: If the 11th position of the **LCA** MCNP6 input card is not defined (i.e., we use the default), MCNP6 will use now **nevtype = 66** for both CEM and LAQGSM. But if we like to change the default and to use, e.g., **nevtype = 6**, we simply input **6** on the 11th position of **LCA** MCNP6 input card. An example of using this recent easy way to change the values of **nevtype** is presented in the test-problem # 18 of Ref. [5]; here, we follow the "historical" way, as it was available to us in September, 2010.

For this test-problem, we use the input file **inp01** with the default option **nevtype=6**, and produced the output file **inp01.o**, as discussed above. After that, we have modified **subroutine initial_run** to activate the option **nevtype=66** and did recompiled MCNP6 as described above. For the **nevtype=66** option, we use a very similar input called **inp01a** to produce the corresponding output file **inp01a.o** and the MCTAL file **inp01a.m**.

Let us present below a small portion of the output file **inp01a.o** calculated with the option **nevtype=66**, so that we can compare these results with the first ones obtained using **nevtype=6** shown above.

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
1 Distribution of residual nuclei
     Z =  1  all A     3.72774E+00 0.0010
             A =   2   2.64148E+00 0.0011
             A =   3   1.08626E+00 0.0016
     Z =  2  all A     1.56336E+00 0.0015
             A =   3   2.09100E-01 0.0032
             A =   4   1.34273E+00 0.0016
             A =   6   1.12506E-02 0.0135
             A =   8   2.76052E-04 0.0861
     Z =  3  all A     2.60266E-02 0.0090
             A =   6   8.27338E-03 0.0158
             A =   7   1.33507E-02 0.0125
             A =   8   3.58050E-03 0.0239
             A =   9   8.22021E-04 0.0499
     Z =  4  all A     8.39607E-03 0.0157
             A =   7   9.16083E-04 0.0473
             A =   9   3.31262E-03 0.0249
             A =  10   3.75840E-03 0.0233
             A =  11   3.76249E-04 0.0737
             A =  12   3.27173E-05 0.2500
     Z =  5  all A     3.64593E-03 0.0238
             A =   8   1.02241E-05 0.4472
             A =  10   1.14919E-03 0.0422
             A =  11   1.39253E-03 0.0384
             A =  12   9.44711E-04 0.0465
             A =  13   1.49273E-04 0.1170
     Z =  6  all A     2.80551E-03 0.0270
             A =  10   1.63586E-05 0.3536
             A =  11   1.22690E-04 0.1291
             A =  12   7.52497E-04 0.0521
```

```
             A =  13   8.40425E-04 0.0493
             A =  14   8.26111E-04 0.0497
             A =  15   2.18797E-04 0.0967
             A =  16   2.86276E-05 0.2673
     Z =  7  all A     1.13897E-03 0.0424
             A =  12   2.04483E-06 1.0000
             A =  13   8.17932E-06 0.5000
             A =  14   2.37200E-04 0.0928
             A =  15   5.25521E-04 0.0624
             A =  16   1.32914E-04 0.1240
             A =  17   2.33110E-04 0.0937
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     Z = 35  all A     7.15465E-02 0.0053
             A =  73   1.43138E-05 0.3780
             A =  74   3.29217E-04 0.0788
             A =  75   1.24530E-03 0.0405
             A =  76   2.92206E-03 0.0264
             A =  77   5.38608E-03 0.0195
             A =  78   6.02611E-03 0.0184
             A =  79   9.08926E-03 0.0150
             A =  80   7.63744E-03 0.0163
             A =  81   8.99316E-03 0.0150
             A =  82   6.54959E-03 0.0176
             A =  83   7.09147E-03 0.0170
             A =  84   4.52930E-03 0.0212
             A =  85   4.75627E-03 0.0207
             A =  86   2.40881E-03 0.0291
             A =  87   2.05096E-03 0.0316
             A =  88   1.10421E-03 0.0430
             A =  89   7.66811E-04 0.0516
             A =  90   3.35352E-04 0.0781
             A =  91   2.04483E-04 0.1000
             A =  92   6.33897E-05 0.1796
             A =  93   2.45379E-05 0.2887
             A =  94   1.63586E-05 0.3536
             A =  95   2.04483E-06 1.0000
     Z = 36  all A     9.17208E-02 0.0046
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

Now, we see in the output file **inp01a.o** four isotopes of Li, including ^{9}Li of interest for our problem, and much larger cross sections for the production of ^{17}N and ^{16}C. These results are presented in Fig. 2, showing a reasonable agreement with the experimental data and results by other codes.

The results by MCNP6 calculated with **nevtype=66** are in the output files **inp01a.o** and the MCTAL file **inp01a.m** of subdirectory **/VALIDATION_CEM/Templates/LINUX/**. To aid in plotting our results with **xmgrace**, the yields of Br, C, Li, and N isotopes are also copied in separate files pU8_Br_MCNP6C66.dat, pU8_C_MCNP6C66.dat, pU8_Li_MCNP6C66.dat,

and pU8_N_MCNP6C66.dat, respectively, in the subdirectory **/VALIDATION_CEM/Experimental_data/inp01/**.

In the same subdirectory, we present results by CEM03.03 as a stand alone code for all isotopes of Br, C, Li, and N, respectively in the files pU8_Br_CEM0302_Bench.dat, pU8_C_CEM0302_Bench.dat, pU8_Li_CEM0302_Bench.dat, and pU8_N_CEM0302_Bench.dat. Results by INCL4.5+ABLA07 [43]-[46] and by ISABEL+ABLA07 [47, 45] for the production of Br and N are presented there respectively in the files pU8_Br_INCL-ABLA7_Bench.dat, pU8_N_INCL-ABLA7_Bench.dat, pU8_Br_ISABEL_ABLA07.dat, and pU8_N_ISABEL_ABLA07.dat, (no results for the production of Li and C were presented at the International Benchmark by other codes [19] except for CEM). Results by MCNPX 2.6.0 [35] with default options, i.e., using the Bertini INC [48], Multistage Preequilibrium Model (MPM) [49], Dresner evaporation model [50], and the RAL fission model [26, 27], for the production of Br are presented there in the file pU8_Br_MCNPX_Bert.dat (true, we observe some problems with these results, just as several other problems for other results by MCNPX 2.6.0 presented at the International Benchmark [19] were observed and discussed at the Second Advanced Workshop on Model Codes for Spallation Reactions, 8-11 February 2010, CEA-Saclay, France; see Ref. [51] for details).

For convenience, all the mentioned results are plotted with **xmgrace** and presented in the **/Experimental_data/** subdirectory as pdf files: pU8_BrNLiC.pdf, pU8_Br.pdf, pU8_C.pdf, pU8_Li.pdf, and pU8_N.pdf. Templates for these figures from **xmgrace** are presented in files: pU8_Br.fig, pU8_C.fig, pU8_Li.fig, and pU8_N.fig, respectively.

Finally, let us discuss briefly the "extra-results" obtained with MCNP6, because of using a nonzero value (=1) for the parameter **NCASE** in the INXC input file **inxc01**. NCASE=1 together with NTYPE=9 and the flags (numbers) 1, 5, 6, 7, 8, 21, 22, 23, and 24 on the 6th card of the INXC input file **inxc01** provide in the MCNP6 outputs energy spectra and multiplicities for the produced n, p, d, t, ^{3}He, ^{4}He, π^+, π^0, and π^-. Let us show here a small portion of the MCNP6 output file **inxc01.o** with results for the energy spectrum and multiplicity of neutrons:

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
1 GENXS tally  1: Cross Section Edit

                                        neutron  production cross section

     E(MeV)        angle integrated     mu max    deg min  energy integrated
    5.000000E+00    4.941E+00 0.000
    1.000000E+01    1.924E+00 0.001
    1.500000E+01    6.610E-01 0.001
    2.000000E+01    2.947E-01 0.001
    2.500000E+01    1.697E-01 0.002
    3.000000E+01    1.155E-01 0.002
    3.500000E+01    8.636E-02 0.002
    4.000000E+01    6.781E-02 0.003
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
    8.000000E+02    3.052E-04 0.018
    8.200000E+02    3.241E-04 0.018
Some tallies at energies/momenta above table maximum =   8.20000E+02
```

```
total neutron  production cross section =  4.470E+01 0.0004 yield =  2.18585E+01
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

These energy spectra $d\sigma/dT$ are in units of [b/MeV]. We have compared the current MCNP6 spectra with the results by CEM03.03 as a stand alone code calculated for the International Benchmark of Spallation Models organized by IAEA during 2008-2009 [19] and have found very good agreement. The total production cross sections of particles are presented in the MCNP6 outputs after the corresponding table with spectra, and are given in units of barns. Note that the mean **"multiplicities"** of particles, i.e., the mean number of particles produced per one inelastic interaction are listed in the MCNP6 outputs as **"yields"**; so, we see that the mean multiplicity of neutrons $< n >$ from this reaction is equal to 21.8585. Table 2 below presents a comparison of the mean multiplicities of n, p, d, t, ^{3}He, ^{4}He, π^+, π^0, and π^- calculated with MCNP6 using the **nevtype=6** and **nevtype=66** options for CEM03.03, together with results by CEM03.03 (with **nevtype=66**) presented at International Benchmark of Spallation Models [19] and available on-line on the web-page of the Benchmark [19] as the file **p_U238_1000_info_cem0303.txt** in the **Additional Information** Section of **Calculated Results** for CEM03.02.

Table 2. Mean multiplicities of n, p, d, t, ^{3}He, ^{4}He, π^+, π^0, and π^- and the total reaction cross sections σ_{in} [mb] calculated with MCNP6 using the CEM03.03 event-generator with **nevtype=66** and **nevtype=6** compared with results by CEM03.03 used as a stand alone code with **nevtype=66**

Ejectiles	MCNP6, **nevtype=66**	MCNP6, **nevtype=6**	CEM03.03, **nevtype=66**
$< n >$	21.859	21.905	21.862
$< p >$	2.158	2.166	2.155
$< d >$	1.292	1.297	1.290
$< t >$	0.531	0.533	0.531
$<^3 He >$	0.102	0.103	0.102
$<^4 He >$	0.657	0.662	0.656
$< \pi^+ >$	0.113	0.113	0.114
$< \pi^0 >$	0.251	0.251	0.251
$< \pi^- >$	0.175	0.175	0.175
σ_{in} [mb]	2044.83	2044.83	1866.14

For completeness sake, we show in Table 2 also the the total reaction cross sections σ_{in} [mb] calculated by MCNP6 and predicted by CEM03.03. Note that the total reaction cross section is listed in the MCNP6 output files with the GENXS option (in barns) before the spectra, and is called as **"nonelastic cross section"**, as shown below for the file **inp01a.o**:

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
                    total cross section        =  2.04483E+00 0.0000

                    nonelastic cross section   =  2.04483E+00 0.0000
                         fission cross section =  1.40035E+00 0.0007
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

The results presented in Table 2 are quite interesting: First, we see a very good agreement between the results by MCNP6 and by CEM03.03. More interesting is to see an almost coincidence between the results by MCNP6 using **nevtype=66** and results obtained with **nevtype=6** for multiplicities of all ejectiles tallied here (for energy spectra, we see a similar perfect agreement). This indicates once again that calculations with **nevtype=6** are very reliable for some problems, providing almost the same results as calculations with **nevtype=66**, but requiring much less computing time. So, we recommend again MCNP6 calculations with **nevtype=6** when users are not interested in the production of fragments heavier than ^4He from heavy nuclei-targets. But if/when the users are not sure which values for **nevtype** must be used for a particular problem, to avoid unreliable results, they should use **nevtype=66**. Just for this reason the default value of **nevtype** was set for both CEM and LAQGSM to 66 in MCNPX [35], and, by Grady Hughes, in the current version of MCNP6, as mentioned above.

Last, in Table 2, we see a little difference between the total reaction cross section provided by MCNP6 for this reaction (2044.83 mb for both cases) and the value predicted by CEM03.03 (1866.14 mb). This difference (of less than 10%) is caused by different normalizations for the total reaction cross sections used by MCNP6 and CEM03.03 (as well as CEM03.01 and CEM03.02): Historically, as was done by Dick Prael in LAHET [25] and adopted also by Nikolai Mokhov in MARS15 [11], MCNP6 and MCNPX use the parameterizations by Barashenkov and Polanski for the total reaction cross sections [52]. On the other hand, for CEM03.01, CEM03.02, and CEM03.03 we developed a more recent approximation [53] trying to describe as good as possible different nuclear reactions at different incident energies, which is based on a combination of several parameterizations, like the NASA systematics by Tripathi *et al.* [54] and the Kalbach systematics [55] for neutrons of lower energy (see more details in [7, 53]).

3.2. Test-problem #2: Fe1200

This MCNP6 problem is to test the applicability of MCNP6 using the CEM03.03 event generator to describe backward emission of particles from thick targets bombarded by intermediate-energy (400–1200 MeV) protons. To be specific, the main aim of this problem is to study neutron emission at 175 degrees from a 1.2 GeV proton beam hitting a face plane of a cylindrical iron target that is 20 cm in diameter and 25 cm thick.

First, we need such information for shielding consideration, to be able to prevent cases when personnel may receive radiation from backward fluxes.

Second, it is much more difficult for all models to describe particle production at very backward angles than at intermediate or forward angles; that is, this problem is a good test to see how the CEM03.03 event generator does work in such a "difficult" kinematics region.

Third, spectra of secondary particles at very backward angles are of great academic interest, to understand the mechanisms of cumulative particle production, under investigation for four decades already, but still with many open questions (see, e.g., Ref. [56]).

The experimental data for this problem were measured at the Institute of High Energy Physics in Protvino, Russia using the calorimetric-time-of-flight (CTOF) technique and are published in Ref. [57].

Thought the current problem is to model only interaction of 1200 MeV protons with a cylindrical iron target of 20 cm in diameter and 25 cm thick, the measurements were performed also at 400, 600, 800, and 1000 MeV; therefore, we performed calculations with MCNP6 using the CEM03.03 event-generator at all these energies. In addition, for comparison, we performed similar calculations with MCNP6, but using the LAQGSM03.01 [8] event-generators, as well as

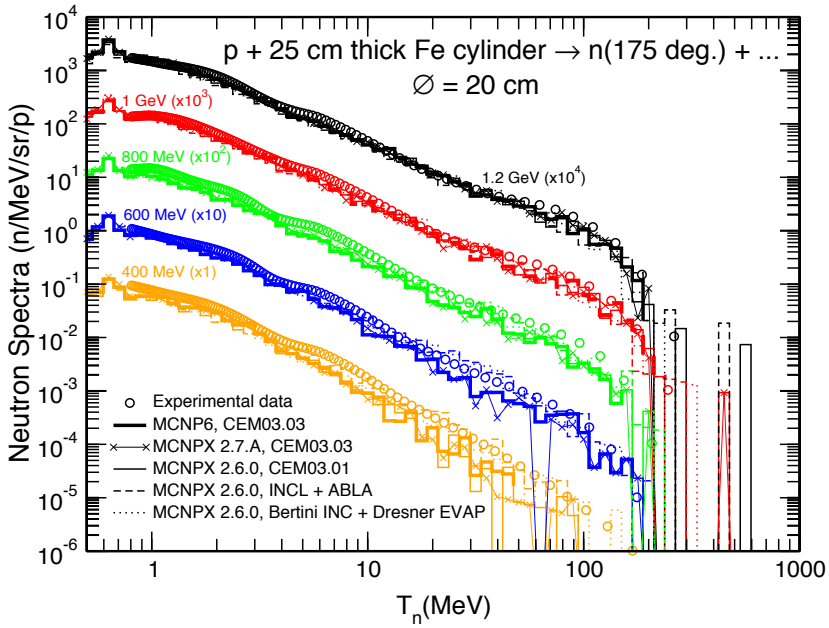

Figure 3: Experimental [57] neutron spectra at 175 degrees (symbols) from a thick Fe cylinder bombarded with 400, 600, 800, 1000, and 1200 MeV protons compared with results by MCNP6 using the CEM03.03 event-generator, by MCNPX 2.7.A [12] using the CEM03.03 event-generator, and by the 2.6.0 version of MCNPX [35] using the CEM03.01, Bertini INC [48] followed by the Multistage Preequilibrium Model (MPM) [49] and the evaporation model described with the Dresner code EVAP [50], and by the INCL+ABLA [42, 44] event-generators, as indicated in legend.

with MCNPX 2.7.A [12] using the CEM03.03 event-generator. For a broader comparison, we use here also the results obtained at ORNL and kindly supplied us by Wei Lu and Franz Gallmeier with the 2.6.0 version of MCNPX [35] using the CEM03.01 [7], Bertini INC [48] followed by the Multistage Preequilibrium Model (MPM) [49] and the evaporation model described with the Dresner code EVAP [50], and using the INCL+ABLA [42, 44] (see more details in Ref. [57]). All these results are shown in Fig. 3 together with the experimental data from Ref. [57].

Below, we present only the MCNP6 input for the case of 1200 MeV bombarding protons; it is called **Fe1200**. This input is more complicated than we had for the previous test-problem, therefore we provide also all the necessary information to help MCNP6 users understand all its details.

Fe1200:

```
MCNP6 test: 175 deg. n-spec. by CEM03.03 to compare with Belyakov data
c
c     **cellcards **
c
    1   1 -7.874   -1 2 -3     $ m1 is iron
    2   2 -0.001168   #1 -5 .
    3   0          5  -6
    6   0          6
  999   0        -999
```

```
c
c  *****surface card
c
    1  cz    10      $ diameter = 20 cm
    2  pz    0.0
    3  pz    25.0    $ 25 cm thick
    5  so    600
    6  so    800
    7  pz    -597.8168189
    8  pz    -597.6168189
  999  cz    10.000001

c  *
c  * Data Cards
c  *
c
c         Material cards
c
m1       26054.70h  5.845
         26056.70h 91.754
         26057.70h  2.119
m2       7014.70h 1.555901784
         7015.60c 0.005778216
         8016.70h 0.448606754
         8017.60c 0.001079246
         1001.70h 0.06
        18000.35c 0.00934
         6000.60c 0.000383
c
c  importances
imp:n 1 1 1 0 0
imp:h 1 1 1 0 0
imp:p 1 1 1 0 0
imp:d 1 1 1 0 0
imp:t 1 1 1 0 0
imp:s 1 1 1 0 0
imp:a 1 1 1 0 0
imp:/ 1 1 1 0 0
imp:z 1 1 1 0 0
c *
c * source definition
c *
sdef erg=1200 par=h dir=1 vec= 0 0 1 x=d1 y=d2 z=0 ccc=999
sp1  -41 2.4 0
sp2  -41 2.4 0
nps   1e7
```

```
C nps   1000
lost 100 100
print   10 110   40
prdmp 2.e7 1.e6 1 10 1e6
LCA  8j 1
c
c  tally
c
F11:n   5
SD11    1 753.9822369 1
FS11    -7 -8
FQ11    e u
TF11    6j 21
E11   1.059254E-03 1.188502E-03 1.333521E-03 1.496236E-03 1.678804E-03
      1.883649E-03 2.113489E-03 2.371374E-03 2.660725E-03 2.985383E-03
      3.349654E-03 3.758374E-03 4.216965E-03 4.731513E-03 5.308844E-03
      5.956621E-03 6.683439E-03 7.498942E-03 8.413951E-03 9.440609E-03
      1.059254E-02 1.188502E-02 1.333521E-02 1.496236E-02 1.678804E-02
      1.883649E-02 2.113489E-02 2.371374E-02 2.660725E-02 2.985383E-02
      3.349654E-02 3.758374E-02 4.216965E-02 4.731513E-02 5.308844E-02
      5.956621E-02 6.683439E-02 7.498942E-02 8.413951E-02 9.440609E-02
      1.059254E-01 1.188502E-01 1.333521E-01 1.496236E-01 1.678804E-01
      1.883649E-01 2.113489E-01 2.371374E-01 2.660725E-01 2.985383E-01
      3.349654E-01 3.758374E-01 4.216965E-01 4.731513E-01 5.308844E-01
      5.956621E-01 6.683439E-01 7.498942E-01 8.413951E-01 9.440609E-01
      1.059254E+00 1.188502E+00 1.333521E+00 1.496236E+00 1.678804E+00
      1.883649E+00 2.113489E+00 2.371374E+00 2.660725E+00 2.985383E+00
      3.349654E+00 3.758374E+00 4.216965E+00 4.731513E+00 5.308844E+00
      5.956621E+00 6.683439E+00 7.498942E+00 8.413951E+00 9.440609E+00
      1.059254E+01 1.188502E+01 1.333521E+01 1.496236E+01 1.678804E+01
      1.883649E+01 2.113489E+01 2.371374E+01 2.660725E+01 2.985383E+01
      3.349654E+01 3.758374E+01 4.216965E+01 4.731513E+01 5.308844E+01
      5.956621E+01 6.683439E+01 7.498942E+01 8.413951E+01 9.440609E+01
      1.059254E+02 1.188502E+02 1.333521E+02 1.496236E+02 1.678804E+02
      1.883649E+02 2.113489E+02 2.371374E+02 2.660725E+02 2.985383E+02
      3.349654E+02 3.758374E+02 4.216965E+02 4.731513E+02 5.308844E+02
      5.956621E+02 6.683439E+02 7.498942E+02 8.413951E+02 9.440609E+02
      1000

c
mode n h p d t s a / z
phys:h   1500.
phys:n   1500.
phys:p   1500
phys:/   1500
phys:z   1500
DBCN 28j 1
```

First, in the the input file **Fe1200**, we see that the iron cylinder, 20 cm in diameter and lying in the Z-axis from $Z = 0$ cm to $Z = 25$ cm, serves as the target for this problem and fills **cell #1**:

```
    1  1 -7.874  -1 2 -3    $ m1 is iron
```

defined by the **surface cards**:

```
    1  cz    10      $ diameter = 20 cm
    2  pz    0.0
    3  pz    25.0    $ 25 cm thick .
```

Its **material** is defined also as #1, **m1**, as indicated by the useful comment on the cell card. The density of Fe is defined on the cell card as equal to 7.874 g/cm^3, and its composition is defined by the **material cards**:

```
m1       26054.70h  5.845
         26056.70h 91.754
         26057.70h  2.119 .
```

As in the real experiment [57], the target was in a room filled with air. We surround in our MCNP6 test-problem the Fe-cylinder also with air, composed in our example of N, O, H, Ar, and C. The air is defined as material #2:

```
m2       7014.70h 1.555901784
         7015.60c 0.005778216
         8016.70h 0.448606754
         8017.60c 0.001079246
         1001.70h 0.06
        18000.35c 0.00934
         6000.60c 0.000383 .
```

In our problem, the air fills cell #2 and has a density of 0.001168 g/cm^3:

```
    2  2 -0.001168  #1 -5 .
```

The surface #5 is a sphere centered at origin with a radius $R = 600$ cm. Later, we tally our neutrons with the **tally card F11** just on the surface of this sphere

```
 F11:n   5 .
```

This means, we are not interested in what happens outside this sphere and can define all the "outside world", beyond this sphere, as "void"; the outside cells #3, #6, and #999 are of zero-density:

```
    3  0        5  -6
    6  0        6
  999  0       -999 .
```

This also means that we do not need to track particles in cells #6 and #999, and can set "importances" of all particles to 0 in these cells:

```
imp:n 1 1 1 0 0
imp:h 1 1 1 0 0
imp:p 1 1 1 0 0
imp:d 1 1 1 0 0
imp:t 1 1 1 0 0
imp:s 1 1 1 0 0
imp:a 1 1 1 0 0
imp:/ 1 1 1 0 0
imp:z 1 1 1 0 0 .
```

The beam of 1.2 GeV bombarding protons is defined on the **sdef** card:

```
sdef erg=1200 par=h dir=1 vec= 0 0 1 x=d1 y=d2 z=0 ccc=999 .
```

It is a mono-directional beam (**dir=1**) of protons (**par=h**) in the Z-direction (**vec= 0 0 1**) starting at $Z = 0$ (**z=0**) but, to account for the profile of the real experimental beam [57], it has a Gaussian distribution in both X- and Y-directions, as defined by the **Source Probability** cards:

```
sp1  -41 2.4 0
sp2  -41 2.4 0 .
```

The built-in function number **41**, used as a negative number on both **sp1** and **sp1** cards with the same parameters (**2.4 0**) identify Gaussian distributions in both X- and Y-directions with the widths at half maximum (FWHM) of 2.4 cm and the mean of 0, i.e., with their maximum at $X = 0$ and $Y = 0$.

Note that on the **sdef** card, we use also the "Cookie-cutter rejection" (**ccc=999**), which accepts the simulated distribution of protons if it is within the cell #999, i.e., inside the cylinder of radius $R_{999} = 10.000001$ cm in the Z-direction, as defined by the surface #999

```
  999  cz    10.000001
```

and reject and resample it (truncate, so that all protons are inside this cylinder), if is not (see pages 3-52 to 3-68 in [3] for more details).

As our problem is symmetric about the Z-axis, we can tally the neutrons on a "ring" we cut from the sphere with a radius $R = 600$ cm defined by the surface #5. If we cut this "ring" from the sphere with planes perpendicular to the Z-axis, $Z_7 = -597.8168189$ and $Z_8 = -597.6168189$, as defined by the surface cards

```
    7  pz    -597.8168189
    8  pz    -597.6168189 ,
```

then the middle of the ring $Z_m = -597.7168189$ determines an angle of 175 degree about the beam direction (600 cm$\times \cos 5^\circ = 597.7168189$ cm), i.e., exactly the angle where we have to tally the neutrons. Then, we can use the **Tally Segment Card**:

```
FS11    -7 -8
```

allowing us to subdivide the surface of the whole sphere into three sections, below $Z_7 = -597.8168189$, above $Z_8 = -597.6168189$, and between $Z_7 = -597.8168189$ and $Z_8 = -597.6168189$ and to calculate the neutron current with the card

```
F11:n   5
```

integrated over each of them, separately. The middle segment will provide us the current of neutrons emitted from the cylinder-target exactly at 175° — what we need in this problem.

Let us mention that MCNP6 provides the results in units of **neutrons per incident proton**, while the experimental spectra were measured in units of **neutrons/sr/MeV per incident proton**. It is very easy to get the units of [1/MeV] for the MCNP6 spectra: For this, we need to divide the final MCNP6 results of the middle segment (**7 -8**) by the values of the corresponding energy bins, whose 121 boundaries are defined by the **Tally Energy Card**:

```
E11   1.059254E-03 1.188502E-03 1.333521E-03 1.496236E-03 1.678804E-03
      - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
      5.956621E+02 6.683439E+02 7.498942E+02 8.413951E+02 9.440609E+02
      1000 .
```

MCNP6 could do this division for us providing [1/MeV] in the calculated spectra, if we would instruct MCNP6 to do so with a corresponding **Energy Multiplier Card** in our input file. We do so later, in other test-problems (see, *e.g.*, test-problems #6, #7, and #8) which have a simpler input file. In the current test-problem, to keep the input file as simple as possible, we chose to not use this capability, but to divide instead the spectra from the final MCNP6 output files by the corresponding energy bins using a little post processing routine after the calculations are completed, just to get the needed units for plotting the final MCNP6 spectra.

It is a little more complicated to get the units of [1/sr] in the final spectra in this test-problem: For this, we have to divide the neutron spectrum tallied in the middle segment by the value of the solid angle of this segment. The solid angle Ω (in [sr]) of the "ring" where we tally neutrons is equal to the area of this ring, $S_{ring} = 2\pi Rh$ (where h is the "height" of the ring, i.e., $h = (Z_8 - Z_7) = 0.2$ cm, and R is the radius of the sphere, $R = 600$ cm), divided by the area of the whole sphere, $S_{sphere} = 4\pi R^2$, and multiplied by 4π: $\Omega = (2\pi Rh/4\pi R^2) \times 4\pi$. This is the same as multiplying the tallied spectra by the inverse of this quantity, $\Omega^{-1} = R^2/2\pi Rh$. This is, to get [1/sr] in our final spectrum, we need to divide the tallied spectrum by $2\pi Rh = 753.9822369$ ([cm^2]) and to multiply it by $R^2 = 360000$ ([cm^2]). Here, we do the division for our middle segment with the **Segment Divisor Card (SD11)**

```
SD11    1 753.9822369 1
```

and multiply our spectra, at all 121 energy bins with the **Energy Multiplier Card (EM11)**:

```
EM11  360000 120r  $ unit: n/sr/p .
```

Note, that we need to detect all the emitted neutrons from our thick target, and the energy of the bombarding proton beam is quite high, 1.2 GeV. Some of the emitted neutrons are produced not directly by the bombarding protons, but via subsequent interactions inside the target of all types of secondary particles produced in an initial proton-iron collision. CEM03.03 can produce n, p, d, t, ^{3}He, ^{4}He, π^+, π^0, and π^- from an p+Fe interaction, therefore we need to transport all these particles through our target. This is guaranteed using the **Mode Card**:

```
mode n h p d t s a / z
```

together with the **Phys Cards**:

```
phys:h   1500.
phys:n   1500.
phys:p   1500
phys:/   1500
phys:z   1500 .
```

Note that we do not need to specify additional **phys** cards to obtain the maximum energies of d, t, ^{3}He, and ^{4}He: They will be set to 1500 MeV for all particles. We can check this with **Print Table 101**, which provides us detailed information about all tracked particles, by adding **101** on the **print card**, like:

```
print   10 110 40 101 .
```

Let us mention here an important point about using the **Mode Card** and **Phys Cards** in MCNP6: Initially, MCNP6 adopted the MCNPX concept to transport both particles and antiparticles, if particles are listed on the **mode** and **phys** cards. This is why we list on these cards in the current input file only the π^+, with its **designator** "/", but do not list its antiparticle, the π^-. This was valid in the version of MCNP6 we had and used when we run this test-problem, in March 2010. This approach really makes physics sense only for the electron/positron instance, and is contrary to the usual practice among other high-energy codes, where particles and their antiparticles are generally separate and separately-treated particle types (because their physics is usually quite different). In other words, the initial MCNP6 approach adopted from MCNPX would tally both π^+ and π^- together and would not allow us to calculate separately π^+ and π^- spectra, as discussed in some other of our test-problems with MCNP6 using LAQGSM [5]. In the initial version of MCNP6, the compromise has been to assume that the presence of a particle on the **Mode Card**, and on appropriate tallies, implies the presence of the corresponding antiparticle when MCNPX emulation is in force (specified by **DBCN(29)=1**, the last card of our current input file), but to keep particles and antiparticles separate when MCNP emulation is effective (specified by **DBCN(29)=0**). This compromise was reasonable, but we understand that the MCNP6 users need the capability to select this behavior independently of the **DBCN(29)** setting. This deficiency was solved in MCNP6 by Grady Hughes, when on May 11, 2010 he produced a new and more universal version of MCNP6 implementing an extra (backward compatibility) DBCN control, namely the **DBCN(27)** flag. Specifically, the logic implemented by Grady Hughes in the new version of MCNP6 is now as follows:

1) There will be no promotion of antiparticles in KCODE problems;
2) There will be no promotion of antiparticles for at most N, P, E problems;
3) Otherwise, **DBCN(27) = 1** turns **on** promotion regardless of DBCN(29);
4) Or, **DBCN(27) = -1** turns **off** promotion regardless of DBCN(29);
5) Otherwise, promotion is turned **on** when **DBCN(29) = 1**;
6) Or, **off** when **DBCN(29) = 0**.

To summarize, if users have an old version of MCNP6, older than of May 11, 2010, they can use the input file provided here. But with a newer version of MCNP6, in order to transport π^-, the user should add the **designator** of π^- (which is "*" in MCNP6) on the **mode card**

```
mode n h p d t s a / * z
```

and to add it on a **phys card** as well. In addition, the last card of the current input file activating here the MCNPX emulation should be replaced with the following card:

```
dbcn 20j 0 5j -1 j 1 2j 0 1 $ dbcn(27)=-1 transports pi+ separately of pi-.
```

More details on the use of the DBCN options in MCNP6 calculations can be found in the recent report by Grady Hughes [58]. Let us note here that we are working at present to simplify the use of the DBCN option for MCNP6 users; many details described in Ref. [58] will be of interest only for MCNP6 developers, while the users will not need to know and/or (explicitly) use them in their applications.

Finally, let us note here that the **Print Hierarchy Card (FQ)**

```
FQ11    e u
```

and the **Tally Fluctuation Card (TF)**

```
TF11    6j 21
```

are very useful for ordering of printed output and, respectively, to change the default bin for a given tally and to specify for which tally bin the chart and all the statistical analysis output will be printed. Both these cards are highly recommended for some problems in the MCNP5 and MCNPX manuals [3, 35]. However, in this particular test-problem, these cards are included more like examples and do not actually affect the neutron spectra we calculate here; in principle, we could omit both these cards in our MCNP6 input file and would get the same results.

As this problem requires quite a long computing time, we calculate it in several steps, using the **Continue-Run** option. Initially, we have run MCNP6 for several hours using the initial input file shown above with the command: **mcnp6 i=Fe1200 n=Fe1200.**. This initial run provides us the output file **Fe1200.o**, the **RUNTPE** file **Fe1200.r**, and the **MCTAL** file **Fe1200.m**. In a second run, we would use only the **RUNTPE** file **Fe1200.r** from the first run and an auxiliary simple input file **inp-con** of only two cards

```
nps   1e7
continue
```

using the command: **mcnp6 c i=inp-con o=Fe1200c.o r=Fe1200.r**. Thereafter, if needed, we can make a third run, and so on (changing every time only the name of the corresponding output file) until we get the needed statistics.

The initial output file of this test-problem, **Fe1200.o**, together with the final output file **Fe1200ccc.o** are presented in the subdirectory **/VALIDATION_CEM/Templates/LINUX/**. As mentioned above, the MCNP6 output file **Fe1200ccc.o** provides for the middle segment **7 -8** the neutron spectrum at 175° in units of [neutrons/sr/proton], looking like:

```
- - - - - - - - - - - - - - - - - - -
surface  5
 segment:           7       -8
      energy
    1.0593E-03   1.83951E-04 0.4598
    1.1885E-03   4.46308E-05 1.0000
    1.3335E-03   0.00000E+00 0.0000
- - - - - - - - - - - - - - - - - - -
    1.0000E+03   0.00000E+00 0.0000
      total      4.87678E-01 0.0098 .
- - - - - - - - - - - - - - - - - - -
```

To plot this spectrum and compare it with the experimental data and results by other codes (see Fig. 3), we have to convert it so that we get for it also the unit of [1/MeV]. We do this separately with a little post processing routine written especially for this.

We present the final neutron spectrum already in units of [neutrons/sr/MeV/proton] in the file **Fe1200C.dat** of subdirectory **/VALIDATION_CEM/Experimental_data/Fe1200/**. Let us note that we performed the calculations for the current test-problem using the option **nevtype=6** in CEM03.03. We use here **nevtype=6** but not **nevtype=66** because in this problem we are interested only in the neutron spectra and do not need any information about the production of fragments heavier than ^{4}He. If users forgot or are not sure what value of **nevtype** was used in a particular problem, they can check this easily by looking at **table 41** which is printed in the beginning of the output file and looks like:

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
1LAHET physics options:                                          print table 41

 lca  ielas ipreq iexisa ichoic jcoul nexite npidk noact  icem  ilaq nevtype
 lca      2     1     1     23     1      1     0     1      1     0      6 .
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

This table shows us that we have used **nevtype=6**. It also shows us that this calculation was done using the CEM event generator, **icem=1**, but not using LAQGSM, **ilaq=0**.

As the measurements [57] and calculations by other codes were done not only for incident protons of 1200 MeV, but also at 1000 MeV, 800 MeV, 600 MeV, and 400 MeV, we performed calculations with MCNP6 at all these energies as well. For this, we had to change in the input file shown above only the incident energy of protons on the **sdef** card.

Our final MCNP6 results using CEM03.03 for the incident proton energies of 1200, 1000, 800, 600, and 400 MeV are presented in the files Fe1200C.dat, Fe1000C.dat, Fe800C.dat, Fe600C.dat, and Fe400C.dat of the subdirectory **/VALIDATION_CEM/Experimental_data/Fe1200/** and are plotted with **xmgrace**, as shown in Fig. 3 and in the pdf file pFe_n_C6etc.pdf of the same subdirectory. A template to plot this figure with **xmgrace** is presented there as well in the file pFe_n_C6etc.fig.

Experimental spectra in units of [neutron/MeV/sr/projectile] as functions of the neutron energy at incident proton energies of 1200, 1000, 800, 600, and 400 MeV are presented in the same subdirectory in the files fe1200exp.dat, fe1000exp.dat, fe800exp.dat, fe600exp.dat, and fe400exp.dat, respectively (the experimental errors are of the order of (8.5-9)%, depending on the neutron energy).

For comparison, MCNP6 results using the LAQGSM03.01 event-generator [8] are presented for the incident proton energies of 1200, 1000, 800, 600, and 400 MeV in the files Fe1200Lb.dat, Fe1000Lb.dat, Fe800Lb.dat, Fe600Lb.dat, and Fe400Lb.dat, respectively.

Results by MCNPX2.7.A [12] using our CEM03.03 event-generator [6] are presented for the incident proton energies of 1200, 1000, 800, 600, and 400 MeV in the files Fe1200_27A.dat, Fe1000_27A.dat, Fe800_27A.dat, Fe600_27A.dat, and Fe400_27A.dat, respectively.

Finally, results by MCNPX2.6.0 [35] using the CEM03.01 [7], Bertini+MPM+Dresner [48, 49, 50], and the INCL+ABLA [42, 44] event-generators obtained at ORNL and kindly supplied us by Wei Lu and Franz Gallmeier as published in Ref. [57] for the incident proton energies of 1200, 1000, 800, 600, and 400 MeV are presented in the files 1200CEM.dat, 1000CEM.dat, 800CEM.dat, 600CEM.dat, 400CEM.dat, Fe1200Bert.dat, Fe1000Bert.dat, Fe800Bert.dat,

Fe600Bert.dat, Fe400Bert.dat, Fe1200INCL.dat, Fe1000INCL.dat, Fe800INCL.dat, Fe600INCL.dat, and Fe400INCL.dat, respectively.

All these results are shown in Fig. 3. We see that MCNP6 using CEM03.03 describes well the experimental spectra [57] and agrees very well with results obtained using LAQGSM03.01 in MCNP6, and with results by MCNPX using several different event-generators.

3.3. Test-problem #3: A) p18-H2O-TTY_C; B) p18-H2O-TTY (for the Bertini+Dresner option)

This MCNP6 problem is to test the applicability of MCNP6 using the CEM03.03 event generator for some medical problems and to see if CEM03.03 provides reliable results at incident energies below 150 MeV, in cases when we do not have data libraries for some particular isotopes or when using CEM03.03 instead of data libraries would provide better results.

In recent years, positron emission tomography (PET) has become a common technique for the functional imaging of brains and organs. A number of cyclotrons are installed in medical facilities to produce radionuclides for PET. In PET, one of the most commonly used radiopharmaceuticals is fluorodeoxyglucose (FDG), which is tagged with the radioactive ^{18}F isotope. The isotope is obtained from the ^{18}O(p,n)^{18}F reaction when ^{18}O-enriched water ($H_2^{18}O$) is bombarded with a proton beam. The nuclear reaction produces neutrons and γ-rays simultaneously. The energy spectrum and angular distribution should be estimated for radiation safety and clearance of the facility. However, experimental data on the energy spectrum and angular distribution for neutrons and γ-rays from the $H_2^{18}O$ target are not available, especially for proton energies from 10 to 20 MeV that are used in the PET cyclotrons. Currently, shielding of the neutrons and γ-rays, as well as activation of accelerator components and the room wall, are calculated based on transport codes like PHITS or MCNPX. The accuracy of all transport codes for such a low energy region should be tested against experimental data, because most physical models implemented in such codes were developed to describe reactions induced by high-energy particles or nuclei.

This problem is to compare neutron spectra at 15, 30, 60, 90, 120, and 150 degrees and angle-integrated energy spectrum of photons emitted from a 2.5x2.5x1 cm box of $H_2^{18}O$ (thick target) bombarded with 18 MeV protons calculated with MCNP6 using CEM03.03 and Bertini+Dresner event generators. We also compare our results with experimental data and calculations with MCNPX 2.6.E using Bertini+Dresner event generator by Dr. Hagiwara published in Ref. [59].

From a computational point of view this test-problem is similar in many aspects to the previous one, test-problem #2. Therefore, we do not need to discuss in detail either the input or the output files of the current test-problem; we direct the interested readers to Sec. 3.2.

The input file for this problem while using the CEM03.03 event generator is **p18-H2O-TTY_C**. It is provided in subdirectory **/VALIDATION_CEM/Inputs/**, and we provide it also below.

p18-H2O-TTY_C:

```
MCNP6 test: neutrons bombarded by protons of 18 MeV
c -------------------------------------------------------------
c 18 MeV protons on a box H2O18 target (5*5*2cm).
```

```
c Source uniformly distributed over circle of 1.0 cm radius.
c Tallies of proton, photon and neutron current.
c ---------------------------------------------------------------
c Cells
c ---------------------------------------------------------------
c density
  1  1  -1.000   1 -2 3 -4 5 -6
  2  0          -7 (-1:2:-3:4:-5:6)
  3  0           7

c ---------------------------------------------------------------
c Surfaces
c ---------------------------------------------------------------
  1  px  -2.5
  2  px   2.5
  3  py  -2.5
  4  py   2.5
  5  pz  -1.00
  6  pz   1.00
  7  so  100.0
  8  pz  99.62    $0-deg +5deg
  9  pz  98.48    $15-deg +-5deg
 10  pz  93.97
 11  pz  90.63    $30-deg +-5deg
 12  pz  81.92
 13  pz  57.36    $60-deg +-5deg
 14  pz  42.26
 15  pz  8.716    $90-deg +-5deg
 16  pz -8.716
 17  pz -42.26    $120-deg +-5deg
 18  pz -57.36
 19  pz -81.92    $150-deg +-5deg
 20  pz -90.63

c ---------------------------------------------------------------
c Materials - H2O(18O enriched)
c ---------------------------------------------------------------
  m1 8018 0.333
     1001 0.667
c ---------------------------------------------------------------
c Source
c ---------------------------------------------------------------
  sdef sur = 5
       erg = 18
       par = 9
       dir = 1
       pos = 0 0 -1.00
```

```
       rad = d1
  si1  0.5
c ------------------------------------------------------------
c Options
c ------------------------------------------------------------
  imp:n 1 1 0
  imp:h 1 0 0
c  phys:n 18.5 j j j 0 -1 j
c  phys:n 19.5 tabl 0.0
  phys:n 19.5
  phys:h 18.5 j 0 j j j j
  mode p n h
  lca 8j 1     $ use CEM03.03
c  lcb 8j
c  lea 8j
c  leb 4j
c ------------------------------------------------------------
c Tallies
c ------------------------------------------------------------
f4:n   1
sd4    1000
f2:n   7
fs2    8 9 10 11 12 13 14 15 16 17 18 19 20 T
sd2    1 1 1 1 1 1 1 1 1 1 1 1 1 1
f14:p   1
sd14    1000
f12:p   7
fs12    8 9 10 11 12 13 14 15 16 17 18 19 20 T
sd12    1 1 1 1 1 1 1 1 1 1 1 1 1 1
e0     1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
c  print
c  cut:n  0 0.4
  nps 3e7
c nps 100000
DBCN 28j 1
```

For brevity sake, we show here the whole MCNP6 input file only for the case of using CEM03.03, **p18-H2O-TTY_C**. The only difference in the input file **p18-H2O-TTY** for the case of using the Bertini+MPM+Dresner [48, 49, 50] event generator is in the **LCA** card; in this case it looks like:

```
lca 2j 1 .
```

All the other cards of the input file for the Bertini+MPM+Dresner case, **p18-H2O-TTY** are exactly the same as in the MCNP6 input file for the case of using the CEM03.03 event-generator showed above. The whole text of the input file for the Bertini+MPM+Dresner case, **p18-H2O-TTY**, is presented in subdirectory **/VALIDATION_CEM/Inputs/**.

Neutron spectra calculated by MCNP6 with CEM03.03 using the input p18-H2O_TTY_C at angles of 15, 30, 60, 90, 120, and 150 ($\pm$ 5) degrees are tabulated in units of [neutrons/sr/proton]

in the output file **/VALIDATION_CEM/Templates/LINUX/p18-H2O_TTY_C.o** as tally 2 for "segments":
1) segment: -8 -9 10
2) segment: -8 -9 -10 -11 12
3) segment: -8 -9 -10 -11 -12 -13 14
4) segment: -8 -9 -10 -11 -12 -13 -14 -15 16
5) segment: -8 -9 -10 -11 -12 -13 -14 -15 -16 -17 18
6) segment: -8 -9 -10 -11 -12 -13 -14 -15 -16 -17 -18 -19 20.

The use of the **sd2** card (together with the **fs2** card) in the input provides the neutron spectra in units of [neutrons/sr/proton]. However, the measured spectra are published in units of [neutrons/sr/MeV/microCoulomb]. To get [1/MeV], the tables from the MCNP6 output should be divided by the energy bin widths, equal to 1 MeV in this particular case.

We present all the experimental data, our calculation results, and all figures for this test-problem in the subdirectory **/VALIDATION_CEM/Experimental_data/p18-H2O-TTY_C/**.

To help plotting the results with **xmgrace**, the n-spectra, in units of [neutrons/sr/MeV/proton] at angles of 15, 30, 60, 90, 120, and 150 ($\pm$ 5) degrees, from the MCNP6 output file are copied to separate files: 15_MCNP6C.dat, 30_MCNP6C.dat, 60_MCNP6C.dat, 90_MCNP6C.dat, 120_MCNP6C.dat, and 150_MCNP6C.dat, respectively. To convert the units of [1/proton] provided by MCNP6 to the final units of experimental data in [1/microCoulomb], all the calculated spectra are multiplied by 6.2415×10^{12}, while plotting them with **xmgrace**.

Neutron spectra calculated by MCNP6 with Bertini+Deresner option using the input file **/VALIDATION_CEM/Inputs/p18-H2O-TTY** are tabulated for the same angles in the same "segments" of the output file **IDATION_CEM/Templates/LINUX/p18-H2O-TTYc.o**. To plot them with **xmgrace**, they are also copied (in units of [neutrons/sr/MeV/proton]) to the separates files 15_MCNP6B.dat, 30_MCNP6B.dat, 60_MCNP6B.dat, 90_MCNP6B.dat, 120_MCNP6B.dat, and 150_MCNP6B.dat, respectively, as in case of CEM03.03.

Results by MCNPX 2.6.E with Bertini+Dresner option kindly sent to us by Dr. Hagiwara are presented in the same units in the files 15_MCNPX.dat, 30_MCNPX.dat, 60_MCNPX.dat, 90_MCNPX.dat, 120_MCNPX.dat, and 150_MCNPX.dat, respectively.

Experimental data for neutron spectra kindly sent to us by Dr. Hagiwara are presented in units of [neutrons/sr/MeV/microCoulomb] in the files 15_exp.dat, 30_exp.dat, 60_exp.dat, 90_exp.dat, 120_exp.dat, and 150_exp.dat, respectively.

All the mentioned neutron spectra are plotted with **xmgrace** and presented in the pdf file p18H2O_n_l.pdf. A **xmgrace** template for this figure is presented in the file p18H2O_n_l.fig.

The angle-integrated energy spectra of photons by MCNP6 with CEM03.03 using the input p18-H2O_TTY_C is tabulated in units of [photons/proton] in the output file **/VALIDATION_CEM/Templates/LINUX/p18-H2O_TTY_C.o** as tally 14 in the "segment": **segment: whole surface**.

To plot them with **xmgrace**, they are divided by the energy bin widths and copied (in units of [photons/MeV/proton]) to the separate file g_Tot_CEM_d.dat. To convert the units of [1/proton] provided by MCNP6 to the final units of experimental data of [1/microCoulomb], the calculated gamma spectrum is multiplied by 6.2415×10^{12}, while plotting it with **xmgrace**.

Similar results in the same units obtained with Bertini+Dresner are presented in a similar "segment" of the output file **/VALIDATION_CEM/Templates/LINUX/p18-H2O-TTYc.o**. To plot them with **xmgrace**, they are also copied (in units of [photons/MeV/proton]) to a separate file, g_Tot_B_d.dat.

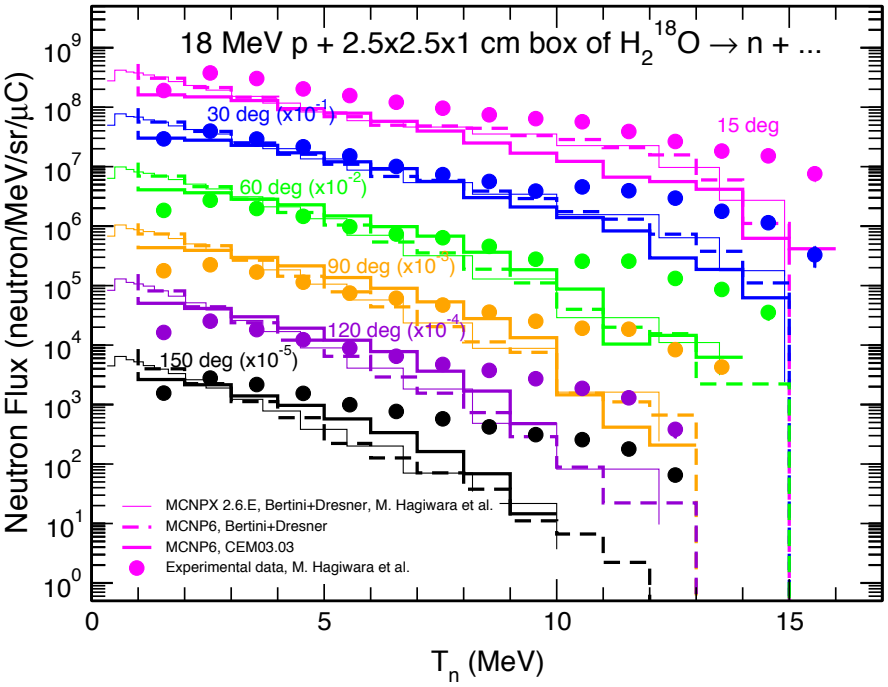

Figure 4: The measured [59] neutron energy spectra at 15, 30, 60, 90, 120, and 150 degrees from a thick $H_2^{18}O$ target bombarded with 18 MeV protons compared with our MCNP6 results using the Bertini+MPM+Dresner [48, 49, 50] and the CEM03.03 [6] event generators, as well as with results by MCNPX 2.6.E [35] from [59] kindly provided us by Dr. Masayuki Hagiwara, as indicate.

Experimental data for gamma spectrum were taken from Fig. 2 of work by Hagiwara et al. [59], and are presented in units of [photons/MeV/microCoulomb] in the file g_Tot_exp.dat.

All the gamma spectra are plotted with **xmgrace** and are presented in the pdf file p18H2O_g.pdf. A **xmgrace** template for this figure is presented in the file p18H2O_g.fig.

Neutron and gamma spectra are shown here in Figs. 4 and 5, respectively. As one can see from Figs. 4 and 5, MCNP6 with CEM03.03 describes well the recently measured [59] spectra of neutrons and of prompt γ-ray from this reaction and agrees reasonably with similar results obtained using the Bertini INC [48] + Multistage Preequilibrium Model (MPM) [49] + Dresner evaporation [50] event-generator.

3.4. Test-problem #4: A) inppfe with inxcpfe; B) inppfe_6 with inxcpfe

This MCNP6 problem is to test the applicability of MCNP6 using the CEM03.03 event generator for problems of interest for the Threat Reduction of the US Defense Department (to estimate yields of delayed-neutron emitters ^{9}Li, ^{16}C, and ^{17}N), as well as for other different intermediate-energy nuclear applications where iron is used as a construction material.

The recent GSI measurements for this test problem are published in the papers [60, 61]. Unfortunately, production of the delayed-neutron emitters ^{9}Li and ^{16}C from this reaction was not measured at GSI. However, production of ^{9}Li and ^{16}C (and of ^{17}N) by 1 GeV protons from a thin target of natural Copper was measured almost 50 years ago by Dostrovsky et al. These old data are published in Ref. [41]. We use here these old data for copper as a rough estimator

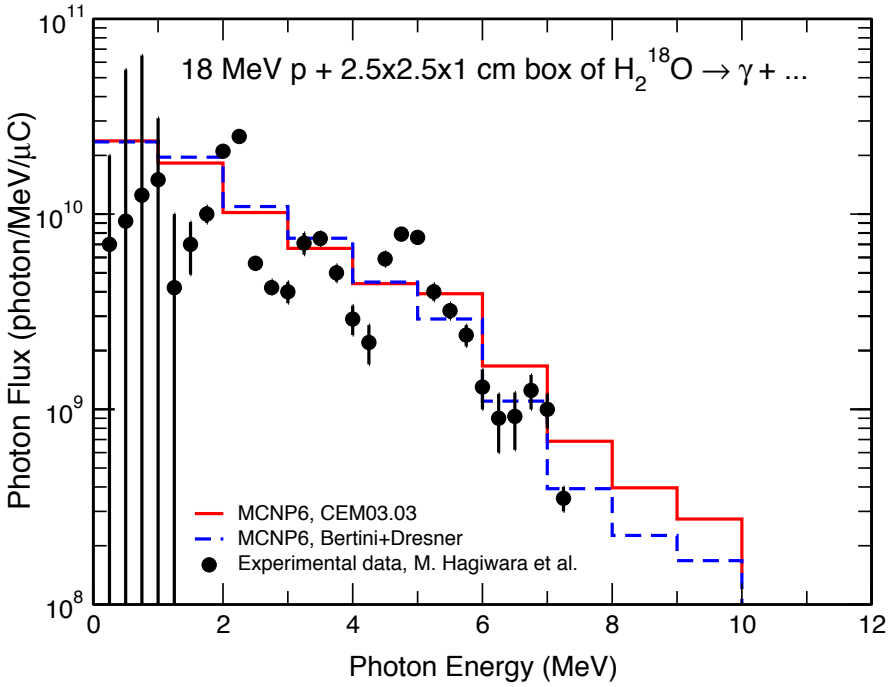

Figure 5: Comparison of the measured [59] energy spectrum of prompt γ-rays from a thick $H_2^{18}O$ target bombarded with 18 MeV protons with our MCNP6 results using the CEM03.03 [6] and the Bertini+MPM+Dresner [48, 49, 50] event generators, as indicated.

for our iron target.

In this test problem, we validate MCNP6 with CEM03.03 against experimental data for the production ^{9}Li, ^{16}C, and ^{17}N delayed-neutron emitters, as well as for the production of the light fragments of Be, B, O, and for heavier products with Z=11, 13, 15, 17, 19, 21, 23, and 25. In addition, we compare the results from MCNP6 with charge and mass distributions of all products produced in this reaction. To evaluate the influence of the value of the parameter **nevtype** on final results, we performed calculations with both **nevtype=66** (output file **inppfe.o** and MCTAL file **inppfe.m**) and using **nevtype=6** (output file **inppfe_6.o** and MCTAL file **inppfe_6.m**).

Let us mention that from a computational point of view, this test-problem is very similar to test-problem # 1 described in depth in Sec. 3.1. Therefore, for this example, we do not need to discuss in detail either the input or the output files; we direct the interested readers to Sec. 3.1. As discussed in Sec. 3.1, some of the MCNP6 yields of products calculated using the CEM and LAQGSM event generators can depend very strongly on the values of **nevtype** used in calculations. Just like in the case of the test-problem # 1, this example was developed and the MCNP6 calculations were performed when MCNP6 was still in its "historical" version, i.e., when its default of **nevtype** was 66 for LAQGSM03.03 and only 6 for CEM03.03, i.e., considering in the later case evaporation of only n, p, d, t, ^{3}He, and ^{4}He. To account for the possibility of evaporating up to 66 different types of particles, from n to ^{28}Mg, we had to change the value of **lcaopt(11)** in **subroutine initial_run** of the **module imcn.F90** in subdirectory **/Source/src/** from 6 to 66.

Let us recall here one more time that in the current version of MCNP6, the default value of **nevtype** is set to 66 for both CEM and LAQGSM. As described in Sec. 3.1, users of MCNP6 can now change the value of **nevtype** they want to use in a particular application with the

11th parameter of the **LCA** MCNP6 input card. The most important comment to MCNP6 users about **nevtype**: if/when the MCNP6 users are not sure which values for **nevtype** must be used for a particular problem, to avoid unreliable results, they should use the default option (**nevtype=66**).

This test-problem was developed before such a useful capability was added recently to MCNP6 by Grady Hughes. Therefore, at that time, we had to change by hand the value of **nevtype** and to recompile MCNP6, as described in Sec. 3.1.

As we change by hand the value of **nevtype** modifying the value of **lcaopt(11)** in **subroutine initial_run** of the **module imcn.F90**, we did not need to change anything in the MCNP6 input. To not confuse our results calculated with different values of **nevtype**, we wrote initially the main MCNP6 input file **inppfe**, with the second, auxiliary input file **inxcpfe** required by the GENXS option of MCNP6 and run MCNP6 compiled for the **nevtype=66** case with the command: **mcnp6 i=inppfe n=inppfe.**. As a result, we got the output file **inppfe.o** and the MCTAL file **inppfe.m**. After that, we simply copied the main MCNP6 input file to a new file with the name **inppfe_6**, changed the value of **nevtype** from 66 to 6, recompiled MCNP6, and run it with the command: **mcnp6 i=inppfe_6 n=inppfe_6.**. In this case, we got the output file **inppfe_6.o** and the MCTAL file **inppfe_6.m**, naturally, different from the ones obtained already with **nevtype=66**. As the input files for these two cases are actually the same, we present below only **inppfe** with its companion **inxcpfe**, as well as in the subdirectory **/VALIDATION_CEM/Inputs/**. (But we present both versions of the output and MCTAL files in the subdirectory **/VALIDATION_CEM/Templetes/LINUX/**.)

inppfe:

```
MCNP6 GENXS test of CEM03.03: p+Fe56 at 1 GeV (nevtype=66)
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ------------------------------------------------------------
  m1   25056 1.0
  sdef erg = 1000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 1000
  mode   h
  tropt genxs inxcpfe  nreact on  nescat off
c ------------------------------------------------------------
  print 40 110 95
c  nps 5000
  nps 10000000
  prdmp 2j -1
```

The INXC Input File **inxcpfe**:

```
MCNP6 GENXS test of CEM03.03: p+Fe56 at 1 GeV (nevtype=66)
1 1 1 /
Cross Section Edit
56 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
1 5 6 7 8 21 22 23 24 /
```

We present all the experimental data, our calculation results, and all figures in the subdirectory **/VALIDATION_CEM/Experimental_data/inppfe/**. The GSI experimental data for the yields of products with Z=3, 4, 5, 6, 7, 8, 11, 13, 15, 17, 19, 21, 23, and 25 in units of [mb] are presented in the files 3_exp.dat, 4_exp.dat, 5_exp.dat, 6_exp.dat, 7_exp.dat, 8_exp.dat, 11_exp.dat, 13_exp.dat, 15_exp.dat, 17_exp.dat, 19_exp.dat, 21_exp.dat, 23_exp.dat, and 25_exp.dat, respectively. The experimental A- and Z-distributions of the yields of all measured products in units of [mb] are presented in the files a_exp.dat and z_exp.dat, respectively. The old Dostrovsky data for the production of ^{9}Li, ^{16}C, and ^{17}N from natural copper are presented in units of [mb] in the files pCu_Li9_exp.dat, pCu_C16_exp.dat, and pCu_N17_exp.dat.

Results by MCNP6 calculated with **nevtype=66** for the yields of products with Z=3, 4, 5, 6, 7, 8, 11, 13, 15, 17, 19, 21, 23, and 25 in units of [mb] are presented in the output file **inppfe.o** and the MCTAL file **inppfe.m** in subdirectory **/VALIDATION_CEM/Templates/LINUX/** and are copied also to separate files 3_6_66.dat, 4_6_66.dat, 5_6_66.dat, 6_6_66.dat, 7_6_66.dat, 8_6_66.dat, 11_6_66.dat, 13_6_66.dat, 15_6_66.dat, 17_6_66.dat, 19_6_66.dat, 21_6_66.dat, 23_6_66.dat, and 25_6_66.dat, respectively, all presented in the subdirectory: **/VALIDATION_CEM/Experimental_data/inppfe/**. A- and Z-distribution of the yields of all products calculated with MCNP6 using **nevtype=66** are presented there in the files a_pfe_6_66.dat and z_pfe_6_66.dat, respectively. Similar results calculated with MCNP6 using **nevtype=6** are presented in the output file **inppfe_6.o** and the MCTAL file **inppfe_6.m** and are copied here to separate files with names similar to the ones used for **nevtype=66** but having "6" instead of "66" in their names before the extension "dat".

For convenience, all the mentioned results are plotted with **xmgrace** and presented in pdf files 1125.pdf, 38.pdf, a.pdf, z.pdf, and in the final file p1000Fe.pdf. Templates for these figures from **xmgrace** are presented in files 1125.fig 38.fig a.fig z.fig, respectively, in the same subdirectory.

All our results for this test-problem are presented here in Fig. 6. We can see a very good agreement between results calculated by CEM03.03 used as a stand alone code and with MCNP6 using CEM. Generally, almost all results calculated with **nevtype=66** agree well with the measured data, especially when the data were measured with small statistical uncertainties. For the production of delayed-neutron emitters ^{16}C and ^{17}N, the agreement with the old Dostrovsky *et al.* data [41] is not good, indicating that a further development and improvement of CEM03.03 is required. It is also true that the Dostrovsky *et al.* data were measured from Cu not from Fe, and their statistical uncertainties are very high.

As we could expect in advance, we see that the yields of products not too far from the target (*i.e.*, for $A \geq 20$ and $Z \geq 9$) calculated with **nevtype=66** agree very well with similar results obtained using **nevtype=6**. But for lighter products, we see a big deference in such

results: *E.g.*, in the case of Li, the calculations with **nevtype=66** agree very well with the measured data, while the results obtained with **nevtype=6** are almost two orders of magnitude below the measurements. With such a situation, let us repeat here one more time the main suggestion to MCNP6 users about **nevtype**: if/when the MCNP6 users are not sure which values of **nevtype** must be used for their problems, to avoid unreliable results, they should use the default option (**nevtype=66**).

3.5. Test-problem #5: inpc05 with inxc05

This MCNP6 problem is to test the applicability of MCNP6 using the CEM03.03 event generator to describe double-differential spectra of protons, deuterons, and tritons from proton-induced reactions on actinide targets at incident energies around/above 1 GeV.

The total production cross section of protons (and to a less degree of deuterons and tritons) from such reactions is very high and only the second by importance after neutron emission (and fission). Therefore, p-, d-, and t-emission determine to a great degree the mass and charge of all final products from such processes, making this problem of interest for Threat Reduction applications. In addition, light charged particle production is important to correctly assess gas production in spallation targets, and tritium is a major contributor to the target radioactivity. Therefore, the capability of MCNP6 to correctly predict production of protons, deuterons, and tritons from reactions similar to the one tested here is of great interest for many other intermediate energy nuclear applications.

The main MCNP6 input for this test-problem is **inpc05**. This problem uses the GENXS option of MCNP6 and requires the second auxiliary input, **inxc05**, both provided in the sub-directory **/VALIDATION_CEM/Inputs/** and also shown below.

inpc05:

```
MCNP6 test: p, d, t, spectra from p + U238 by CEM03.03 at 1041 MeV, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ------------------------------------------------------------
  m1   92238 1.0
  sdef erg = 1041 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 1500
  mode   h
LCA  8j 1    $ use CEM03.03
  tropt genxs inxc05  nreact on  nescat off
c ------------------------------------------------------------
```

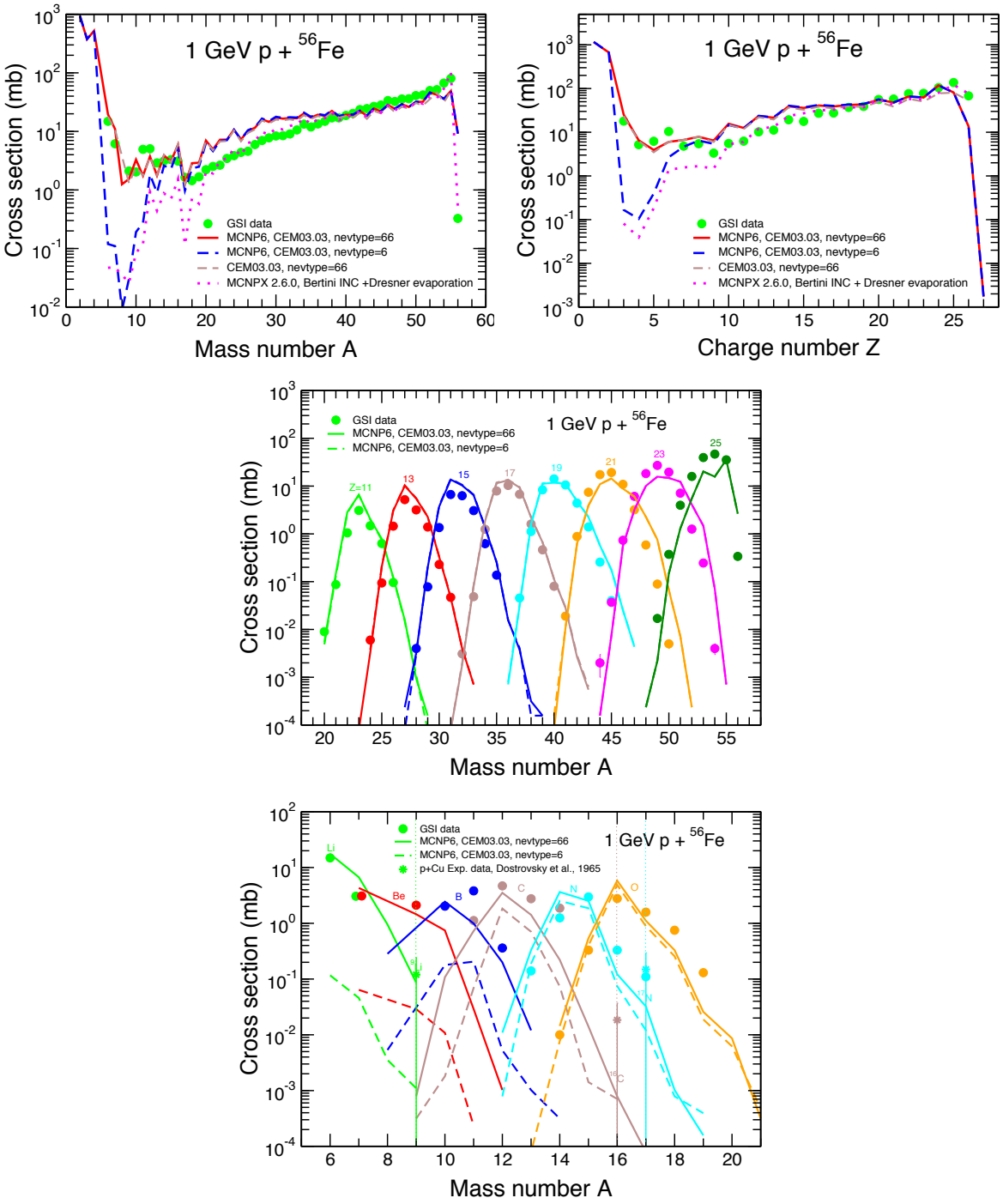

Figure 6: The measured [60, 61] mass and charge distributions of the product yields from the reaction 1 GeV/A ^{56}Fe+p and the mass distributions of the cross sections for the production of elements with the charge Z equal to 25, 23, 21, 19, 17, 15, 13, 11, 8, 7, 6, 5, 4, and 3 (filled color circles) compared with results by CEM03.03 used as a stand-alone code and with results by MCNP6 using CEM03.03 with the option **nevtype=66** and **nevtype=6**, as indicated. The delayed-neutron emitters ^{9}Li, ^{16}C, and ^{17}N are shown with vertical dotted lines of different colors in the bottom plot. As the GSI experiments [60, 61] do not provide measured cross section for the production of ^{9}Li and ^{16}C from Fe, we show here the cross section for the production of ^{9}Li and ^{16}C (as well as of ^{17}N) from Cu measured by Dostrovsky *et al.* at the same energy [41], as indicated in legend of the bottom plot.

```
  print 40 110 95
  nps 5000000
c  nps 10000
  prdmp 2j -1
```

inxc05:

```
MCNP6 test: p, d, t, spectra from p + U238 by CEM03.03 at 1041 MeV, nevtype=66
1 1 1 /
Cross Section Edit
72 -11 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
155. 145. 115. 105. 95. 85. 55. 45. 25. 15. 0. /
1 5 6 7 8 21 22 23 24 /
```

We calculate here with MCNP6 using CEM03.03 double differential spectra of protons, deuterons, and tritons at 20, 50, 90, 110, and 150 degrees and compare the results with experimental data and with predictions by CEM03.03 and LAQGSM03.03 used as stand alone codes.

The experimental spectra at 20, 50, 90, 110, and 150 degrees for protons, deuterons, and tritons are from the paper [62] and are presented here in units of [mb/MeV/sr] as functions of the kinetic energy of particles (in MeV) in the files: p1041U_20_p.dat, p1041U_50_p.dat, p1041U_90_p.dat, p1041U_110_p.dat, p1041U_150_p.dat, p1041U_20_d.dat, p1041U_50_d.dat, p1041U_90_d.dat, p1041U_110_d.dat, p1041U_150_d.dat, p1041U_20_t.dat, p1041U_50_t.dat, p1041U_90_t.dat, p1041U_110_t.dat, and p1041U_150_t.dat, respectively, in the subdirectory **/VALIDATION_CEM/Experimental_data/inpc05**

The calculations for this problem were done using **nevtype=66**. Proton spectra by MCNP6 at 150, 110, and 90 degrees in units of [b/MeV/sr] as functions of the particle (proton) kinetic energy (in MeV) are tabulated in the 2nd, 4th, and 6th pairs of columns of the first part of the "proton production cross section" table of the MCNP6 output file **inpc05.o** (with the proton energy tabulated in the 1st column), and for 50 and 20 degrees, in the 1st and 3rd pairs of columns of the second part of the same table (after the proton energy tabulated in the 1st column), as well as in the MCTAL file **inpc05.m** presented in the same subdirectory **/VALIDATION_CEM/Templates/LINUX/**.

To exemplify these proton spectra and to help MCNP6 users better understand the output file, we show a little portion of the output file relevant to these spectra on the next page. We see that proton spectra are tabulated in the output files in pairs of columns (the first column of a pair provides the calculated spectra and the second column gives its relative statistical error) after the proton energy tabulated (in [MeV]) in the first column. The number of pairs of columns in this table is determined by the number of angle bin boundaries specified for the second (**NABG**) parameter (11, in our case) on the 4th line of the INXC input file (**inxc05**, in our case). But the maximum numbers of pairs allowed in the MCNP6 output file by the GENXS option on a single page is equal to seven. Therefore, if we have in our problem more than seven angle bin boundaries, the table with spectra will be divided in two, or three, or more parts with only seven pairs of columns with results in each of them, depending on the number of angle bin boundaries we have in our problem. As in this test problem we have

proton production cross section

E(MeV)	mu max=-0.90631	mu max=-0.81915	mu max=-0.42262	mu max=-0.25882	mu max=-0.08716	mu max= 0.08716	mu max= 0.57358
5.000000E+00	1.440E-03 0.010	1.403E-03 0.010	1.370E-03 0.005	1.320E-03 0.008	1.283E-03 0.008	1.256E-03 0.008	1.210E-03 0.005
1.000000E+01	9.477E-03 0.004	9.412E-03 0.004	9.143E-03 0.002	8.930E-03 0.003	8.815E-03 0.003	8.601E-03 0.003	8.271E-03 0.002
1.500000E+01	1.484E-02 0.003	1.505E-02 0.003	1.563E-02 0.001	1.638E-02 0.002	1.692E-02 0.002	1.743E-02 0.002	1.825E-02 0.001
2.000000E+01	6.826E-03 0.005	7.041E-03 0.005	7.642E-03 0.002	8.360E-03 0.003	8.804E-03 0.003	9.378E-03 0.003	1.028E-02 0.002
2.500000E+01	3.371E-03 0.006	3.502E-03 0.007	3.937E-03 0.003	4.504E-03 0.004	4.940E-03 0.004	5.379E-03 0.004	6.120E-03 0.002
3.000000E+01	2.079E-03 0.008	2.132E-03 0.008	2.503E-03 0.004	3.000E-03 0.005	3.354E-03 0.005	3.751E-03 0.004	4.435E-03 0.002
3.500000E+01	1.460E-03 0.010	1.544E-03 0.010	1.806E-03 0.004	2.265E-03 0.006	2.584E-03 0.005	2.984E-03 0.005	3.587E-03 0.003
4.000000E+01	1.113E-03 0.011	1.162E-03 0.011	1.420E-03 0.005	1.773E-03 0.007	2.073E-03 0.006	2.446E-03 0.006	3.080E-03 0.003
4.500000E+01	8.832E-04 0.013	9.450E-04 0.013	1.142E-03 0.005	1.444E-03 0.007	1.729E-03 0.007	2.071E-03 0.006	2.691E-03 0.003
5.000000E+01	7.155E-04 0.014	7.699E-04 0.014	9.206E-04 0.006	1.191E-03 0.008	1.451E-03 0.007	1.787E-03 0.006	2.401E-03 0.003
5.500000E+01	5.905E-04 0.015	6.291E-04 0.015	7.667E-04 0.007	9.894E-04 0.009	1.234E-03 0.008	1.537E-03 0.007	2.160E-03 0.004
6.000000E+01	5.129E-04 0.016	5.202E-04 0.017	6.383E-04 0.007	8.537E-04 0.010	1.037E-03 0.009	1.352E-03 0.007	1.952E-03 0.004
6.500000E+01	4.464E-04 0.018	4.495E-04 0.018	5.480E-04 0.008	7.239E-04 0.010	8.992E-04 0.009	1.164E-03 0.008	1.781E-03 0.004
7.000000E+01	3.938E-04 0.019	4.081E-04 0.019	4.720E-04 0.008	6.310E-04 0.011	7.841E-04 0.010	1.031E-03 0.009	1.645E-03 0.004
7.500000E+01	3.410E-04 0.020	3.443E-04 0.021	4.090E-04 0.009	5.465E-04 0.012	6.870E-04 0.011	9.155E-04 0.009	1.527E-03 0.004

E(MeV)	mu max= 0.70711	mu max= 0.90631	mu max= 0.96593	mu max= 1.00000
5.000000E+00	1.146E-03 0.009	1.120E-03 0.008	1.107E-03 0.014	1.045E-03 0.019
1.000000E+01	7.898E-03 0.004	7.609E-03 0.003	7.493E-03 0.005	7.485E-03 0.007
1.500000E+01	1.876E-02 0.002	1.901E-02 0.002	1.944E-02 0.003	1.942E-02 0.004
2.000000E+01	1.079E-02 0.003	1.126E-02 0.002	1.152E-02 0.004	1.155E-02 0.006
2.500000E+01	6.558E-03 0.004	6.855E-03 0.003	7.070E-03 0.006	7.011E-03 0.007
3.000000E+01	4.752E-03 0.005	5.012E-03 0.004	5.228E-03 0.006	5.273E-03 0.009
3.500000E+01	3.895E-03 0.005	4.070E-03 0.004	4.271E-03 0.007	4.383E-03 0.009
4.000000E+01	3.339E-03 0.005	3.545E-03 0.004	3.707E-03 0.008	3.762E-03 0.010
4.500000E+01	2.976E-03 0.006	3.103E-03 0.005	3.269E-03 0.008	3.303E-03 0.011
5.000000E+01	2.592E-03 0.006	2.802E-03 0.005	2.953E-03 0.009	3.070E-03 0.011
5.500000E+01	2.360E-03 0.006	2.566E-03 0.005	2.733E-03 0.009	2.813E-03 0.012
6.000000E+01	2.190E-03 0.007	2.358E-03 0.005	2.576E-03 0.009	2.642E-03 0.012
6.500000E+01	2.015E-03 0.007	2.197E-03 0.005	2.377E-03 0.010	2.445E-03 0.013
7.000000E+01	1.894E-03 0.007	2.044E-03 0.006	2.298E-03 0.010	2.306E-03 0.013
7.500000E+01	1.754E-03 0.007	1.961E-03 0.006	2.116E-03 0.010	2.222E-03 0.013

specified 11 angle bin boundaries, the table with proton spectra will by divided in two parts, with seven spectra in the first part of the table and the remaining four spectra in its second part. To understand what is printed in each pair of columns, the cosine values of the end of corresponding angle bin are printed in the first line of this table for all angles (in **decreasing** order) we specified in our INXC input file.

Note that in this problem, we have indicated in our INXC input file 11 angles in degrees, as specified on the 7th line of the file **inxc05**:

```
155. 145. 115. 105. 95. 85. 55. 45. 25. 15. 0. /,
```

while in the first line of the table with spectra in the output file we have printed the cosines, but not the angles in degrees. However, as we see below form another little portion of the output file (provided almost at the beginning of the output file, before spectra are tabulated), the output file informs us which value of cosine corresponds to which angle.

```
cosine bin boundaries :
    -0.90630778703665   -0.81915204428899   -0.42261826174070   -0.25881904510252   -0.08715574274766
     0.08715574274765    0.57357643635104    0.70710678118655    0.90630778703665    0.96592582628907
     1.00000000000000

degree bin boundaries :
    155.000000000000    145.000000000000    115.000000000000    105.000000000000     95.000000000000
     85.000000000000     55.000000000000     45.000000000000     25.000000000000     15.000000000000
      0.000000000000
```

From this portion of the output file, we easily understand that in the 1st pair of the first part of table with spectra is the spectrum of protons emitted at angles between 180 and 155 degrees (*i.e.* at 167.5 ± 12.5 degrees); the second pairs provides the protons emitted at angles between 155 and 145 degrees (*i.e.* at 150.0 ± 5.0 degrees); the third pairs provides the protons emitted at angles between 145 and 115 degrees (*i.e.* at 130.0 ± 15.0 degrees); the 4th pairs provides the protons emitted at angles between 115 and 105 degrees (*i.e.* at 110.0 ± 5.0 degrees), etc., up to the the protons emitted at angles between 85 and 55 degrees (*i.e.* at 70.0 ± 15.0 degrees), in the last 7th pair. Here, the first part of the table ends and the spectra for the following angles are printed in the second part of this table, following in the output file immediately after the first part of the table. We easily understand that in the 1st pair of the second part of this tables is the spectrum for protons emitted at angles between 55 and 45 degrees (*i.e.* at 50.0 ± 5.0 degrees); the second pairs provides the protons emitted at angles between 45 and 25 degrees (*i.e.* at 35.0 ± 10.0 degrees); the third pairs provides the protons emitted at angles between 25 and 15 degrees (*i.e.* at 20.0 ± 5.0 degrees); and finally, the last, 4th pairs provides the protons emitted at angles between 15 and 0 degrees (*i.e.* at 7.5 ± 7.5 degrees). After the second part of this table, we see in the output file also its last part, with the angle-integrated energy proton spectra, i.e., $d\sigma/dT$ in units of [b/MeV], as well as the energy-integrated angular proton spectra, i.e., $d\sigma/d\Omega$ in units of [b/sr].

```
  E(MeV)   angle integrated          mu max          deg min    energy integrated
5.000000E+00    1.585E-02 0.002     -0.906307787037   155.0000000    2.359E-01 0.002
1.000000E+01    1.075E-01 0.001     -0.819152044289   145.0000000    2.401E-01 0.002
1.500000E+01    2.169E-01 0.001     -0.422618261741   115.0000000    2.572E-01 0.001
2.000000E+01    1.166E-01 0.001     -0.258819045103   105.0000000    2.851E-01 0.001
2.500000E+01    6.650E-02 0.001     -0.087155742748    95.0000000    3.098E-01 0.001

- - - - - - - - - - - - - - - - -
```

Finally, after this last part of the proton spectra, we can see in the output file the mean multiplicity and the total production cross section (in barns) of all protons:

```
total proton   production cross section =  5.276E+00 0.0003 yield =  2.57770E+00
```

Although we have already mentioned this in Sec. 3.2, let us recall here one more time that the mean **"multiplicities"** of particles, i.e., the mean number of particles produced per one inelastic interaction are listed in the MCNP6 outputs as **"yields"**; so, we see that the mean multiplicity of protons $< p >$ from this reaction is equal to 2.5777 and their total production cross section is equal to 5.276 b ($\pm 0.03\%$).

MCNP6 spectra for deuterons and tritons are tabulated in similar pairs of columns of similar MCNP6 output tables entitled "deuteron production cross section" and "triton production cross section," respectively. To help plotting these spectra with xmgrace, all the MCNP6 spectra are copied here to separate files 20_p_m6c.dat, 50_p_m6c.dat, 90_p_m6c.dat, 110_p_m6c.dat, 150_p_m6c.dat, 20_d_m6c.dat, 50_d_m6c.dat, 90_d_m6c.dat, 110_d_m6c.dat, 150_d_m6c.dat, 20_t_m6c.dat, 50_t_m6c.dat, 90_t_m6c.dat, 110_t_m6c.dat, 150_t_m6c.dat, respectively.

Spectra by CEM03.03 as a stand alone code are presented in the files 20_p_c.dat, 50_p_c.dat, 90_p_c.dat, 110_p_c.dat, 150_p_c.dat, 20_d_c.dat, 50_d_c.dat, 90_d_c.dat, 110_d_c.dat, 150_d_c.dat, 20_t_c.dat, 50_t_c.dat, 90_t_c.dat, 110_t_c.dat, 150_t_c.dat, respectively.

Spectra by LAQGSM03.03 as a stand alone code are presented in the files 20_p_l.dat, 50_p_l.dat, 90_p_l.dat, 110_p_l.dat, 150_p_l.dat, 20_d_l.dat, 50_d_l.dat, 90_d_l.dat, 110_d_l.dat, 150_d_l.dat, 20_t_l.dat, 50_t_l.dat, 90_t_l.dat, 110_t_l.dat, 150_t_l.dat, respectively.

For convenience, all the mentioned results are plotted with xmgrace and presented in the pdf files p1041U_p.pdf, p1041U_d.pdf, p1041U_t.pdf, and in the summary file p1041U.pdf. Templates for these figures from **xmgrace** are presented in the files p1041U_p.fig, p1041U_d.fig, and p1041U_t.fig, respectively. All these files are in subdirectory **/VALIDATION_CEM/Experimental_data/inpc05/**.

Here, we present all our results for this test-problem in Fig. 7. We see a very good agreement between results by CEM03.03 used as a stand alone code and results by MCNP6 using CEM. We also observe a good agreement with experimental data. The results by LAQGSM03.03 used as a stand alone code agree a little worse (though, still very reasonably) with some of the measured spectra at this energy, as we observe, *e.g.*, for proton spectra at 150 degrees. We know that for some reactions, CEM describes the measured data a little better that LAQGSM, at incident energies below several GeVs. This is why we recommend use of CEM at such relatively low incident energies, but to "switch" to LAQGSM at energies above ~ 5 GeV and for projectiles not allowed by CEM.

3.6. Test-problem #6: A) p63Pb_GENXS_1 with inxc06; B) p63Pb_n_cemREP with inp_p63Pb_n

This problem is to test the applicability of MCNP6 using the CEM03.03 event generator to calculate neutron production from proton-induced reactions at incident energies below 150 MeV, but above 20 MeV where we have data libraries for most of the nuclides. A need in such calculations may arise when we do not have data libraries for some specific nuclides, or when we believe that using CEM03.03 instead of data libraries would provide more reliable final results.

This test calculates with MCNP6 using CEM03.03 neutron spectra at 24, 35, 55, 80, and 120 degrees from interactions of 62.9 MeV protons with ^{208}Pb; it compares the results with experimental data and with results by CEM03.03 event generator used as a stand alone code, as well as with results by INCL4.5+ABLA07 and by MCNPX using the default options, i.e., using the Bertini INC, preequilibrium emission as described by MPM, Dresner evaporation,

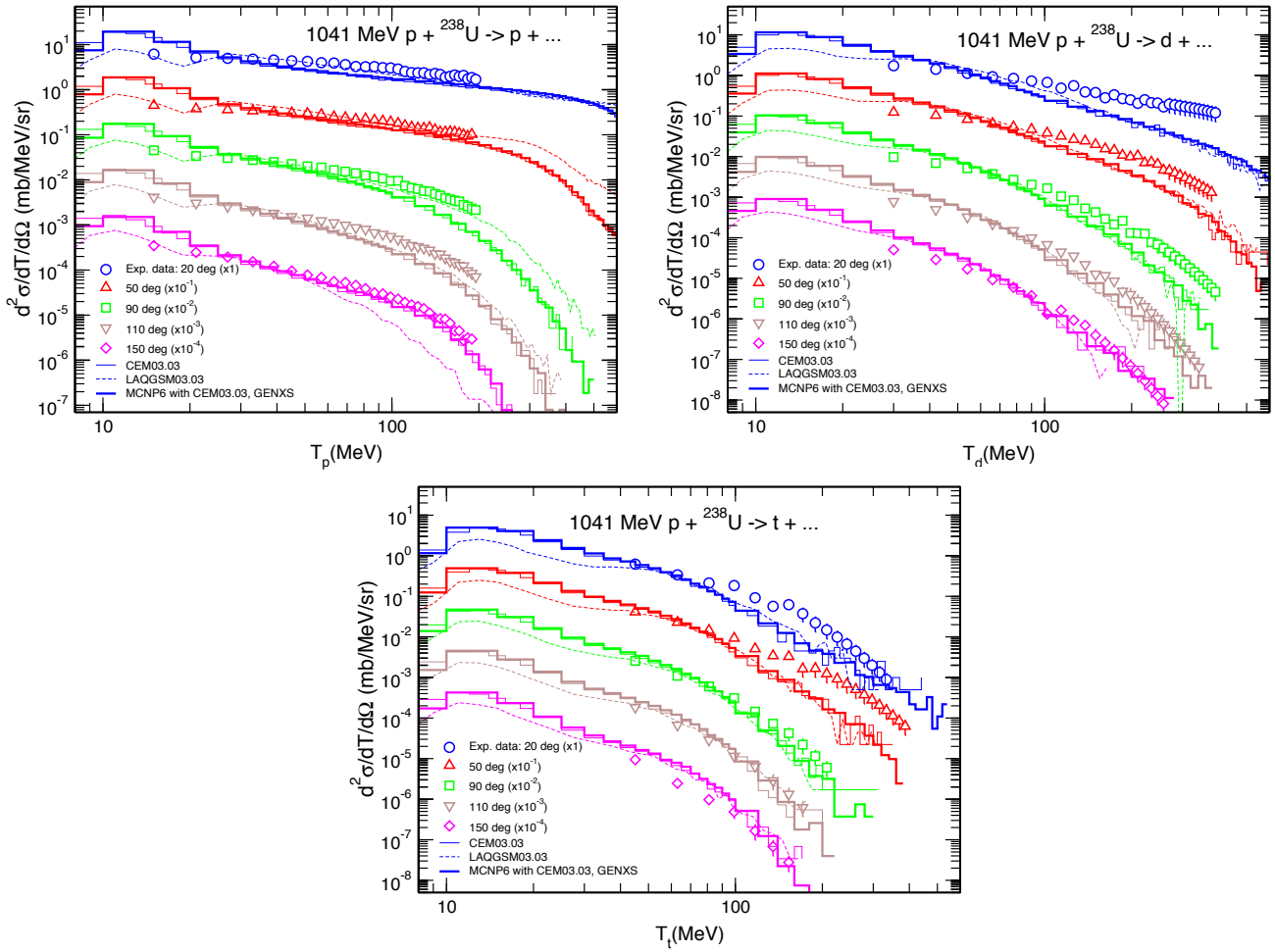

Figure 7: Experimental [62] double-differential spectra of protons, deuterons, and tritons at 20, 50, 90, 110, and 150 degrees from interactions of 1.041 GeV protons with a thin ^{238}U target compared with calculations by CEM03.03 [6] and LAQGSM03.03 [10] used as stand alone codes and with results by MCNP6 using the CEM03.03 event-generator, as indicated.

and the RAL fission, as presented at the recent International Benchmark of Spallation Models organized by IAEA during 2008-2010 [19].

We calculated with MCNP6 these spectra in two different ways:

1) using the GENXS option of MCNP6;

2) using the NOACT=-2 option for the 8th parameter of the LCA card.

1) We have presented a detailed description of the use of GENXS option to calculate particle spectra from thin targets in test-problems #1 and #5, therefore we do not need to discuss in depth either the input or the output files of the current test-problem while using the GENXS option: we direct the readers to Sections 3.1 and 3.5 for details. The main MCNP6 input file for this case is **p63Pb_GENXS_1** and its auxiliary companion required by the GENXS option is **inxc06**. Both files are presented in the subdirectory **/VALIDATION_CEM/Inputs/** and are shown below.

p63Pb_GENXS_1:

```
MCNP6 test: n spectra from p + Pb208 by CEM03.03 at 62.9 MeV, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c -------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c -------------------------------------------------------------
  m1 82208 1.0
  sdef erg = 62.9 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 75
  mode   h
LCA  8j 1    $ use CEM03.03
  tropt genxs inxc06  nreact on  nescat off
c -------------------------------------------------------------
  print 40 110 95
nps 1000000
c  nps 10000
  prdmp 2j -1
```

inxc06:

```
MCNP6 test: n spectra from p + Pb208 by CEM03.03 at 62.9 MeV, nevtype=66
1 1 0 /
Cross Section Edit
72 -11 9 /
1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 11. 12. 13. 14. 15. 16.
17. 18. 19. 20. 21. /
122. 118. 82. 78. 57. 53. 37. 33. 26. 22. 0. /
1 /
```

Neutron spectra calculated by MCNP6 using CEM03.03 with the GENXS option at 120, 80, and 55 (±3) degrees are tabulated in units of [b/sr/MeV] in the 2nd, 4th, and 6th pairs of columns of the first part of the "neutron production cross section" table of the MCNP6 output file p63Pb_GENXS_1.o (after the neutron energy tabulated in the 1st column) and for 35 and 24 degrees, in the 1st and 3rd pairs of columns of the second part of the same tables, following the neutron energy tabulated in the 1st column, as well as in the MCTAL file **p63Pb_GENXS_1.m** presented in the Templates subdirectory **/VALIDATION_CEM/Templates/LINUX/**.

To help plotting these spectra with xmgrace (see file p63Pb_n_REP.pdf), the MCNP6 results are copied also to separate files 24genxs.dat, 35genxs.dat, 55genxs.dat, 80genxs.dat, and

120genxs.dat, respectively, presented in subdirectory
/VALIDATION_CEM/Experimental_data/p63Pb_n.

2) The **NOACT=-2** option for the 8th parameter of the LCA card is very convenient for calculating with MCNP6 nuclear reactions on thin targets, especially when we need to compare our results with experimental data (most of the data are measured on thin targets). This option forces source particles to collide immediately and all progeny to escape (see more details in Sec. 5.4.6.1 of the old MCNPX Manual [35] and in Sec. 5.4.7.1 of the recent MCNPX Manual (Version 2.7.0) [63]). This is, we can have a problem with a really thick target, but the results will correspond to a thin target, as we will account for only the first interaction of a source particle with a nucleus of the target.

Except for using the **noact=-2** option, the rest of the MCNP6 input file (**p63Pb_n_cem**) for this case as well as the output file with MCNP6 results (**p63Pb_n_cemREP_cc.o**) are similar in many aspects to the examples discussed in test-problems #2 and #3. Therefore, we discuss below only several details not addressed above in the test-problems #2 and #3. The MCNP6 input file for this case is **p63Pb_n_cemREP**, presented in the subdirectory **/VALIDATION_CEM/Inputs/** and also shown below.

p63Pb_n_cemREP:

```
MCNP6 test with CEM03.03: 62.9 MeV p+Pb208 -> neutron spectra
c d^2sigma/dT/dOmega [mb/sr/MeV] at 24, 35, 55, 80, and 120 deg (+/- 2 deg)
c to compare with Guertin's et al. measurements, Eur. Phys. J. A 23 (2005) 49,
c and results by CEM03.03 and INCL4.5+ABLA07 as stand alone codes
c as well as by MCNPX 2.6.0 using Bertini+Dresner (default) option
c as presented at the IAEA Benchmark of Spallation Models, 2009-2010
1   1  -10   -501      imp:n=1
2   0         501  -502  imp:n=1
99  0         502      imp:n=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
22     kz    0    0.163237191     1  $ tan(22.0 deg)^2
26     kz    0    0.237883077     1  $ tan(26.0 deg)^2
33     kz    0    0.421730222     1  $ tan(33.0 deg)^2
37     kz    0    0.567843706     1  $ tan(37.0 deg)^2
53     kz    0    1.761047959     1  $ tan(53.0 deg)^2
57     kz    0    2.371184107     1  $ tan(57.0 deg)^2
78     kz    0    22.13354447     1  $ tan(78.0 deg)^2
82     kz    0    50.62848629     1  $ tan(82.0 deg)^2
118    kz    0    3.537132037    -1  $ tan(118.0 deg)^2
122    kz    0    2.561070605    -1  $ tan(122.0 deg)^2

mode n h d t s a
m1  82208 1
```

```
lca 0 6j -2 1    $ CEM03.03, no transport, only the 1st inelastic, no elastic
nps 10000
c nps 2e8
c prdmp 2j -1
sdef par=h erg=62.9 vec=0 0 1 dir 1
phys:h 70 j 0 j j j j
phys:n 70
phys:a 70
phys:d 70
phys:t 70
phys:s 70
c
f1:n  502
c define the "segments" for n at 24, 35, 55, 80, and 120 deg
fs1 -22 -26 -33 -37 -53 -57 -78 -82 118 122 T
c
c The following Segment Divisor card is needed to get 1/sr for n spectra
sd1   0.45752  $ 2pi(cos0 -cos22.0)
      0.17838  $ 2pi(cos22.0 - cos26.0)
      0.37777  $ 2pi(cos26.0 - cos33.0)
      0.25155  $ 2pi(cos33.0 - cos37.0)
      1.23666  $ 2pi(cos37.0 - cos53.0)
      0.35925  $ 2pi(cos53.0 - cos57.0)
      2.11572  $ 2pi(cos57.0 - cos78.0)
      0.43190  $ 2pi(cos78.0 - cos82.0)
      3.82423  $ 2pi(cos82.0 - cos118.0)
      0.37980  $ 2pi(cos118.0 - cos122.0)
      2.95360  $ 2pi(cos122.0 - cos180)
      12.56637 $ 4pi
c
c     Boundaries of the neutron energy bins: 0-1 MeV; 1-2 MeV, ...
c     tabulated exactly as used by CEM03.03 as stand alone code
e0    1     2     3     4     5     6     7     8     9     10
      11    12    13    14    15    16    17    18    19    20
      21    22    23    24    25    26    27    28    29    30
      31    32    33    34    35    36    37    38    39    40
      41    42    43    44    45    46    47    48    49    50
      51    52    53    54    55    56    57    58    59    60
      61    62    63    64    65    66    67    68    69    70
c
em1 1962.23 69r $ multiply to sig_inelastic = 1962.23 mb, as predicted by
c                 CEM03.03 as a stand alone code. This is needed
c                 to get the spectra in [mb/sr/MeV], after dividing the flux
c                 to the energy bins, to get [1/MeV]; we do this for every E-bin
dbcn  28j 1
```

We calculate the neutron spectra using the **F1** tally on the surface of a sphere (surface

502) with a radius equal to 1 cm, using a source of 62.9 MeV monoenergetic protons in its center, with the beam in the Z-axis direction. To get the double-differential spectra of secondary neutrons at needed angles, it is very convenient to divide the surface of the sphere (surface # 502) in "segments", corresponding to our angles, and to tally the neutron separately in all these "segments". For this, we use "tally surfaces" of cones on the Z-axis defined as:

```
22      kz     0     0.163237191      1  $ tan(22.0 deg)^2
26      kz     0     0.237883077      1  $ tan(26.0 deg)^2
33      kz     0     0.421730222      1  $ tan(33.0 deg)^2
37      kz     0     0.567843706      1  $ tan(37.0 deg)^2
53      kz     0     1.761047959      1  $ tan(53.0 deg)^2
57      kz     0     2.371184107      1  $ tan(57.0 deg)^2
78      kz     0     22.13354447      1  $ tan(78.0 deg)^2
82      kz     0     50.62848629      1  $ tan(82.0 deg)^2
118     kz     0     3.537132037     -1  $ tan(118.0 deg)^2
122     kz     0     2.561070605     -1  $ tan(122.0 deg)^2
```

Let us provide here a useful hint: we have chosen the numbers for the surfaces for these cones not arbitrarily, but so that they help us know at once the angle a given cone provides: So, surface #22 is a cone on the Z-axis starting at the origin, Z=0; it provides us an angle of 22 degrees relative to the Z-axis. Similarly, surface #26 provides us an angle of 26 degrees, etc. From here, we have that the "segment" of the sphere (surface # 502) cut by the cones #22 and #26 corresponds to an angle of 24 ± 2 degrees, the first angle for which we need to calculate the neutron spectra. In a similar way, the rest of cones have the surface numbers and provide just the angles to get the remaining 35 ± 2, 55 ± 2, 80 ± 2, and 120 ± 2 degrees in order to calculate our spectra.

Let us recall here that the F1 tally of MCNP6 provides us current of particles (neutrons, in our case) over a surface in units of [particles/projectile], while we need our final neutron spectra in units of [mb/MeV/sr] (per projectile), as they were measured in the experiment. To get the units of mb, we multiply our MCNP6 spectra with the total inelastic cross section, $\sigma_{in} = 1962.23$ mb, as calculated by CEM03.03 used as a stand alone code; for this, we use the Energy Multiplier Card **EM1**

```
em1 1962.23 69r $ multiply to sig_inelastic = 1962.23 mb, as predicted by
c                 CEM03.03 as a stand alone code. This is needed
c                 to get the spectra in [mb/sr/MeV], after dividing the flux
c                 to the energy bins, to get [1/MeV]; we do this for every E-bin
```

with this value for all of the 70 energy bins defined by the **E0** card:

```
e0    1     2     3     4     5     6     7     8     9     10
      11    12    13    14    15    16    17    18    19    20
      21    22    23    24    25    26    27    28    29    30
      31    32    33    34    35    36    37    38    39    40
      41    42    43    44    45    46    47    48    49    50
      51    52    53    54    55    56    57    58    59    60
      61    62    63    64    65    66    67    68    69    70 .
```

To get the needed units of [1/MeV] for our spectra, we need to divide the MCNP6 results by the corresponding energy bin widths (in MeV). If the energy bins would have different values, we could do this with the **EM1** card, using on it σ_{in} divided by different values for the corresponding energy bins. We show such an example below in Sec. 3.8, for the test-problem # 8. Here, to keep this example as simple as possible, we have chosen the easiest way: All the energy bins in this test problem are equal to 1 MeV, so we can use only one number on the **EM1** card for all energy bins, and even a real division is not needed, as all energy bins are exactly 1 MeV.

Finally, to get the units of [1/sr] in our spectra, we need to divide the **F1** MCNP6 tally results by the values of the solid angles for the "segments" where we count the neutrons. It is convenient to do this with the Segment Divisor Card **SD1**, where we provide the solid angle for each "segment" (we calculate them separately with a calculator before starting our MCNP6 run).

```
c The following Segment Divisor card is needed to get 1/sr for n spectra
sd1   0.45752  $ 2pi(cos0 -cos22.0)
      0.17838  $ 2pi(cos22.0 - cos26.0)
      0.37777  $ 2pi(cos26.0 - cos33.0)
      0.25155  $ 2pi(cos33.0 - cos37.0)
      1.23666  $ 2pi(cos37.0 - cos53.0)
      0.35925  $ 2pi(cos53.0 - cos57.0)
      2.11572  $ 2pi(cos57.0 - cos78.0)
      0.43190  $ 2pi(cos78.0 - cos82.0)
      3.82423  $ 2pi(cos82.0 - cos118.0)
      0.37980  $ 2pi(cos118.0 - cos122.0)
      2.95360  $ 2pi(cos122.0 - cos180)
      12.56637 $ 4pi
```

Last, let us note that as was suggested by Dick Prael (REP), to get correct results using the **noact=-2** option for particle-nucleus calculations like in this test-problem, we need to set **IELAS=0** on the LCA card (we do not need to do so for nucleus-nucleus reactions in the current version of MCNP6):

```
lca 0 6j -2 1    $ CEM03.03, no transport, only the 1st inelastic, no elastic.
```

All other details of the input file are either described in previous sections or are self-explanatory; therefore, we do not discuss them here.

Neutron spectra calculated by MCNP6 with CEM03.03 using the **NOACT=-2** option for the 8th parameter of the LCA card, and the **IELAS=0** option for the first parameter of the same LCA card at 24, 35, 55, 80, and 120 (±2) degrees are tabulated in units of [mb/sr/MeV] in the final MCNP6 output file **/VALIDATION_CEM/Templates/LINUX/p63Pb_n_cemREP_cc.o** (calculated with the "continue" option using the auxiliary input file **inp_p63Pb_n**; the first MCNP6 output calculated with the main input file, **p63Pb_n_cemREP**, is: **p63Pb_n_cemREP.o**) as tally 1, respectively in the "segments":
1) segment: 22 -26
2) segment: 22 26 33 -37
3) segment: 22 26 33 37 53 -57
4) segment: 22 26 33 37 53 57 78 -82

5) segment: 22 26 33 37 53 57 78 82 -118 122 .

To help plotting these spectra with xmgrace (see file p63Pb_n_REP.pdf), the final MCNP6 results obtained in the second way are copied to separate files noact24.dat, noact35.dat, noact55.dat, noact80.dat, and noact120.dat, respectively, presented in subdirectory
/VALIDATION_CEM/Experimental_data/p63Pb_n.

Besides the MCNP6 results, for comparison, we show here also results by CEM03.03 as a stand alone code as presented at the mentioned above IAEA Benchmark; see files: 24cem.dat, 35cem.dat, 55cem.dat, 80cem.dat, and 120cem.dat, respectively. Results by INCL4.5+ABLA07 downloaded from the official IAEA Benchmark web-page are presented in the files 24incl.dat, 35incl.dat, 55incl.dat, 80incl.dat, and 120incl.dat, respectively. Finally, results by MCNPX using the default option downloaded from the same IAEA Benchmark web-page are presented in the files 24mcnpx.dat, 35mcnpx.dat, 55mcnpx.dat, 80mcnpx.dat, and 120mcnpx.dat, respectively. All these files as well as files with our figures and with experimental data are presented in the same subdirectory **/VALIDATION_CEM/Experimental_data/p63Pb_n**.

The file p63Pb_n_REP.fig is a template for plotting the spectra with **xmgrace**. The pdf file for the figure with final results for this problem is p63Pb_n_REP.pdf.

The experimental data for this problem were measured at the CYCLONE facility in Louvain-la-Neuve (Belgium) and are published in the paper [64]. Tabulated values of these measurements are available in the EXFOR data base, Entry: O1146, and are presented also on the IAEA web page of the mentioned Benchmark [19].

Experimental neutron spectra $d^2\sigma/dT/d\Omega$ in units of [mb/sr/MeV] as functions of neutron kinetic energy in [MeV] at 24, 35, 55, 80, and 120 degrees are presented here in the files 24exp.dat, 35exp.dat, 55exp.dat, 80exp.dat, and 120exp.dat, respectively.

Here, we present the final results in Fig. 8. First, we see a very good agreement between results by CEM03.03 used as a stand alone code and the MCNP6 results using CEM. We observe also a very good description of the measured spectra by MCNP6 results obtained using the two different ways we tested here: 1) using the GENXS option of MCNP6, and

2) using the NOACT=-2 option for the 8th parameter of the LCA card.

We see that the second set of corrected MCNPX 2.6.0 results calculated by Franz Gallmeier with default options (i.e., Bertini INC [48] + Multistage Preequilibrium Model [49] + Dresner evaporation [50] + RAL fission model [26]) as presented at the recent International Benchmark of Spallation Models [19] also agrees well with the measured data for this reaction (unfortunately, the first set of such MCNPX 2.6.0 results presented by Franz Gallmeier at the IAEA Benchmark [19] was calculated with some errors in the input files, therefore strongly disagreeing with the measured data; see more details about this in Ref. [51]). The INCL4.5 + ABLA07 results presented at the IAEA Benchmark [19] show some problems for these spectra at neutron energies around 10 MeV.

3.7. Test-problem #7: A) p160Au_He4_GENXS with inxc07; B) p160Au_He4_REP

This problem is to test the applicability of MCNP6 using the CEM03.03 event generator to calculate production of alpha particles from intermediate-energy proton-induced reactions of interest for different applications.

This test calculates with MCNP6 using CEM03.03 the ^{4}He spectra at 20, 40, 65, 100, and

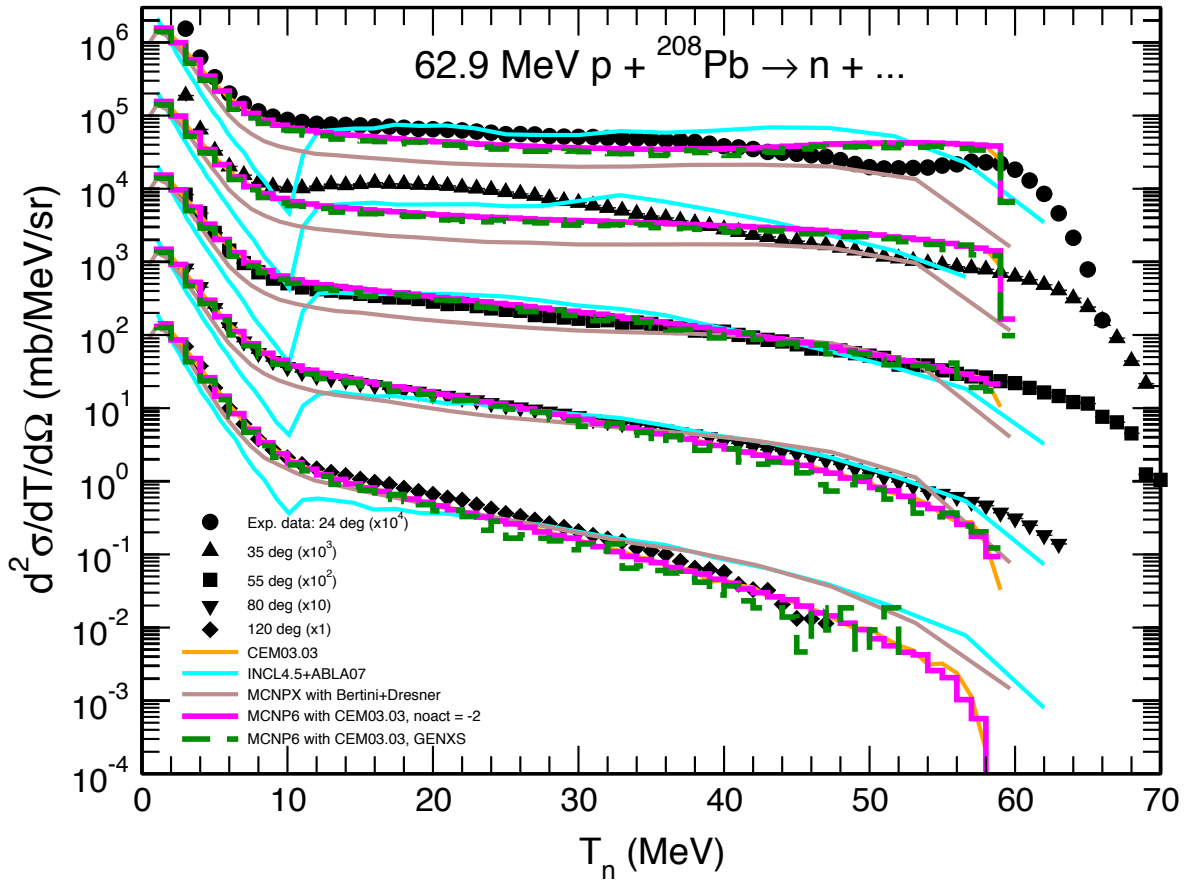

Figure 8: Experimental [64] double-differential spectra of neutrons at 24, 35, 55, 80, and 120 degrees from interactions of 62.9 MeV protons with a thin ^{208}Pb target compared with calculations by CEM03.03 [6] and INCL4.5+ABLA07 [43, 45, 46] codes and with results by MCNPX 2.6.0 calculated by Franz Gallmeier with default options (i.e., Bertini INC [48] + Multistage Preequilibrium Model [49] + Dresner evaporation [50] + RAL fission model [26]) as presented at the recent International Benchmark of Spallation Models [19], as well as with our current results by MCNP6 using the CEM03.03 event generator, as indicated.

140 degrees from interactions of 160 MeV protons with ^{197}Au; it compares the results with experimental data and with results by CEM03.03 event generator used as a stand alone code, as well as with similar results by other codes involved in the recent International Benchmark of Spallation Models organized by IAEA during 2008-2010 (see Ref. [19]).

Like in the previous test-problem #6, we have calculated with MCNP6 these spectra in two different ways:

1) using the GENXS option of MCNP6;

2) using the NOACT=-2 option for the 8th parameter of the LCA card.

As we have presented a detailed description of the use of GENXS option to calculate particle spectra from thin targets in test-problems #1 and #5, and the use of the NOACT=-2 option for the 8th parameter of the LCA card was described in depth in the previous test-problem #6, we will not discuss in detail here the input and output files for both cases. Therefore, we limit ourselves below to only providing the text of the input files for both cases, as well as describing in short where to find the results in the MCNP6 output files.

1) The main MCNP6 input file for the case of using the GENXS option is **p160Au_He4_GENXS** and its auxiliary companion required by the GENXS option is **inxc07**. Both of them are presented in the subdirectory **/VALIDATION_CEM/Inputs/** and are also shown below.

p160Au_He4_GENXS:

```
MCNP6 test: He4 spectra from p + Au197 by CEM03.03 at 160 MeV, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c -------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c -------------------------------------------------------------
  m1   79197 1.0
  sdef erg = 160. par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 175
  mode   h
LCA  8j 1    $ use CEM03.03
  tropt genxs inxc07  nreact on  nescat off
c -------------------------------------------------------------
  print 40 110 95
  nps 40000000
c  nps 10000
  prdmp 2j -1
```

inxc07:

```
MCNP6 test: He4 spectra from p + Au197 by CEM03.03 at 160 MeV, nevtype=66
1 1 0 /
Cross Section Edit
72 -11 9 /
2. 4. 6. 8. 10. 12. 14. 16. 18. 20. 22. 24. 26. 28. 30. 32.
34. 36. 38. 40. 42. /
143. 137. 103. 97. 63. 57. 43. 37. 23. 17. 0. /
24 /
```

^{4}He spectra by MCNP6 using CEM03.03 with the GENXS option at 140, 100, and 60 ($\pm$3) degrees are tabulated in units of [b/sr/MeV] in the 2nd, 4th, and 6th pairs of columns of the first part of the "alpha production cross section" table of the MCNP6 output file **p160Au_He4_GENXS.o** (after the ^{4}He energy tabulated in the 1st column) and for 40 and 20 degrees, in the 1st and 3rd pairs of columns of the second part of the same tables, following the alpha energy tabulated

in the 1st column, as well as in the MCTAL file **p160Au_He4_GENXS.m** presented in the Templates subdirectory **/VALIDATION_CEM/Templates/LINUX/**.

To help plotting these spectra with xmgrace (see file p160Au_He4_lin.pdf), the MCNP6 results are copied to separate files 20genxs.dat, 40genxs.dat, 60genxs.dat, 100genxs.dat, and 140genxs.dat, respectively, presented in subdirectory
/VALIDATION_CEM/Experimental_data/p160Au_He4.

2) The MCNP6 input file for this test-problem using the **NOACT=-2** option for the 8th parameter of the LCA card is **p160Au_He4_REP**. It is presented in the subdirectory **/VALIDATION_CEM/Inputs/** and is also shown below.

p160Au_He4_REP:

```
MCNP6 test with CEM03.03: 160 MeV p+Au197 -> He4 spectra
c d^2sigma/dT/dOmega [mb/sr/MeV] at 20, 40, 60, 100, and 140 deg (+/- 3 deg)
c to compare with Cowley's et al. measurements (Phys. Rev. C54 (1996) 778)
c and results by CEM03.03 and other models used as stand alone codes,
c as presented at the IAEA Benchmark of Spallation Models, 2009-2010
1   1  -10   -501      imp:a=1
2   0         501  -502  imp:a=1
99  0         502      imp:a=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
17     kz    0    0.093471249     1  $ tan(17.0 deg)^2
23     kz    0    0.180178869     1  $ tan(23.0 deg)^2
37     kz    0    0.567843706     1  $ tan(37.0 deg)^2
43     kz    0    0.869584385     1  $ tan(43.0 deg)^2
57     kz    0    2.371184107     1  $ tan(57.0 deg)^2
63     kz    0    3.851839996     1  $ tan(63.0 deg)^2
97     kz    0    66.33037874    -1  $ tan(97.0 deg)^2
103    kz    0    18.76168325    -1  $ tan(103.0 deg)^2
137    kz    0    0.869584385    -1  $ tan(137.0 deg)^2
143    kz    0    0.567843706    -1  $ tan(143.0 deg)^2

mode n h d t s a
m1  79197 1
lca 0 6j -2 1    $ CEM03.03, no transport, only the 1st inelastic, no elastic
c nps 10000
nps 4e7
sdef par=h erg=160. vec=0 0 1 dir 1
phys:h 170 j 0 j j j j
phys:n 170
phys:a 170
phys:d 170
```

```
phys:t 170
phys:s 170
c
f1:a  502
c define the "segments" for He4 at 20, 40, 60, 100, and 140 (+/- 3) deg
fs1 -17 -23 -37 -43 -57 -63 97 103 137 143 T
c
c The following Segment Divisor card is needed to get 1/sr for He4 spectra
sd1   0.49948  $ 2pi(cos0 -cos17.0)
      0.22494  $ 2pi(cos17.0 - cos23.0)
      0.76573  $ 2pi(cos23.0 - cos37.0)
      0.42274  $ 2pi(cos37.0 - cos43.0)
      1.17316  $ 2pi(cos43.0 - cos57.0)
      0.56956  $ 2pi(cos57.0 - cos63.0)
      3.61823  $ 2pi(cos63.0 - cos97.0)
      0.64768  $ 2pi(cos97.0 - cos103.0)
      3.18182  $ 2pi(cos103.0 - cos137.0)
      0.42274  $ 2pi(cos137.0 - cos143.0)
      1.26521  $ 2pi(cos143.0 - cos180.0)
      12.56637 $ 4pi
c
c     Boundaries of the He4 energy bins: 0-2 MeV; 2-4 MeV, ...
c     tabulated exactly as used by CEM03.03 as stand alone code
e0    2     4     6     8     10    12    14    16    18    20
      22    24    26    28    30    32    34    36    38    40
      42    44    46    48    50    52    54    56    58    60
      62    64    66    68    70    72    74    76    78    80
      82    84    86    88    90    92    94    96    98    100
      102   104   106   108   110   112   114   116   118   120
      122   124   126   128   130   132   134   136   138   140
      142   144   146   148   150   152   154   156   158   160
      162   164   166   168   170
c
em1 833.875 84r $ multiply to sig_inelastic = 1667.75 mb, as predicted by
c                 CEM03.03 as a stand alone code, then divided by 2 (the
c                 values of each energy bin in MeV). This is needed
c                 to get the spectra in [mb/sr/MeV]; we do this for every E-bin
dbcn  28j 1
```

[4]He spectra calculated by MCNP6 with CEM03.03 using the **noact=-2** option for the 8th parameter of the LCA card at 20, 40, 60, 100, and 140 (±2) degrees are tabulated in units of [mb/sr/MeV] in the MCNP6 output file **p160Au_He4_cem.o** as tally 1, respectively in the "segments":
1) segment: 17 -23
2) segment: 17 23 37 -43
3) segment: 17 23 37 43 57 -63
4) segment: 17 23 37 43 57 63 -97 103

5) segment: 17 23 37 43 57 63 -97 -103 -137 143.

Note that to get the units of [mb] needed for the normalization of the calculated spectra to the total reaction cross section, we use the Energy Multiplier card EM1 in our input file **p160Au_He4_REP** with the value 1667.75 on it for all the 85 energy bins of our tally F1: 1667.75 is the value of the total inelastic (reaction) cross section in [mb] as predicted by CEM03.03 used for this reaction as a stand alone code. Note also that to get in the MCNP6 calculated spectra $d^2\sigma/dT/d\Omega$ the units of [1/MeV], we divide the tables from the MCNP6 output file for every "segment" described above by the corresponding values of the energy bins: we especially used here all values of the energy bins equal to 2 MeV, and used on the **EM1** card the value of 1667.75/2.=833.875 (i.e., already divided by 2. ([MeV]) for all 85 energy bins of our tally **F1**), so that no a further division is needed in this particular case.

In a similar manner, to get the units of [1/sr] for the calculated spectra, we had to use in our input file the Segment Divisor card **SD1** with values of the solid angles for each "segment" used to identify the needed angles of 20, 40, 60, 100, and 140 ($\pm$2) degrees. To help plotting these spectra with xmgrace (see file p160Au_He4_lin.pdf), the final MCNP6 results obtained by the second way are copied to separate files 20_m6.dat, 40_m6.dat, 60_m6.dat, 100_m6.dat, and 140_m6.dat, respectively, all presented in the subdirectory
/VALIDATION_CEM/Experimental_data/p160Au_He4 together with files with experimental data, results by CEM03.03 used as a stand alone code, as well as a template and final pdf file of the figure with all results for this test-problem.

Besides the MCNP6 results, for comparison, we show here also results by CEM03.03 as a stand alone code as presented at the mentioned above IAEA Benchmark; see files: 20cem0302.dat, 40cem0302.dat, 60cem0302.dat, 100cem0302.dat, and 140cem0302.dat, respectively. Initially, we planned to compare our MCNP6 results also with results by INCL4.5+ABLA07 and by MCNPX (using the default options) which can be downloaded from the IAEA Benchmark web-page. However, after we downloaded the tables, we discovered that the files shown at the IAEA web-page for the p+Au reaction represent actually, by mistake, results of calculations of the p+Al reaction, for all codes involved in the IAEA Benchmark. This is why we are unable to compare our MCNP6 calculations with results posted at the IAEA Benchmark web-page as of the moment of the current writing for this reaction (in the case of CEM03.03, we use here the results we sent ourselves to the organizers of the IAEA Benchmark about two years ago, but not what is posted in error for this reaction for CEM03.03 on the IAEA Benchmark web-page).

The experimental data for this problem were measured at the National Accelerator Center in Faure (South Africa) by an international team and are published in the paper [65].

Tabulated values of these measurements are available in the EXFOR data base, Entry: O0508, and are presented also on the IAEA web page of the mentioned Benchmark [19].

Experimental ^{4}He spectra $d^2\sigma/dT/d\Omega$ in units of [mb/sr/MeV] as functions of ^{4}He kinetic energy in [MeV] at 20, 40, 60, 100, and 140 degrees are presented here in the files 20exp.dat, 40exp.dat, 60exp.dat, 100exp.dat, and 140exp.dat, respectively.

The file p160Au_He4_lin.fig is a template for plotting the spectra with xmgrace. The pdf file for the figure with final results for this problem is p160Au_He4_lin.pdf (see Fig. 9 below).

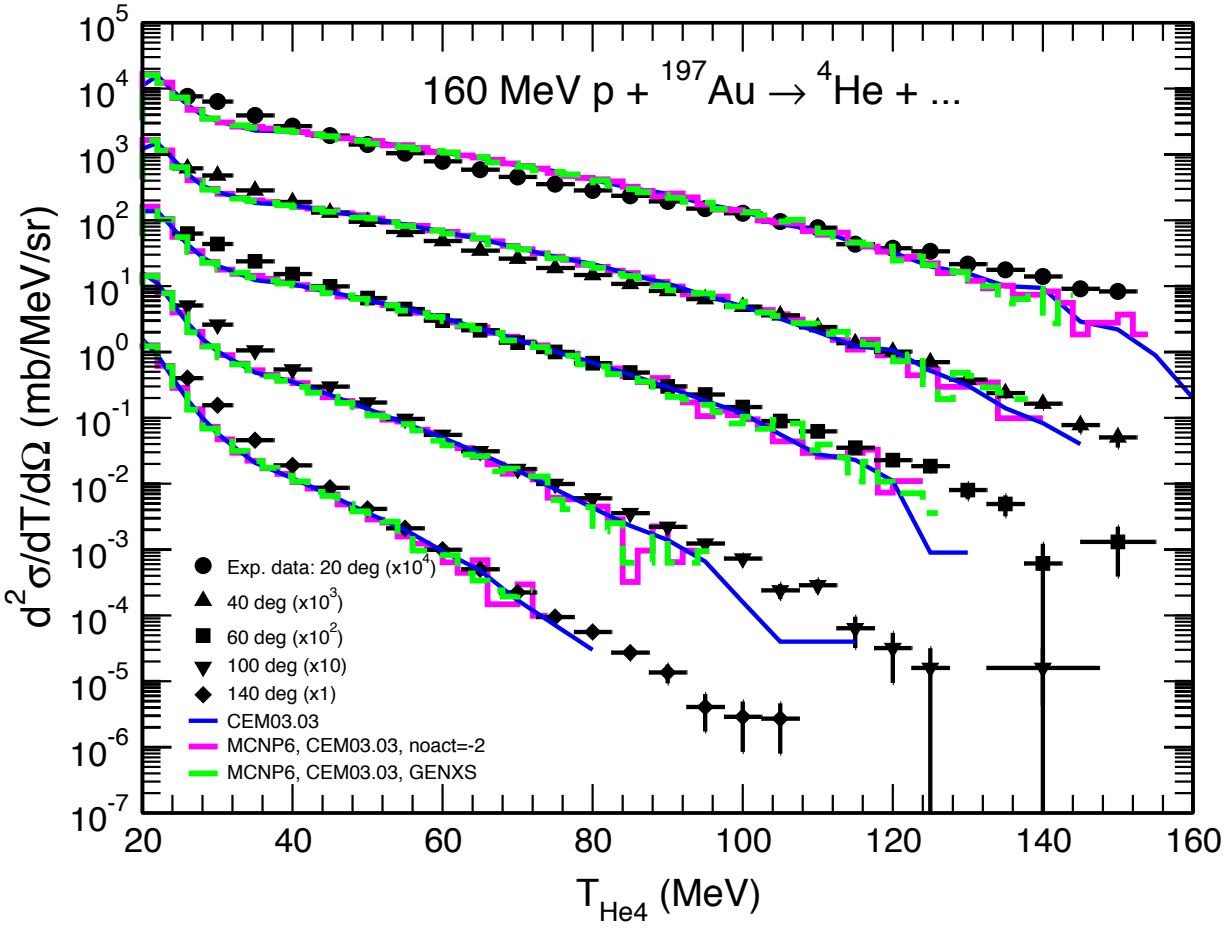

Figure 9: Experimental [65] double-differential spectra of ^{4}He at 20, 40, 60, 100, and 140 degrees from interactions of 160 MeV protons with a thin ^{197}Au target compared with calculations by CEM03.03 [6] as presented at the recent International Benchmark of Spallation Models [19] and with our current results by MCNP6 using the CEM03.03 event generator obtained in two different ways, namely, using the **GENXS** and **noact=-2** options of MCNP6, as indicated.

From Fig. 9 we see very good agreement between MCNP6 results calculated using the **GENXS** option and the results by the **NOACT=-2** option for the 8th parameter of the LCA card. Both these results agree very well with experimental data and with calculations by CEM03.03 used as a stand alone code.

3.8. Test-problem #8: A) n542Bi_GENXS with inxc08; B) n542BiREP

This problem is to test the applicability of MCNP6 using the CEM03.03 event generator to calculate production of protons, deuterons, and tritium from intermediate-energy neutron-induced reactions of interest for many important applications.

To be specific, this test calculates with MCNP6 using CEM03.03 the p, d, and t spectra at 54, 68, 90, 121, and 164 degrees from interactions of 542 MeV neutrons with ^{209}Bi; it is to compare the results with experimental data and with results by CEM03.03 event generator used as a stand alone code, as well as with similar results by INCL4.5+ABLA07 as presented at the recent International Benchmark of Spallation Models organized by IAEA during 2008-2010,

see Ref. [19].

This is the last test-problem we like to show in the current MCNP6 Testing Primer we have calculated in two different ways:

1) using the **GENXS** option of MCNP6;

2) using the **noact=-2** option for the 8th parameter of the LCA card.

As we have presented a detailed description of the use of the GENXS option to calculate particle spectra from thin targets in test-problems #1 and #5, and the use of the **NOACT=-2** option for the 8th parameter of the LCA card was described in depth in test-problem #6, we do not need to discuss in detail here the input and output files for both cases. Therefore, we limit ourselves below to only providing the text of the input files for both cases, as well as to describing in short where to find the results in the MCNP6 output files.

1) The main MCNP6 input file for the case of using the GENXS option is **n542Bi_GENXS** and its auxiliary companion required by the GENXS option is **inxc08**. Both of these are presented in the subdirectory **/VALIDATION_CEM/Inputs/** and are also shown below.

n542Bi_GENXS:

```
MCNP6 test: p, d, and t spectra from n+Bi209 by CEM03.03 at 542 MeV, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c -------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c -------------------------------------------------------------
  m1   83209 1.0
  sdef erg = 542. par = n dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 550
  mode   n
LCA  8j 1    $ use CEM03.03
  tropt genxs inxc08  nreact on  nescat off
c -------------------------------------------------------------
  print 40 110 95
  nps 40000000
c  nps 10000
  prdmp 2j -1
```

inxc08:

```
MCNP6 test: p, d, and t spectra from n+Bi209 by CEM03.03 at 542 MeV, nevtype=66
1 1 0 /
Cross Section Edit
```

```
72 -11 9 /
2.    4.    6.    8.   10.  12.  14.  16.  18.  20.
22.   24.   26.   28.  30.  32.  34.  36.  38.  40.
50.   60.   70.   80.  90.  100. 110. 120. 130. 140.
150.  160.  170.  180. 190. 200. 210. 220. 230. 240.
260.  280.  300.  320. 340. 360. 380. 400. 420. 440.
460.  480.  500.  520. 540. 560. /
167. 161. 124. 118. 93. 87. 71. 65. 57. 51. 0. /
5 21 22 /
```

Proton spectra calculated by MCNP6 using CEM03.03 with the GENXS option at 164, 120, and 90 (±3) degrees are tabulated in units of [b/sr/MeV] in the 2nd, 4th, and 6th pairs of columns, after the proton energy tabulated in the 1st column, of the first part of the "proton production cross section" table of the final MCNP6 output file **n542Bi_GENXS_c2.o** (calculated with the "continue" option using the auxiliary input file **inp_n542Bi**; the first MCNP6 output calculated with the main input file, **n542Bi_GENXS**, is: **n542Bi_GENXS.o**) and for 68 and 54 degrees, in the 1st and 3rd pairs of columns of the second part of the same tables, following the proton energy tabulated in the 1st column. Deuteron spectra at the same angles are tabulated in a similar manner in a very similar table entitled "deuteron production cross section" in the same MCNP6 output file. Triton spectra at the same angles are tabulated in the same manner in a very similar table entitled "triton production cross section" in the same MCNP6 output file. All these output files are presented in the subdirectory **/VALIDATION_CEM/Templates/LINUX/**.

To help plotting these spectra with xmgrace (see files n542Bi_p.pdf, n542Bi_d.pdf, n542Bi_t.pdf, and the summary file n542Bi.pdf), the final MCNP6 results at 54, 68, 90, 121, and 164 degrees for protons, deuterons, and tritons are copied here in separate files: 54p_genxs.dat, 68p_genxs.dat, 90p_genxs.dat, 121p_genxs.dat, 164p_genxs.dat, 54d_genxs.dat, 68d_genxs.dat, 90d_genxs.dat, 121d_genxs.dat, 164d_genxs.dat, 54t_genxs.dat, 68t_genxs.dat, 90t_genxs.dat, 121t_genxs.dat, and 164t_genxs.dat, respectively, presented in subdirectory **/VALIDATION_CEM/Experimental_data/n542Bi/**.

2) The MCNP6 input file for this test-problem using the **NOACT=-2** option for the 8th parameter of the LCA card is **n542BiREP**. It is presented in the subdirectory **/VALIDATION_CEM/Inputs/** and is also shown below.

n542BiREP:

```
MCNP6 test with CEM03.03: 542 MeV n+Bi209 -> p, d, and t spectra
c d^2sigma/dT/dOmega [mb/sr/MeV] at 54, 68, 90, 121, and 164 deg (+/- 3 deg)
c to compare with Franz's et al. measurements (Nucl. Phys. A 510 (19906) 774)
c and results by CEM03.03 and INCL4.5+ABLA07 as stand alone codes
c as well as by MCNPX 2.6.0 using Bertini+Dresner (default) option
c as presented at the IAEA Benchmark of Spallation Models, 2009-2010
1   1  -10   -501      imp:a=1
2   0         501  -502  imp:a=1
99  0         502      imp:a=0

501   so 0.01
```

```
502   so 1
c
c  tally surfaces
c
51     kz    0    1.524970987     1  $ tan(51.0 deg)^2
57     kz    0    2.371184107     1  $ tan(57.0 deg)^2
65     kz    0    4.598909932     1  $ tan(65.0 deg)^2
71     kz    0    8.434440822     1  $ tan(71.0 deg)^2
87     kz    0    364.0897773     1  $ tan(87.0 deg)^2
93     kz    0    364.0897773    -1  $ tan(93.0 deg)^2
118    kz    0    3.537132037    -1  $ tan(118.0 deg)^2
124    kz    0    2.197987025    -1  $ tan(124.0 deg)^2
161    kz    0    0.118561505    -1  $ tan(161.0 deg)^2
167    kz    0    0.053300121    -1  $ tan(167.0 deg)^2

mode n h d t s a / z *
m1  83209 1
lca 0 6j -2 1    $ CEM03.03, no transport, only 1st inelastic, no elastic cols.
nps 10000
c nps 4e7
sdef par=n erg=542. vec=0 0 1 dir 1
phys:h 560 j 0 j j j j
phys:n 560
phys:a 560
phys:d 560
phys:t 560
phys:s 560
phys:/ 560
phys:z 560
phys:* 560
c
f1:h  502
c define the "segments" for protons at 54, 68, 90, 121, and 164 (+/- 3) deg
fs1 -51 -57 -65 -71 -87 93 118 124 161 167 T
c
c The following Segment Divisor card is needed to get 1/sr for proton spectra
sd1   2.32290  $ 2pi(cos0 - cos51.0)
      0.53207  $ 2pi(cos51.0 - cos57.0)
      0.76668  $ 2pi(cos57.0 - cos65.0)
      0.60978  $ 2pi(cos65.0 - cos71.0)
      1.71677  $ 2pi(cos71.0 - cos87.0)
      0.65767  $ 2pi(cos87.0 - cos93.0)
      2.62094  $ 2pi(cos93.0 - cos118.0)
      0.56374  $ 2pi(cos118.0 - cos124.0)
      2.42736  $ 2pi(cos124.0 - cos161.0)
      0.18128  $ 2pi(cos161.0 - cos167.0)
      0.16104  $ 2pi(cos167.0 - cos180.0)
```

```
      12.56637 $ 4pi
c
c     Boundaries of the energy bins: 0-2 MeV; 2-4 MeV, ...
c     tabulated exactly as used by CEM03.03 as stand alone code
e0    2     4     6     8     10    12    14    16    18    20
      22    24    26    28    30    32    34    36    38    40
      50    60    70    80    90    100   110   120   130   140
      150   160   170   180   190   200   210   220   230   240
      260   280   300   320   340   360   380   400   420   440
      460   480   500   520   540   560
c
em1 1040.445 19r 208.089 19r 104.0445 15r
c  Multiply to sig_inelastic = 2080.89 mb, as predicted by CEM03.03 as a stand
c  alone code, then divided by 2 [MeV] for the first 20 bins (the value of these
c  energy bins in MeV), by 10 [MeV] for the next 20 bins, and by 20 [MeV] for the
c  last 16 bins. This is needed to get the final spectra in [mb/sr/MeV]
c
f11:d  502
c define the "segments" for deutrons at 54, 68, 90, 121, and 164 (+/- 3) deg
fs11 -51 -57 -65 -71 -87 93 118 124 161 167 T
c
c The following Segment Divisor card is needed to get 1/sr for deuteron spectra
sd11   2.32290  $ 2pi(cos0 - cos51.0)
      0.53207  $ 2pi(cos51.0 - cos57.0)
      0.76668  $ 2pi(cos57.0 - cos65.0)
      0.60978  $ 2pi(cos65.0 - cos71.0)
      1.71677  $ 2pi(cos71.0 - cos87.0)
      0.65767  $ 2pi(cos87.0 - cos93.0)
      2.62094  $ 2pi(cos93.0 - cos118.0)
      0.56374  $ 2pi(cos118.0 - cos124.0)
      2.42736  $ 2pi(cos124.0 - cos161.0)
      0.18128  $ 2pi(cos161.0 - cos167.0)
      0.16104  $ 2pi(cos167.0 - cos180.0)
      12.56637 $ 4pi
c
em11 1040.445 19r 208.089 19r 104.0445 15r
c  Multiply to sig_inelastic = 2080.89 mb, as predicted by CEM03.03 as a stand
c  alone code, then divided by 2 [MeV] for the first 20 bins (the value of these
c  energy bins in MeV), by 10 [MeV] for the next 20 bins, and by 20 [MeV] for the
c  last 16 bins. This is needed to get the final spectra in [mb/sr/MeV]
c
f21:t  502
c define the "segments" for tritium at 54, 68, 90, 121, and 164 (+/- 3) deg
fs21 -51 -57 -65 -71 -87 93 118 124 161 167 T
c
c The following Segment Divisor card is needed to get 1/sr for tritium spectra
sd21   2.32290  $ 2pi(cos0 - cos51.0)
```

```
      0.53207  $ 2pi(cos51.0 - cos57.0)
      0.76668  $ 2pi(cos57.0 - cos65.0)
      0.60978  $ 2pi(cos65.0 - cos71.0)
      1.71677  $ 2pi(cos71.0 - cos87.0)
      0.65767  $ 2pi(cos87.0 - cos93.0)
      2.62094  $ 2pi(cos93.0 - cos118.0)
      0.56374  $ 2pi(cos118.0 - cos124.0)
      2.42736  $ 2pi(cos124.0 - cos161.0)
      0.18128  $ 2pi(cos161.0 - cos167.0)
      0.16104  $ 2pi(cos167.0 - cos180.0)
      12.56637 $ 4pi
c
em21 1040.445 19r 208.089 19r 104.0445 15r
c  Multiply to sig_inelastic = 2080.89 mb, as predicted by CEM03.03 as a stand
c  alone code, then divided by 2 [MeV] for the first 20 bins (the value of these
c  energy bins in MeV), by 10 [MeV] for the next 20 bins, and by 20 [MeV] for the
c  last 16 bins. This is needed to get the final spectra in [mb/sr/MeV]
dbcn  28j 1
```

Proton spectra by MCNP6 with CEM03.03 using the **noact=-2** option for the 8th parameter of the LCA card at 54, 68, 90, 121, and 164 (±3) degrees are tabulated in units of [mb/sr/MeV] in the final MCNP6 output file **n542BiREP_cc.o** (calculated with the "continue" option using the auxiliary two-line input file **inp_n542Bi**; the first MCNP6 output calculated with the main input file, **n542BiREP**, is: **n542BiREP.o**) as **tally 1**, respectively in the "segments":
1) segment: 51 -57
2) segment: 51 57 65 -71
3) segment: 51 57 65 71 87 93
4) segment: 51 57 65 71 87 -93 -118 124
5) segment: 51 57 65 71 87 -93 -118 -124 -161 167.

Deuteron spectra at the same angles are tabulated in the same manner in very similar "segments" for **tally 11** of the same MCNP6 output file. Triton spectra at the same angles are tabulated in the same manner in very similar "segments" for **tally 21** of the same MCNP6 output file.

Note that to get the units of [mb] needed for the normalization of the calculated spectra to the total reaction cross section, we would have to use the Energy Multiplier card **EM1** for protons, **EM11** for deuterons, and **EM21** for tritons in our input file **n542BiREP** with the value 2080.89 on it for all the 56 energy bins of our tallies **F1**, **F11**, and **F21**, respectively: 2080.89 is the value of the total inelastic (reaction) cross section in [mb] for this reaction as predicted by CEM03.03 used as a stand alone code. Note also that to normalize MCNP6 calculated spectra to units of [1/MeV], we have to divide the tables from the MCNP6 output file for every "segment" described above by the corresponding values of the energy bins. Here, for all p, d, and t MCNP6 spectra, we use the value of the 2 MeV for the first 20 energy bins, 10 MeV for the next 20 energy bins, and 20 MeV for the last 16 energy bins. Having this done, we can use on the **EM1**, **EM11**, and **EM21** cards not the value of the total reaction cross section 2080.89 [mb], but this value divided by 2 MeV for the first 20 energy bins, by 10 MeV

for the next 20 energy bins, and by 20 MeV for the last 16 energy bins. This way we do not need a further division of the final tables from our MCNP6 output to the values of the p, d, and t energy bins.

In a similar manner, to get the units of [1/sr] for the calculated spectra, we had to use in our input file the Segment Divisor Cards **SD1** for protons, **SD11** for deuterons, and **SD21** for tritons with values of the solid angles for each "segment" used to identify the needed angles of 54, 68, 90, 121, and 164 (± 3) degrees.

To help plotting these spectra with xmgrace, the final MCNP6 results obtained by the second way at 54, 68, 90, 121, and 164 degrees for protons, deuterons, and tritons are copied here to separate files: 54p_m6.dat, 68p_m6.dat, 90p_m6.dat, 121p_m6.dat, 164p_m6.dat, 54d_m6.dat, 68d_m6.dat, 90d_m6.dat, 121d_m6.dat, 164d_m6.dat, 54t_m6.dat, 68t_m6.dat, 90t_m6.dat, 121t_m6.dat, and 164t_m6.dat, respectively, presented in subdirectory **/VALIDATION_CEM/Experimental_data/n542Bi/** together with all files with other results, with experimental data, and with figures.

Besides the MCNP6 results, for comparison, we show here also results by CEM03.03 as a stand alone code as presented at the mentioned above IAEA Benchmark; see files: 54p_cem.dat, 68p_cem.dat, 90p_cem.dat, 121p_cem.dat, 164p_cem.dat, 54d_cem.dat, 68d_cem.dat, 90d_cem.dat, 121d_cem.dat, 164d_cem.dat, 54t_cem.dat, 68t_cem.dat, 90t_cem.dat, 121t_cem.dat, and 164t_cem.dat, respectively.

Results by INCL4.5+ABLA07 downloaded from the official IAEA Benchmark web-page are presented in the files: 54p_incl.dat, 68p_incl.dat, 90p_incl.dat, 121p_incl.dat, 164p_incl.dat, 54d_incl.dat, 68d_incl.dat, 90d_incl.dat, 121d_incl.dat, 164d_incl.dat, 54t_incl.dat, 68t_incl.dat, 90t_incl.dat, 121t_incl.dat, and 164t_incl.dat, respectively.

The experimental data for this problem were measured at the Swiss Institute for Nuclear Research (SIN, now Paul Schrrer Institut, PSI) in Villigen (Switzerland) by an international team and are published in the paper [66].

Tabulated values of these measurements are available in the EXFOR data base, Entry: 22173, and are presented also on the IAEA web page of the mentioned Benchmark [19].

Experimental spectra $d^2\sigma/dT/d\Omega$ in units of [mb/sr/MeV] as functions of particle kinetic energy in [MeV] at 54, 68, 90, 121, and 164 degrees for protons, deuterons, and tritons are presented here in the files 54p_exp.dat, 68p_exp.dat, 90p_exp.dat, 121p_exp.dat, 164p_exp.dat, 54d_exp.dat, 68d_exp.dat, 90d_exp.dat, 121d_exp.dat, 164d_exp.dat, 54t_exp.dat, 68t_exp.dat, 90t_exp.dat, 121t_exp.dat, and 164t_exp.dat, respectively.

The files n542Bi_p.fig, n542Bi_d.fig, and n542Bi_t.fig are templates for plotting the proton, deuteron, and triton spectra with xmgrace. The pdf files for the figures with final results for this problem are n542Bi_p.pdf, n542Bi_d.pdf, and n542Bi_t.pdf. The summary file n542Bi.pdf shows all spectra, of proton, deuteron, and tritons, on a single plot; it is presented below in Fig. 10.

From Fig. 10, we see very good agreement between MCNP6 results calculated using the **GENXS** option and the results by the **NOACT=-2** option for the 8th parameter of the LCA card. Both these results agree well with experimental spectra of protons, deuterons, and tritons from this reaction and with calculations by CEM03.03 used as a stand alone code. The agreement with the results by INCL4.5+ABLA07 used as a stand alone code is not so good, especially for high-energy tails of deuteron and triton spectra, but is still reasonable.

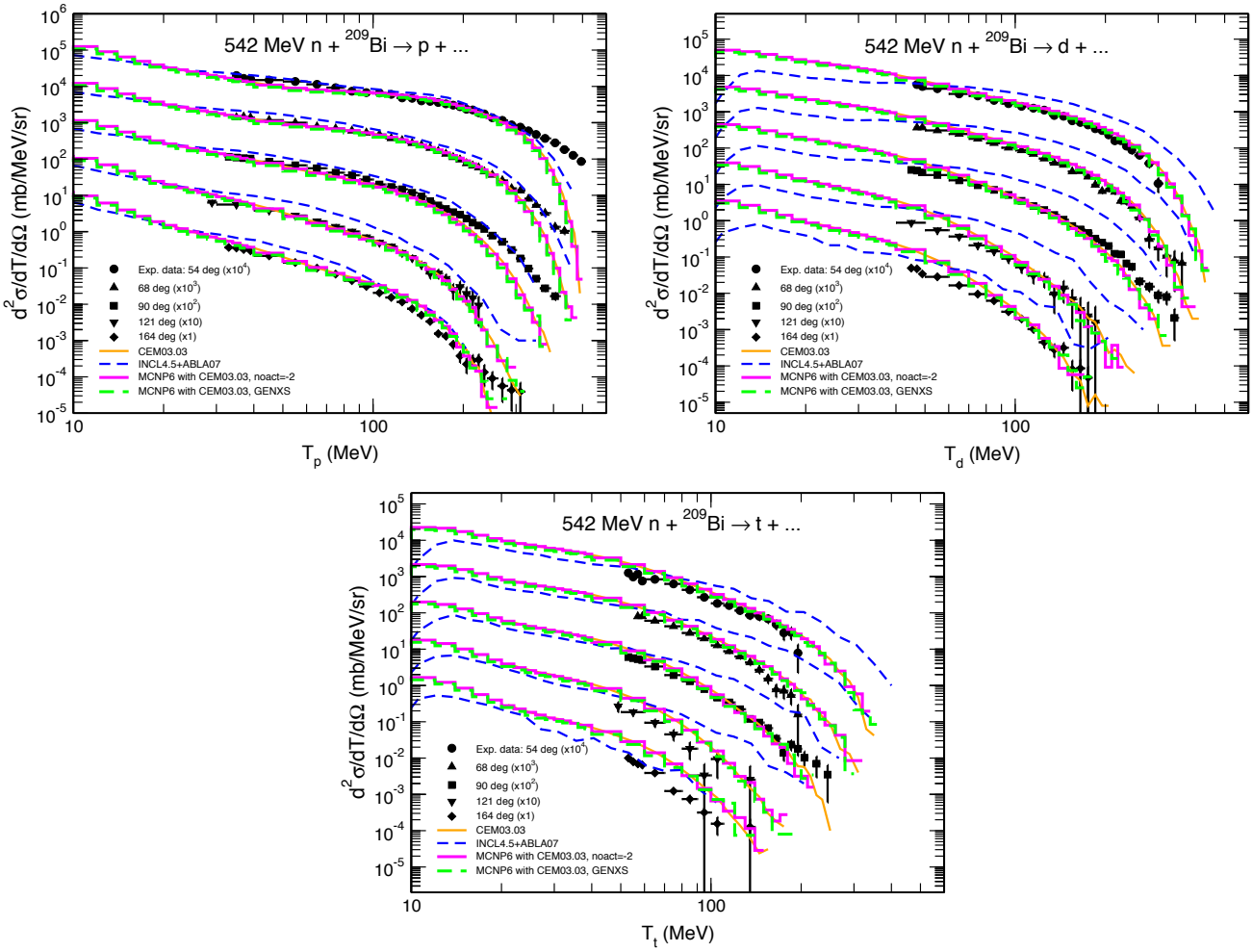

Figure 10: Experimental [66] double-differential spectra of protons, deuterons, and tritons at 54, 68, 90, 121, and 164 degrees from interactions of 542 MeV neutrons with a thin ^{209}Bi target compared with calculations by CEM03.03 [6] and INCL4.5+ABLA07 [43, 45, 46] codes as presented at the recent International Benchmark of Spallation Models [19], as well as with our current results by MCNP6 using the CEM03.03 event generator, obtained in two different ways, namely, using the **GENXS** and **noact=-2** options of MCNP6, as indicated.

3.9. Test-problem #9: p730C_pi with xpc12s

This problem is to test the applicability of MCNP6 using the CEM03.03 event-generator to calculate pions production from intermediate-energy nucleon-induced reactions — of interest to almost all nuclear applications at energies above the pion production threshold.

To be specific, this test calculates with MCNP6 using CEM03.03 the π^+ and π^- spectra at 30, 60, 90, 120, and 150 degrees from interaction of 730 MeV protons with carbon. It compares the MCNP6 results with experimental data and with results by CEM03.03 event-generator used as a stand alone code. Such reactions are of vital interest to determine the viability of muon interrogation technique using charged pions produced by an intermediate-energy proton beam. This exercise can also be used to compare MCNP6 results with similar calculations by the other 15 codes involved in the recent International Benchmark of Spallation Models organized by IAEA during 2008-2010, see Ref. [19]. As an additional test of MCNP6, we calculate and

compare here with experimental data and with calculations by CEM03.03 used as a stand alone code proton spectra from this reaction.

In this test-problem, the GENXS option of MCNP6 is used. As we have presented a detailed description of the use of GENXS option to calculate particle spectra from thin targets in test-problems #1 and #5, we do not need to discuss in detail here the input and output files for this case. Therefore, we limit ourselves below to only providing the text of the input files (let us recall here again that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to its main input file), as well as describing in short where to find the results in the MCNP6 output file.

The main MCNP6 input file for the case of using the GENXS option is **p730C_pi** and its auxiliary companion required by the GENXS option is **xpc12s**. Both of these are present in the subdirectory **/VALIDATION_CEM/Inputs/** and are also shown below.

p730C_pi:

```
MCNP6 using CEM03.03 test of pion spectra from 730 MeV p + C12
C for applications of interest to Andrea Palounek of ISR-6
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c -------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c -------------------------------------------------------------
  m1   6012 1.0
  sdef erg = 730 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 800
  mode   h
  tropt genxs xpc12s  nreact on  nescat off
c -------------------------------------------------------------
  print 40 110 95
c  nps 10000
  nps 10000000
  prdmp 2j -1
```

xcp12s:

```
Problem for Andrea Palounek: pion spectra from 730 p+C12 by MCNP6 with CEM03.03
1 1 1 /
Cross section edit
52 -11 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
```

```
85. 90. 95. 100. 120. /
155. 145. 125. 115. 95. 85. 65. 55. 35. 25. 0. /
1 5 6 7 8 21 22 23 24 /
```

π^+ spectra calculated by MCNP6 using CEM03.03 with the GENXS option at 150, 120, 90, 60, and 30 ($\pm$5.0) degrees are tabulated in units of [b/sr/MeV] in the 2nd, 4th, and 6th pairs of columns of the first part of the "pi_plus production cross section" table of the MCNP6 output file **p730C_pi.o** (after the particle energy tabulated in the 1st column) and in the 1st, and 3rd pairs of columns of the second part of the same table, as well as in the MCTAL file **p730C_pi.m**, both present in the Templates subdirectory **/VALIDATION_CEM/Templates/LINUX/**.

π^- and proton MCNP6 spectra are tabulated exactly the same way and in the same pairs of columns of the tables with captions "pi_minus production cross section" and "proton production cross section", respectively.

To help plotting our results with xmgrace (see files p730Cpip_MCNP6.pdf, p730Cpim_MCNP6.pdf, and p730Cp_MCNP6.pdf), the MCNP6 spectra of pi+, pi-, and protons at 30, 60, 90, 120, and 150 degrees are copied to separate files cpip30_GENXS.dat, cpip60_GENXS.dat, cpip90_GENXS.dat, cpip120_GENXS.dat, and cpip150_GENXS.dat, for pi+, cpim30_GENXS.dat, cpim60_GENXS.dat, cpim90_GENXS.dat, cpim120_GENXS.dat, and cpim150_GENXS.dat, for pi-, and cp30_GENXS.dat, cp60_GENXS.dat, cp90_GENXS.dat, cp120_GENXS.dat, and cp150_GENXS.dat, for protons, respectively.

Besides the MCNP6 results, for comparison, we show here also results by CEM03.03 used as a stand alone code; see files: cpip30_0302.dat, cpip60_0302.dat, cpip90_0302.dat, cpip120_0302.dat, and cpip_0302.dat, for pi+, cpim30_0302.dat, cpim60_0302.dat, cpim90_0302.dat, cpim120_0302.dat, and cpim_0302.dat, for pi-, and cp30_0302.dat, cp60_0302.dat, cp90_0302.dat, cp120_0302.dat, and cp_0302.dat, for protons, respectively.

We present all the experimental data, our calculation results, and all figures in the subdirectory **/VALIDATION_CEM/Experimental_data/p730C_pi/**.

The experimental data for this problem were measured at the Los Alamos Meson Physics Facility (LAMPF) and are published in the paper [67]. Experimental spectra of π^+, π^-, and protons $d^2\sigma/dT/d\Omega$ in units of [mb/sr/MeV] as functions of particle kinetic energy in [MeV] at 30, 60, a90, 120, and 150 degrees are presented here in the files cpip1e.dat, cpip2e.dat, cpip3e.dat, cpip4e.dat, and cpip5e.dat, for π^+; cpim1e.dat, cpim2e.dat, cpim3e.dat, cpim4e.dat, and cpim5e.dat, for π^-; and cp30.dat, cp60.dat, cp90.dat, cp120.dat, cp150.dat, for protons, respectively.

The files p730Cpip_MCNP6.fig, p730Cpim_MCNP6.fig, and p730Cp_MCNP6.fig are templates for plotting these spectra with xmgrace. The pdf files for these figures are p730Cpip_MCNP6.pdf, p730Cpim_MCNP6.pdf, and p730Cp_MCNP6.pdf, with the summary file p730C_MCNP6.pdf showing spectra of all particles in one plot, as shown below in Fig. 11.

From Fig. 11, we see very good agreement between the MCNP6 results obtained using the **GENXS** option with the CEM03.03 event generator and the calculations by CEM03.03 used as a stand alone code, for all spectra of π^+, π^-, and protons, at all angles studied here. We observe also reasonably good agreement of our results agree with the experimental data.

3.10. Test-problem #10: inp_pTi100 with inxct9

This problem is to test the applicability of MCNP6 using the CEM03.03 event-generator to calculate excitation functions of nuclear reactions leading to the soft-radiation emitting

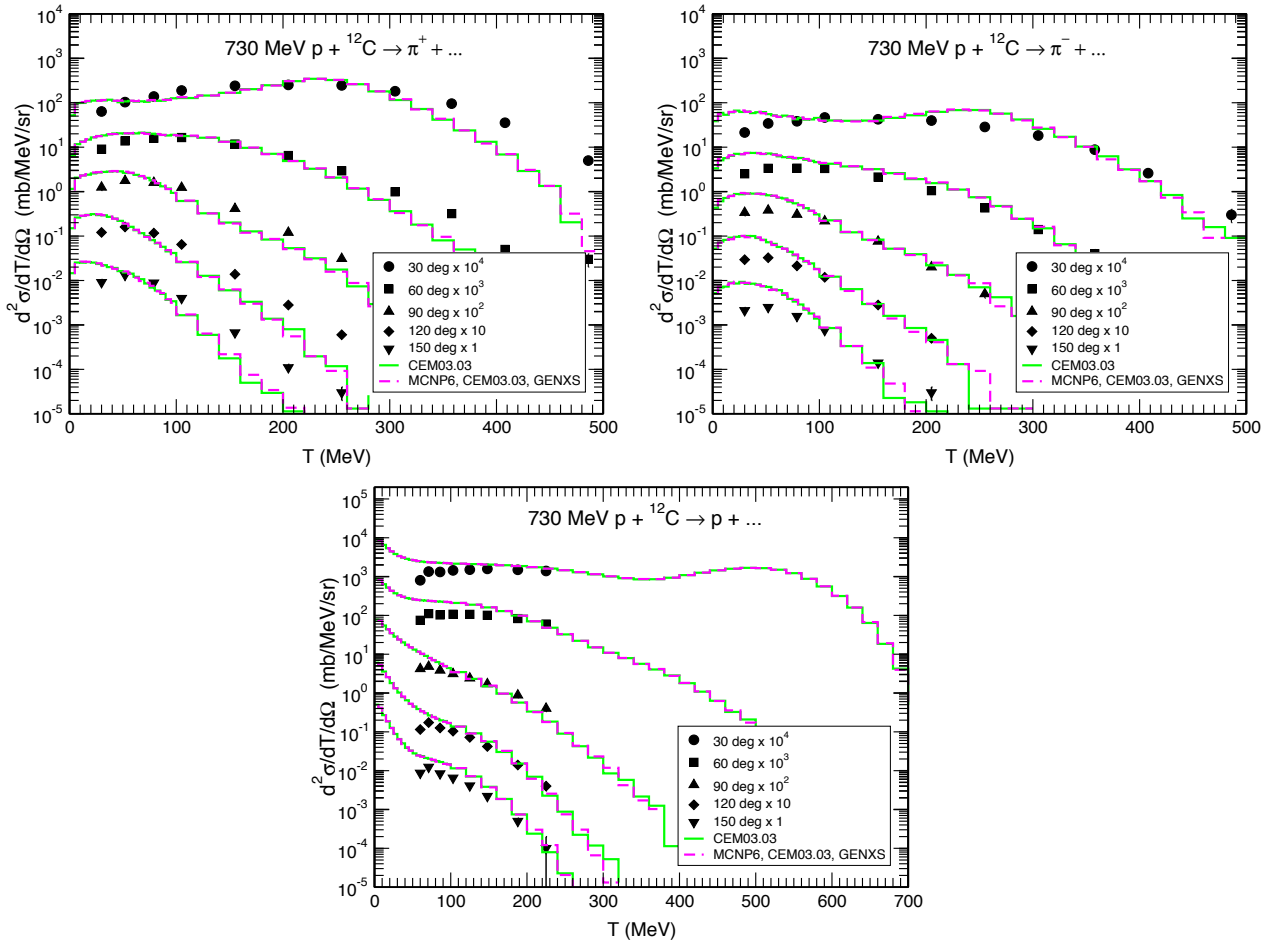

Figure 11: Experimental [67] double-differential spectra of π^+, π^-, and protons at 30, 60, 90, 120, and 150 degrees from interactions of 730 MeV protons with a thin ^{12}C target compared with calculations by CEM03.03 [6] used as a stand alone code and with results by MCNP6 using the CEM03.03 event generator with the **GENXS** option [36], as indicated.

radionuclides in beam collimator materials used in proton therapy.

To be specific, this test calculates with MCNP6 using CEM03.03 excitation functions for the production of radioactive ^{49}V and ^{45}Ca isotopes from ^{nat}Ti bombarded with protons at energies from 10 to 210 MeV. It compares the MCNP6 results with experimental data and with results by CEM03.03 event-generator used as a stand alone code, as well as with published results by the TALYS and ALICE-IPPE codes. Such reactions are of interest to radiation protection of cancer therapy personnel: In proton therapy of deep-lying tumors, the projectile energy is generally varied between 60 and 230 MeV, and the beam collimation to the desired shape is achieved using special collimators. Many collimators used today in such therapy are made of Titanium. Due to the generally low beam current incident on the tumor, often not much attention is paid to the activation of the collimator, although the beam extracted from the cyclotron/accelerator loses a considerable part of its intensity in the collimator during its fine tuning and shaping.

This test-problem uses the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate particle spectra from thin targets in test-problems #5 and #1, we do not need to discuss in detail here the input and output files for

this case. Therefore, we limit ourselves below to only providing the text of the input files (let us recall here again that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to its main input file), as well as describing where to find the results in the MCNP6 output file.

Note that, in the subdirectory **/VALIDATION_CEM/Inputs/**, we present only the MCNP6 input for a single incident proton energy, of 100 MeV, **inp_pTi100**, with its companion, the second, auxiliary input file required by the GENXS option of MCNP6, **inxct9**, both shown below.

inp_pTi100:

```
MCNP6 test: p + Ti-nat by CEM03.03 at 100 MeV, nevtype=66       !!!
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c -------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c -------------------------------------------------------------
  m1   22046 0.0825 22047 0.0744 22048 0.7372 22049 0.0541 22050 0.0518
  sdef erg = 100 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 1000
  mode   h
LCA  8j 1    $ use CEM03.03, nevtype = 66                   !!!
  tropt genxs inxct9  nreact on  nescat off
c -------------------------------------------------------------
  print 40 110 95
  nps 5000000
  prdmp 2j -1
```

inxct9

```
MCNP6 test: p + Ti-nat for medical applications
0 0 1 /
Cross Section Edit
0 0 0 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
1 5 6 7 8 21 22 23 24 /
```

In the subdirectory **/VALIDATION_CEM/Templates/LINUX/**, we present the MCNP6 output file **inp_pTi100.o** for this energy, where the cross sections for the production of ^{49}V

and ^{45}Ca (as well as of other products) are listed in units of barns in the table "Cross Section (b)", as shown below.

```
- - - - - - - - - - - - - - - - - - - - -

1 Distribution of residual nuclei:

                        Cross Section (b)
- - - - - - - - - - - - - - - - - - - - -

 Z = 20  all A     1.28987E-01 0.0009
             A =  39   2.35298E-05 0.0758
             A =  40   5.35749E-03 0.0050
             A =  41   1.17205E-02 0.0034
             A =  42   3.61893E-02 0.0019
             A =  43   3.33393E-02 0.0020
             A =  44   3.41577E-02 0.0019
             A =  45   5.94371E-03 0.0047
             A =  46   2.03411E-03 0.0081

- - - - - - - - - - - - - - - - - - - - -

    Z = 23  all A     2.68708E-02 0.0022
             A =  44   5.13869E-06 0.1622
             A =  45   1.52538E-04 0.0298
             A =  46   2.71702E-03 0.0070
             A =  47   7.46774E-03 0.0042
             A =  48   1.36101E-02 0.0031
             A =  49   2.05642E-03 0.0081
             A =  50   8.61813E-04 0.0125
- - - - - - - - - - - - - - - - - - - - -
```

To get the needed "excitation functions," i.e., cross sections for the production of ^{49}V and ^{45}Ca at different incident energies as functions of the proton bombarding energy, we must perform several calculations at the corresponding energies, changing only the value of the incident proton energy on the **SDEF** card (shown below) of the MCNP6 input file.

```
sdef erg = 100 par = H dir = 1 pos = 0 0 0 vec 0 0 1
```

As this is such a trivial change, we do not show examples of MCNP6 input and output files at other energies.

The MCNP6 ^{nat}Ti(p,x)^{49}V and ^{nat}Ti(p,x)^{45}Ca excitation functions calculated with CEM03.03 using the GENXS option are given in the files pTi_V49_GENXS.dat and pTi_Ca45_GENXS.dat, respectively, presented in the subdirectory **/VALIDATION_CEM/Experimental_data/pTi/** together with experimental data and results by CEM03.03, TALYS, and ALICE-IPPE used as stand alone codes.

The experimental data for this problem were obtained with targets irradiated at three cyclotrons, namely, the injector of COSY at FZ Julich (Germany), the injector cyclotron at

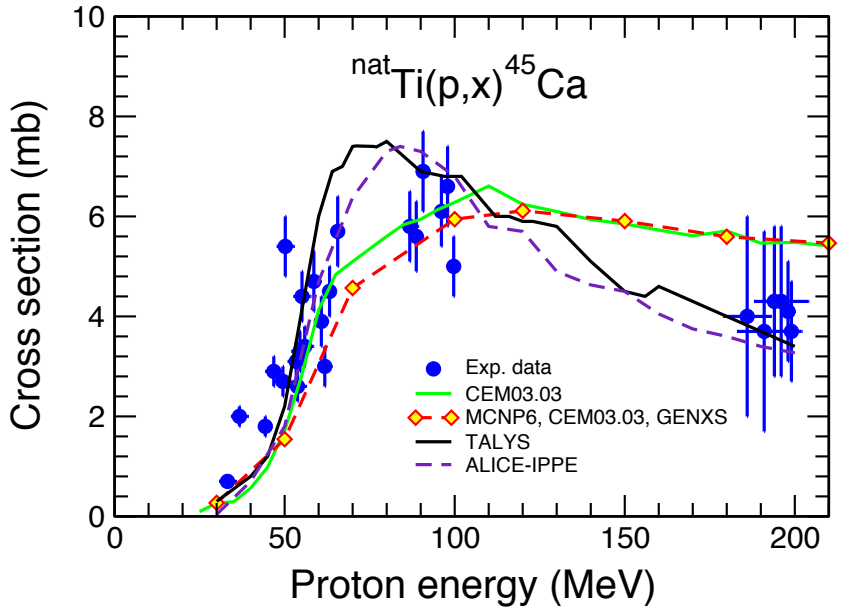

Figure 12: Comparison of the measured [69] excitation function for the production of the radionuclide ^{45}Ca from a thin ^{nat}Ti target bombarded with protons of energies below 210 MeV with our results by CEM03.03 used as a stand alone code, with results by MCNP6 with the GENXS option using the CEM03.03 event-generator, as well as with results by TALYS [70] and ALICE-IPPE [71] from Ref. [69], as indicated.

PSI Villigen (Switzerland), and the Separated Sector Cyclotron (SSC) at the iThemba LABS in Somerset West (South Africa), and are published in the paper [69].

The experimental cross section for the production of ^{49}V from ^{nat}T in units of [mb] as a function of the bombarding proton energy in [MeV], i.e., the ^{nat}Ti(p,x)^{49}V excitation function is presented here in the file pTi_V49_exp.dat, while the experimental excitation function ^{nat}Ti(p,x)^{45}Ca is presented in the file pTi_Ca45_exp.dat.

Results by the TALYS code for the ^{nat}Ti(p,x)^{49}V and ^{nat}Ti(p,x)^{45}Ca excitation functions extracted from enlarged Figs. 7 and 8 of the paper [69] are presented here in the files pTi_Ca45_TALYS.dat and pTi_Ca45_TALYS.dat, respectively. Similar results by the ALICE-IPPE code extracted in the same way from the same figures are shown in files pTi_Ca45_ALICE.dat and pTi_V49_ALICE.dat, respectively.

Results by CEM03.03 used as a stand alone code for the ^{nat}Ti(p,x)^{49}V and ^{nat}Ti(p,x)^{45}Ca excitation functions are shown in files pTi_V49_CEM.dat and pTi_Ca45_CEM.dat, respectively.

The files pTi_V49_TAL.fig and pTi_Ca45_TAL.fig are templates for plotting the ^{nat}Ti(p,x)^{49}V and ^{nat}Ti(p,x)^{45}Ca excitation functions with xmgrace. The pdf files for these figures are pTi_V49_TAL.pdf and pTi_Ca45_TAL.pdf, shown below in Figs. 12 and 13.

From Figs. 12 and 13, we see good agreement between the MCNP6 results obtained using the **GENXS** option with the CEM03.03 event generator and the calculations by CEM03.03 used as a stand alone code, for both ^{nat}Ti(p,x)^{49}V and ^{nat}Ti(p,x)^{45}Ca excitation functions. We also can see a not so good, but still a reasonable agreement of our results with experimental data and with calculations by TALYS and ALICE-IPPE published in the paper [69].

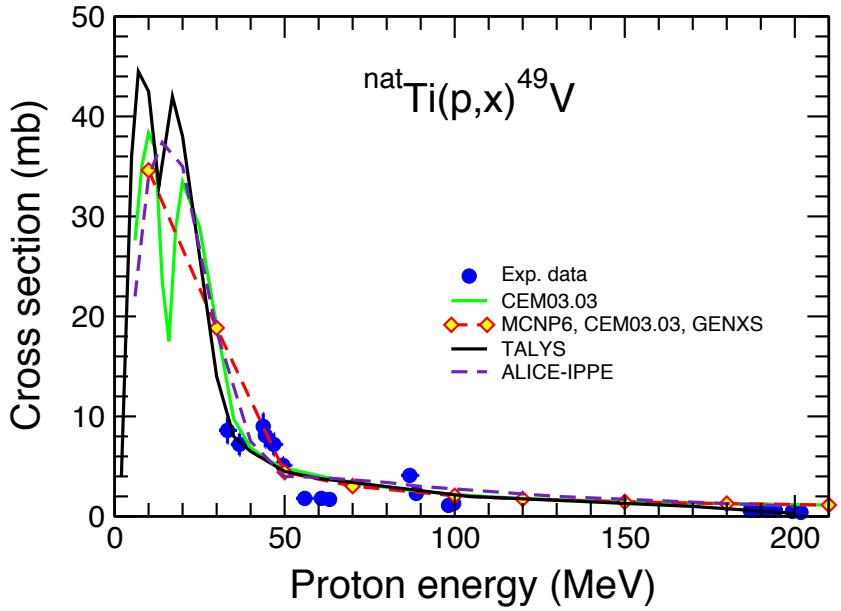

Figure 13: Comparison of the measured [69] excitation function for the production of the radionuclide ^{49}V from a thin ^{nat}Ti target bombarded with protons of energies below 210 MeV with our results by CEM03.03 used as a stand alone code, with results by MCNP6 with the GENXS option using the CEM03.03 event-generator, as well as with results by TALYS [70] and ALICE-IPPE [71] from Ref. [69], as indicated.

3.11. Test-problem #11: A) p800Th_CEM; B) p800Th_Bert; C) p800Th_INCL (all using inxc95)

This problem is to test the applicability of MCNP6 using the CEM03.03, Bertini+Dresner+RAL, and INCL+ABLA event-generators to calculate cross sections for the production of the therapy isotope ^{225}Ac from ^{232}Th bombarded with protons of energies of 800 and from 40 to 200 MeV.

Clinical trials for acute myeloid leukemia have been promising, with about 25% of terminal patients going into remission when using the Alpha Particle Therapy with ^{225}Ac and its daughter product ^{213}Bi. Researchers throughout the world are examining approaches for prostate cancer, bladder cancer, ovarian cancer, pancreatic cancer, melanoma, and non-Hodgkin's lymphoma. Unfortunately, there is not enough supply of the medical ^{225}Ac to support the current world research needs; much less is available for therapeutic use. This is why the US DOE Office of Science (Nuclear Physics) decided recently to fund the **"Accelerator-Based Production of ^{225}Ac"** project in order to determine the commercial viability of ^{225}Ac production using appropriate accelerators.

Limited experimental data for this problem, at only 100 and 800 MeV, were measured during 1997-1999 at the Institute for Theoretical and Experimental Physics (ITEP) in Moscow, Russia, and were published in Ref. [72]. These ITEP data are also available in the EXFOR database, as Entry No. 00997. In subdirectory **/VALIDATION_CEM/Experimental_data/pTh/**, we present the 800 MeV part of these data in the file p800Th_A_Titarenko.dat and plot them in the figure p800Th_A.pdf.

New measurements for this reaction at many energies from 40 to 200 MeV and also at 800

MeV are in progress at present at LANSCE, LANL, in the framework of the mentioned above US DOE **Ac-225 Project**. Preliminary data from these measurements are presented in the file p800Th_Ac225_LA.dat of the same subdirectory (together with all our calculation results and other files needed for the final figure). These preliminary data are from a 2010 presentation by John Weidner at the LANL Chemistry Division [73]; the final LANL data will be published after the completion of their analysis.

This test-problem uses the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate problems on thin targets in test-problems #5 and #1, we do not need to discuss here in detail the input and output files for this case. Therefore, we limit ourselves below to only providing the text of the input files (let us recall here again that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output file for this test-problem.

As a special study-case, we calculate this test-problem with three different models available for such type of reactions in MCNP6, namely, using the CEM03.03 [6], Bertini[48]+MPM[49]+ Dresner[50]+RAL[26], and the INCL[42]+ABLA[44] event-generators. We show below the main MCNP6 input files for all three cases: **p800Th_CEM**, for CEM03.03; **p800Th_Bert**, for Bertini+MPM+Dresner+RAL; and **p800Th_INCL**, for INCL+ABLA. All of them use the same companion, auxiliary second input file, **inxc95**, shown below as well.

p800Th_CEM:

```
MCNP6 test: p + Th232 by CEM03.03 at 800 MeV, nevtype=66
C Medical Ac-225 production for alpha cancer therapy
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ------------------------------------------------------------
  m1   90232 1.0
  sdef erg = 800 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 1000
  mode   h
LCA  8j 1    $ use CEM03.03, nevtype = 66                  !!!
  tropt genxs inxc95  nreact on  nescat off
c ------------------------------------------------------------
  print 40 110 95
  nps 1000000
  prdmp 2j -1
```

inxc95:

```
MCNP6 test: p + Th232 by CEM03.03 at 800 MeV, nevtype=66
1 0 1 /
Cross Section Edit
50 0 9 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
1 5 6 7 8 21 22 23 24 /
```

p800Th_Bert:

```
MCNP6 test: p + Th232 by Bertini+Dresner+RAL at 800 MeV,
C Medical Ac-225 production for alpha cancer therapy
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ------------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ------------------------------------------------------------------
  m1   90232 1.0
  sdef erg = 800 par = h dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 1000
  mode   h
  lca 2 1 5j -1
  lea 2j 0
c  LCA  8j 0    $ use Bertini+Dresner+RAL                  !!!
  tropt genxs inxc95  nreact on  nescat off
c  tropt genxs inxc95
c ------------------------------------------------------------------
  print 40 110 95
  nps 1000000
  prdmp 2j -1
dbcn  28j 1
```

p800Th_INCL:

```
MCNP6 test: p + Th232 by INCL+ABLA at 800 MeV,
```

```
C Medical Ac-225 production for alpha cancer therapy
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ------------------------------------------------------------
  m1   90232 1.0
  sdef erg = 800 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 1000
  mode   h
  LCA  2 1 0 4j -1 2    $ use INCL+ABLA                  !!!
  lea 2j 0
  tropt genxs inxc95  nreact on  nescat off
c ------------------------------------------------------------
  print 40 110 95
  nps 1000000
  prdmp 2j -1
  dbcn  28j 1
```

The MCNP6 mass-distribution of products from the reaction 800 MeV p + ^{232}Th calculated with the CEM03.03 event generator is printed in the table entitled "Summary by mass number:" of the MCNP6 output file **p800Th_CEM.o** present in the subdirectory **/VALIDATION_CEM/Templates/LINUX/** (together with output files with results calculated with the Bertini+MPM+Dresner+RAL and INCL+ABLA event-generators). It is also copied in a separate auxiliary file, p800Th_A_M6CEM.dat provided in subdirectory **/VALIDATION_CEM/Experimental_data/pTh/**, to help plotting this A-distribution with **xmgrace**. To help the users understand better our output file, we show below a small part of it, with only a little part of this table.

```
- - - - - - - - - - - - - - - - - - - - - - - - - -
Summary by mass number:

   A    Cross Section (b)    Mean Recoil (MeV)
   2   1.94210E+00 0.0012   3.81400E+01 0.0017
   3   8.96690E-01 0.0016   3.11142E+01 0.0019
   4   9.87166E-01 0.0017   2.62148E+01 0.0016
   6   1.01789E-02 0.0139   2.96702E+01 0.0044
   7   7.48509E-03 0.0163   3.53946E+01 0.0042
   8   1.96005E-03 0.0317   3.43503E+01 0.0077

- - - - - - - - - - - - - - - - - - - - - - - - - -
```

```
 227   3.37054E-02 0.0076   1.59811E-01 0.0087
 228   3.83770E-02 0.0071   1.29079E-01 0.0083
 229   3.68447E-02 0.0073   9.81487E-02 0.0094
 230   2.87788E-02 0.0082   9.71503E-02 0.0090
 231   5.02688E-02 0.0062   5.19686E-02 0.0086
 232   9.23716E-03 0.0146   8.41757E-02 0.0143
- - - - - - - - - - - - - - - - - - - - - - - - - -
```

Cross sections for the production of all isotopes from this reaction, including the ^{225}Ac of interest for us, are printed in table entitled "Distribution of residual nuclei:" of the MCNP6 output file. A little part of it is shown below.

```
- - - - - - - - - - - - - - - - - - - - - - - - - -
1 Distribution of residual nuclei:

                        Cross Section (b)
     Z =  1  all A     2.69183E+00 0.0011
             A =   2   1.94210E+00 0.0012
             A =   3   7.49727E-01 0.0018
- - - - - - - - - - - - - - - - - - - - - - - - - -
     Z = 89  all A     1.55776E-01 0.0034
             A = 211   1.17721E-05 0.4082
             A = 212   3.72783E-05 0.2294
             A = 213   3.15884E-04 0.0788
- - - - - - - - - - - - - - - - - - - - - - - - - -
             A = 224   1.03418E-02 0.0137
             A = 225   1.40088E-02 0.0118
             A = 226   1.36438E-02 0.0119
- - - - - - - - - - - - - - - - - - - - - - - - - -
```

Results by MCNP6 using the Bertini+Dresner+RAL event-generator are presented in the output file **p800Th_Bert.o**, with the mass-distribution of all products copied also in the auxiliary file p800Th_A_M6Bert.dat, to help plotting this A-distribution with **xmgrace**. Similarly, results by MCNP6 using the INCL+ABLA event-generator are presented in the output file **p800Th_INCL.o**, with the mass-distribution of all products copied also in the auxiliary file p800Th_A_M6INCL.dat, to help plotting this A-distribution with **xmgrace**.

The file p800Th_A.fig is a template for plotting the mass distribution of all products from our p + ^{232}Th reaction with with xmgrace. The pdf file for the figure is p800Th_A.pdf. It is shown here in Fig. 14.

From Fig. 14, we see very good agreement between the MCNP6 results obtained using the **GENXS** option with the CEM03.03 event generator and the calculations by CEM03.03 used as a stand alone code for all products from this reaction. We see also a quite reasonable agreement between results calculated with MCNP6 using different event generators for the spallation ($A \geq 190$), fission fragment ($30 \leq A \leq 150$), and very light ($A \leq 5$) products: If we were interested in only such products, we could use any event generator from the ones we tested here and the final results would be good enough and reliable. However, we see a very big difference between results obtained with different event generators for products at the border between fragmentation and fission ($5 \leq A \leq 30$) and between fission and spallation

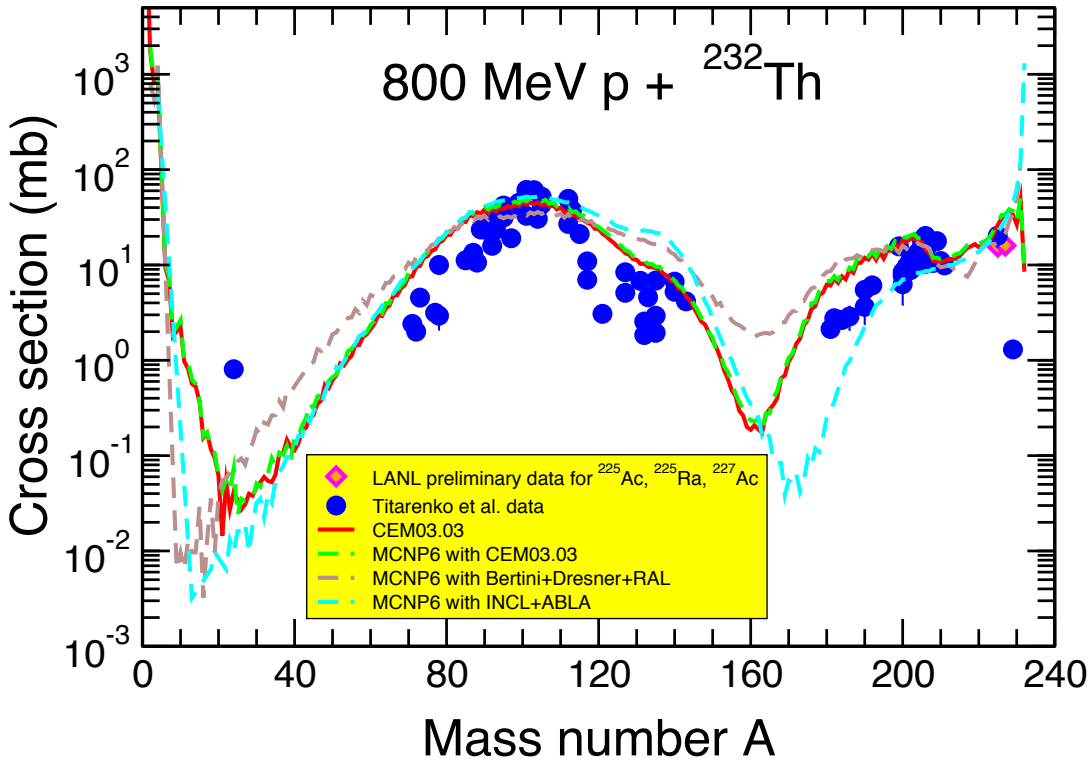

Figure 14: Comparison of the measured [72, 73] mass distribution of products from the reaction 800 MeV p + ^{232}Th with results by CEM03.03 used as a stand alone code and with results by MCNP6 with the GENXS option using the CEM03.03 [6], Bertini+MPM+Dresner+RAL [48, 49, 50, 26], and INCL+ABLA [42, 44] event-generators, as indicated.

($150 \leq A \leq 190$). Unfortunately, just for such products we do not have experimental data (their yields are lower and much more difficult to measure). In situations like this, we need predictions by several different models, so that we can make at least a rough estimation about the uncertainties in our results due to a good and reliable or to a bad and not so reliable physics considered by the models we use.

Note, that in the subdirectory **/VALIDATION_CEM/Templates/LINUX/**, for this test-problem, we present the MCNP6 output files only for the proton incident energy of 800 MeV. As we had in the previous test-problem #10, to get the yield of ^{225}Ac from this reaction as a function of the incident proton energy, i.e., the "excitation function" ^{232}Th(p,x)^{225}Ac of interest to us, we must perform several calculations at different energies, changing only the value of the incident proton energy on the **SDEF** card of the MCNP6 input file. As this is such a trivial change, we do not show examples of MCNP6 input and output files at other energies.

3.12. Test-problem #12: A) p392Pb with inxc18; B) p392Bi with inxc18

This problem is to test the applicability of MCNP6 using the CEM03.03 event generator to calculate production of secondary protons from intermediate-energy proton-induced reactions

on heavy nuclei-targets, of interest for various nuclear applications at energies above the pion production threshold.

To be specific, this test calculates with MCNP6 using CEM03.03 the proton spectra at 20, 25, 30, 40, 45, 50, 60, 75, 90, and 105 degrees from interactions of 392 MeV protons with ^{208}Pb and ^{209}Bi. It compares the MCNP6 results with experimental data and with results by CEM03.03 event-generator used as a stand alone code.

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate particle spectra from thin targets in test-problem #5, we do not need to discuss the input and output files for this case. Therefore, we limit ourselves to only providing the text of the input files (let us recall here again that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output files.

The main MCNP6 input files for the case of using the GENXS option are **p392Pb** (for p+^{208}Pb) and **p392Bi** (for p+^{209}Bi). Both of these use the same auxiliary companion requires by the GENXS option input file **inxc18**. All of these are presented in the subdirectory **/VALIDATION_CEM/Inputs/** and are also shown below.

p392Pb_GENXS:

```
MCNP6 test: p spectra from p+Pb208 by CEM03.03 at 392 MeV, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ------------------------------------------------------------
  m1   82208 1.0
  sdef erg = 392. par = h dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 400
  mode   h
LCA  8j 1    $ use CEM03.03
  tropt genxs inxc18  nreact on  nescat off
c ------------------------------------------------------------
  print 40 110 95
  nps 10000000
c  nps 10000
  prdmp 2j -1
```

inxc18:

```
MCNP6 test: p spectra from p+Pb208 by CEM03.03 at 392 MeV, nevtype=66
1 0 0 /
Cross Section Edit
41 -17 9 /
10.    20.    30.    40.   50.  60.  70.  80.  90.  100.
110.  120.   130.   140.  150. 160. 170. 180. 190.  200.
210.  220.   230.   240.  250. 260. 270. 280. 290.  300.
310.  320.   330.   340.  350. 360. 370. 380. 390.  400. /
107.5 102.5 92.5 87.5 77.5 72.5 62.5 57.5 52.5 47.5 42.5
37.5 32.5 27.5 22.5 17.5 0./
5 /
```

p392Bi_GENXS:

```
MCNP6 test: p spectra from p+Bi209 by CEM03.03 at 392 MeV, nevtype=66
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ---------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ---------------------------------------------------------------
  m1   83209 1.0
  sdef erg = 392. par = h dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 400
  mode   h
LCA  8j 1    $ use CEM03.03
  tropt genxs inxc18  nreact on  nescat off
c ---------------------------------------------------------------
  print 40 110 95
  nps 10000000
c  nps 10000
  prdmp 2j -1
```

Proton spectra calculated by MCNP6 using CEM03.03 with the GENXS option at 105, 90, 75, 60, 50, 45, 40, 30, 25, and 20 (±2.5) degrees from ^{208}Pb are tabulated in units of [b/sr/MeV] in the 2nd, 4th, and 6th pairs of columns of the first part of the "proton production cross section" table of the MCNP6 output file **p392Pb_GENXS.o** (presented in the Templates subdirectory **/VALIDATION_CEM/Templates/LINUX/**), after the proton energy tabulated in the 1st column; in the 1st, 3rd, 4th, 5th, and 7th pairs of columns of the second part of the same table (after the proton energy tabulated in the 1st column); and the 1st, and 2nd pairs of columns of the third part of the same table (after the proton energy tabulated in the 1st column); the

angle-integrated energy-spectrum of all protons is printed in the fourth part of the same table. To help plotting these spectra with **xmgrace** (see file p392Pb_p.pdf), these MCNP6 spectra are also copied to separate auxiliary files: 20_PbGENXS.dat, 25_PbGENXS.dat, 30_PbGENXS.dat, 40_PbGENXS.dat, 45_PbGENXS.dat, 50_PbGENXS.dat, 60_PbGENXS.dat, 75_PbGENXS.dat, 90_PbGENXS.dat, and 105_PbGENXS.dat, respectively, provided in the subdirectory **/VALIDATION_CEM/Experimental_data/p393Pb_Bi/** together with other our results, experimental data, and files with figures for this test-problem.

Proton spectra calculated by MCNP6 using CEM03.03 with the GENXS option at 105, 90, 75, 60, 50, 45, 40, 30, 25, and 20 ($\pm$2.5) degrees from ^{209}Bi are tabulated in units of [b/sr/MeV] in the 2nd, 4th, and 6th pairs of columns of the first part of the "proton production cross section" table of the MCNP6 output file **p392Bi_GENXS.o** (presented in the Templates subdirectory **/VALIDATION_CEM/Templates/LINUX/**), after the proton energy tabulated in the 1st column; the 1st, 3rd, 4th, 5th, and 7th pairs of columns of the second part of the same table (after the proton energy tabulated in the 1st column); and the 1st, and 2nd pairs of columns of the third part of the same table (after the proton energy tabulated in the 1st column); the angle-integrated energy-spectrum of all protons is printed in the fourth part of the same table. To help plotting these spectra with xmgrace (see file p392Bi_p.pdf), these MCNP6 spectra are copied also to separate auxiliary files: 20_BiGENXS.dat, 25_BiGENXS.dat, 30_BiGENXS.dat, 40_BiGENXS.dat, 45_BiGENXS.dat, 50_BiGENXS.dat, 60_BiGENXS.dat, 75_BiGENXS.dat, 90_BiGENXS.dat, and 105_BiGENXS.dat, respectively, in the subdirectory **/VALIDATION_CEM/Experimental_data/p393Pb_Bi/**.

Besides the MCNP6 results, for comparison, we show here also results by CEM03.03 used as a stand alone code; see files: 20_PbCEM.dat, 25_PbCEM.dat, 30_PbCEM.dat, 40_PbCEM.dat, 45_PbCEM.dat, 50_PbCEM.dat, 60_PbCEM.dat, 75_PbCEM.dat, 90_PbCEM.dat, and 105_PbCEM.dat, for the Pb209 target, and 20_BiCEM.dat, 25_BiCEM.dat, 30_BiCEM.dat, 40_BiCEM.dat, 45_BiCEM.dat, 50_BiCEM.dat, 60_BiCEM.dat, 75_BiCEM.dat, 90_BiCEM.dat, and 105_BiCEM.dat, for the Bi209 target, respectively.

The experimental neutron spectra for this problem were measured at the Research Center for Nuclear Physics (RCNP), Osaka University, Japan and are published in the paper [74]. Numerical values of the measured data were kindly sent us by Dr. Yusuke Uozumi.

Experimental proton spectra $d^2\sigma/dT/d\Omega$ from Pb in units of [mb/sr/MeV] as functions of proton kinetic energy in [MeV] at 20, 25, 30, 40, 45, 50, 60, 75, 90, and 105 degrees are presented here in the files: 20_pb392exp.dat, 25_pb392exp.dat, 30_pb392exp.dat, 40_pb392exp.dat, 45_pb392exp.dat, 50_pb392exp.dat, 60_pb392exp.dat, 75_pb392exp.dat, 90_pb392exp.dat, and 105_pb392exp.dat, respectively. Similar experimental data from the Bi-target are shown in the files: 20_bi392exp.dat, 25_bi392exp.dat, 30_bi392exp.dat, 40_bi392exp.dat, 45_bi392exp.dat, 50_bi392exp.dat, 60_bi392exp.dat, 75_bi392exp.dat, 90_bi392exp.dat, and 105_bi392exp.dat, respectively.

The files p392Pb_p.fig and p392Bi_p.fig are templates for plotting these spectra with xmgrace. The pdf files for the figures are p392Pb_p.pdf and p392Bi_p.pdf, with the summary file p392PbBi.pdf showing spectra for both Pb and Bi. Our final results are shown below in Fig. 15.

From Fig. 15, we see very good agreement between the MCNP6 results obtained using the **GENXS** option with the CEM03.03 event generator and the calculations by CEM03.03 used as a stand alone code, for all proton spectra from these reactions. We observe also reasonably good agreement of our results with the experimental data.

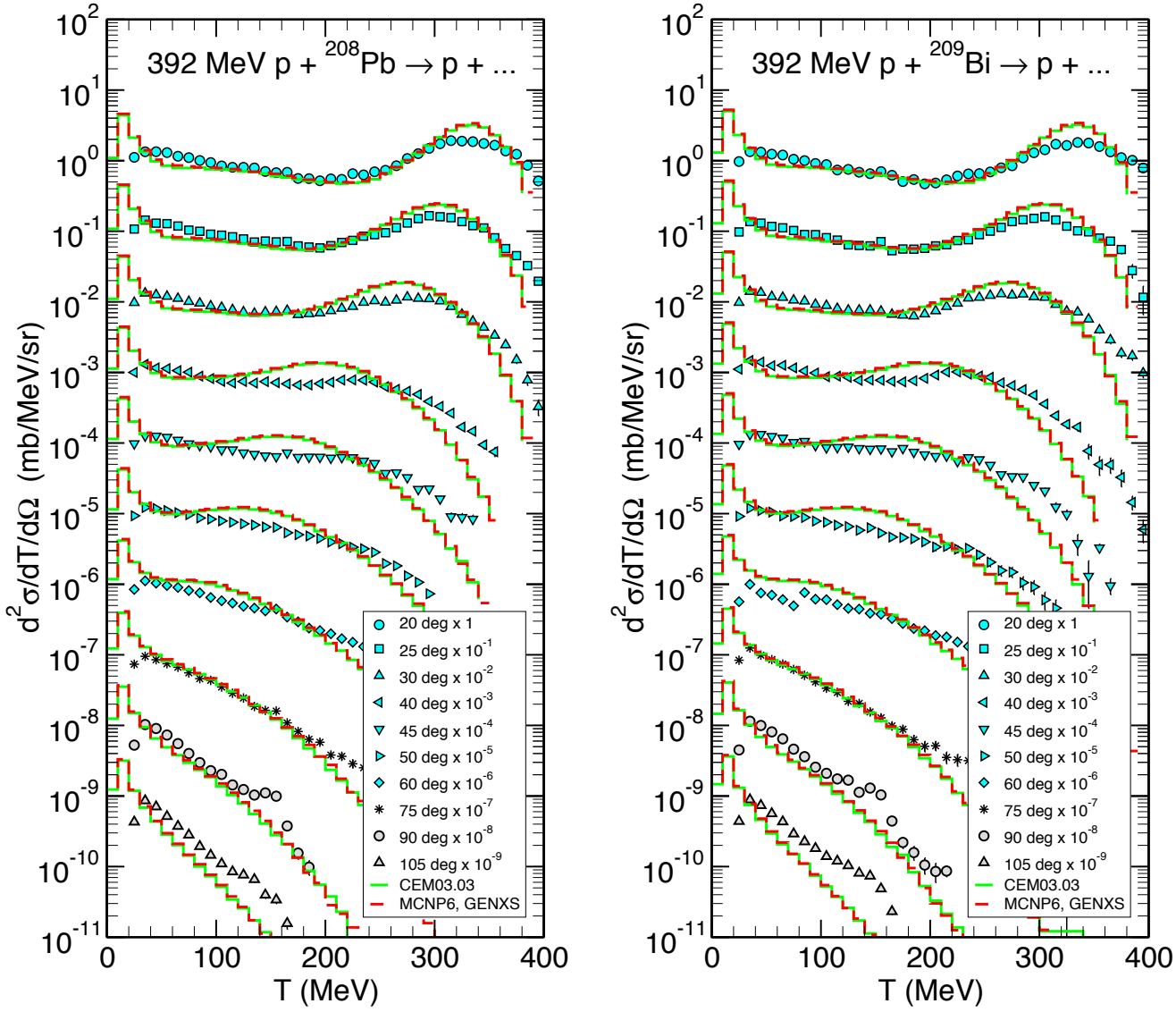

Figure 15: Experimental [74] double-differential spectra of protons at 20, 25, 30, 40, 45, 50, 60, 75, 90, and 105 degrees from interactions of 392 MeV protons with thin ^{208}Pb and ^{209}Bi targets compared with calculations by CEM03.03 [6] used as a stand alone code and with results by MCNP6 using the CEM03.03 event-generator with the GENXS option [36], as indicated.

3.13. Test-problem #13: g300Cu with inxcg1

This problem tests the applicability of MCNP6 using the CEM03.03 event generator to calculate a new type of reaction at intermediate energies which is of interest for many different applications but was not addressed so far in our Primer, namely, photonuclear reactions.

To be specific, this test calculates with MCNP6 using CEM03.03 the proton spectra at 45, 90, and 135 degrees from interactions of effectively 300 MeV monoenergetic photons with Cu. It compares the MCNP6 results with experimental data and with results by CEM03.03 event generator used as a stand alone code.

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate particle spectra from thin targets in test-problem #5, we do not need to discuss in detail here the input and output files for this

case. Therefore, we limit ourselves below to only providing the text of the input files (let us recall here again that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well describing where to find the results in the MCNP6 output files.

The main MCNP6 input file for this test-problem is **g300Cu**. Its auxiliary companion file required by the GENXS option is **inxcg1**. Both of these are presented in the subdirectory **/VALIDATION_CEM/Inputs/** and are also shown below.

g300Cu:

```
MCNP6 test with CEM03.03, GENXS: 300 MeV gamma + Cu64
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ------------------------------------------------------------
  m1   29064 1.0
  sdef erg = 300 par = 2 dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 1000
  mode   p
  tropt genxs inxcg1  nreact on  nescat off
c ------------------------------------------------------------
  print 40 110 95
  nps 1000000
c  nps 1000
  prdmp 2j -1
```

inxcg1:

```
MCNP6 test with CEM03.03, GENXS: 300 MeV gamma + Cu64
1 1 1 /
Cross Section Edit
80 -7 9 /
2.     3.   4.   5.   6.   7.   8.   9.  10.  11.
12.   13.  14.  15.  16.  17.  18.  19.  20.  21.
22.   24.  26.  28.  30.  32.  34.  36.  38.  42.
44.   46.  48.  50.  54.  56.  58.  60.  62.  64.
68.   70.  72.  74.  76.  78.  80.  84.  86.  88.
92.   98. 102. 104. 106. 108. 110. 112. 114. 116.
```

```
118. 120. 130. 140. 150. 160. 170. 180. 190. 200.
210. 220. 230. 240. 250. 260. 270. 290. 300. /
137.5 132.5 92.5 87.5 47.5 42.5 0. /
5 /
```

Proton spectra calculated by MCNP6 using CEM03.03 with the GENXS option at 135, 90, and 45 ($\pm$2.5) degrees are tabulated in units of [b/sr/MeV] in the 2nd, 4th, and 6th pairs of columns of the first part of the "proton production cross section" table of the MCNP6 output file **g300Cu.o** (after the proton energy tabulated in the 1st column); the angle-integrated energy-spectrum of all protons is printed in the second part of the same table, as well as in the MCTAL **g300Cu.m**, presented in subdirectory **/VALIDATION_CEM/Templates/LINUX/**. To help plotting these spectra with xmgrace (see file g300Cu_sf4.pdf), the MCNP6 results are copied to separate files 45_GENXS.dat, 90_GENXS.dat, and 135_GENXS.dat, respectively,

Besides the MCNP6 results, for comparison, we show also results by CEM03.03 used as a stand alone code; see files: 45CEM.dat, 90CEM.dat, and 135CEM.dat, respectively.

The experimental proton spectra for this problem were measured using the bremsstrahlung "difference method" (i.e., data for each proton energy were taken in pairs of runs with the electron energy varied by 10 MeV such that the peak of the difference between the corresponding bremsstrahlung spectra was centered at 300 MeV; this way, the "difference method" provides data for "effectively" monochromatic photons) at the Massachusetts Institute of Technology (MIT) Bates Linear Accelerator and are published in the paper [75].

Experimental proton spectra $d^2\sigma/dT/d\Omega$ in units of [microbarns/sr/MeV] as functions of proton kinetic energy in [MeV] at 45, 90, and 135 degrees are presented in the files 45.dat, 90.dat, and 135.dat, respectively, in the above mentioned subdirectory
/VALIDATION_CEM/Experimental_data/g300Cu/.

The file g300Cu_sf4.fig is a template for plotting the spectra with xmgrace. The pdf file for the figure is g300Cu_sf4.pdf; it is presented below in Fig. 16.

From Fig. 16, we see very good agreement between the MCNP6 results obtained using the **GENXS** option with the CEM03.03 event generator and the calculations by CEM03.03 used as a stand alone code, for all proton spectra from this photonuclear reaction. We observe also reasonably good agreement of our results with the experimental data.

3.14. Test-problem #13: n175F

This problem tests the applicability of MCNP6 using the CEM03.03 event generator to calculate production of alpha particles from intermediate-energy neutron-induced reactions of interest for many different applications.

To be specific, this test calculates with MCNP6 using CEM03.03 the ^{4}He spectra at 20, 40, 60, 80, 100, 120, 140, and 160 degrees from interactions of 175 MeV neutrons with ^{56}Fe. It compares the MCNP6 results with the new Uppsala experimental data [76] and with results by CEM03.03 event generator used as a stand alone code; it also could be used to compare MCNP6 results with similar calculations by the TALYS code [70], usually used to analyze such Uppsala measurements.

We calculate this test-problem using the **NOACT=-2** option for the 8th parameter of the LCA card of the MCNP6 input file. As we have presented a detailed description of the use of **NOACT=-2** option to calculate particle spectra from thin targets in test-problem #6, and have provided additional examples of its use in test problems #7 and #8, we do not need to

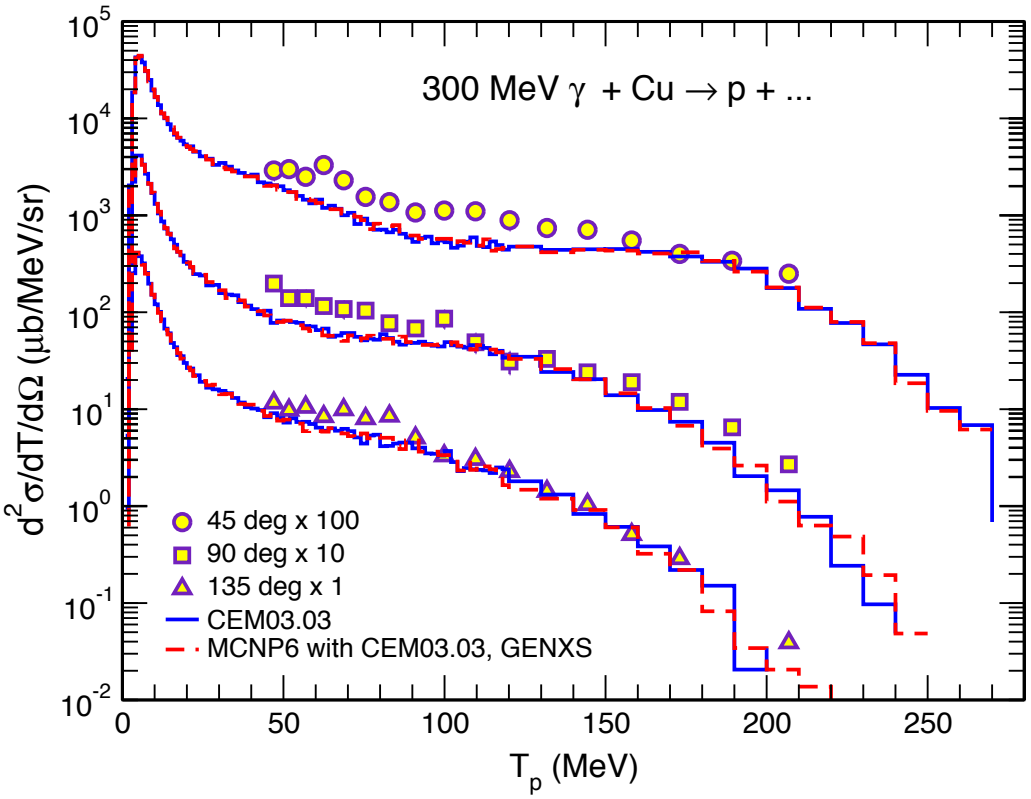

Figure 16: Experimental [75] double-differential spectra of protons at 45, 90, and 135 degrees from interactions of 300 MeV photons with a thin Cu target compared with calculations by CEM03.03 [6] used as a stand alone code and with results by MCNP6 using the CEM03.03 event-generator with the GENXS option [36], as indicated.

discuss in detail here the input and output files for this case. Therefore, we limit ourselves below to only providing the text of the input file as well as describing where to find the results in the MCNP6 output files. The input file for this test problem is **n175F**. It is presented in the subdirectory **/VALIDATION_CEM/Inputs/** and is also shown below.

n175Fe:

```
MCNP6 test with CEM03.03: 175 MeV p+ Fe56 -> n, p, d, t, He3, and $^4$He spectra
c d^2sigma/dT/dOmega [mb/MeV/sr] at 20, 40, 60, 80, 100, 120, 140, and 160 deg
c to compare with Bevilacqua's et al. measurements (Proc. ND2010)
c and results by CEM03.03 used as a stand alone code
1   1  -10   -501      imp:h=1
2   0         501  -502  imp:h=1
99  0         502      imp:h=0

501   so 0.01
502   so 1
c
c  tally surfaces
c
5      kz    0    0.007654253     1
```

```
10     kz    0    0.031091151     1
15     kz    0    0.071796643     1
20     kz    0    0.132474088     1
25     kz    0    0.217442414     1
30     kz    0    0.333332652     1
35     kz    0    0.49028952      1
40     kz    0    0.704086505     1
45     kz    0    0.999997346     1
50     kz    0    1.420272373     1
55     kz    0    2.03959969      1
60     kz    0    2.999987744     1
65     kz    0    4.598886921     1
70     kz    0    7.548583695     1
75     kz    0    13.92808003     1
80     kz    0    32.16299385     1
85     kz    0    130.6423246     1
90     pz    0
95     kz    0    130.6503105    -1
100    kz    0    32.16399202    -1
105    kz    0    13.92837571    -1
110    kz    0    7.548708346    -1
115    kz    0    4.598950644    -1
120    kz    0    3.000024513    -1
125    kz    0    2.039622728    -1
130    kz    0    1.420287681    -1
135    kz    0    1.000007961    -1
140    kz    0    0.704094093    -1
145    kz    0    0.490295058    -1
150    kz    0    0.333336738    -1
155    kz    0    0.217445427    -1
160    kz    0    0.132476276    -1
165    kz    0    0.071798167    -1
170    kz    0    0.031092115    -1
175    kz    0    0.007654721    -1

mode n h d t s a / * z
m1  26056 1    $ we use only Fe-56 as the target meterial
lca 0 6j -2 1    $ CEM03.03, no transport, only the 1st inelstic interaction
c nps 1000
nps 1e7
c prdmp 2j -1
sdef par=n erg=175 vec=0 0 1 dir 1
phys:h 200
phys:n 200
phys:a 200
phys:d 200
phys:t 200
```

```
phys:s 200
phys:/ 200
phys:* 200
phys:z 200
c
f11:n  502  $ tally n
f21:h  502  $ tally p
f31:d  502  $ tally d
f41:t  502  $ tally t
f51:s  502  $ tally He3
f61:a  502  $ tally He4
c defining our "segments" for n at 20, 40, 60, 80, 100, 120, 140, and 160 deg
fs11 -15 -25 -35 -45 -55 -65 -75 -85 95 105 115 125 135 145 155 165 T
c
c defining our "segments" for p at 20, 40, 60, 80, 100, 120, 140, and 160 deg
fs21 -15 -25 -35 -45 -55 -65 -75 -85 95 105 115 125 135 145 155 165 T
c
c defining our "segments" for d at 20, 40, 60, 80, 100, 120, 140, and 160 deg
fs31 -15 -25 -35 -45 -55 -65 -75 -85 95 105 115 125 135 145 155 165 T
c
c defining our "segments" for t at 20, 40, 60, 80, 100, 120, 140, and 160 deg
fs41 -15 -25 -35 -45 -55 -65 -75 -85 95 105 115 125 135 145 155 165 T
c
c defining our "segments" for He3 at 20, 40, 60, 80, 100, 120, 140, and 160 deg
fs51 -15 -25 -35 -45 -55 -65 -75 -85 95 105 115 125 135 145 155 165 T
c
c defining our "segments" for He4 at 20, 40, 60, 80, 100, 120, 140, and 160 deg
fs61 -15 -25 -35 -45 -55 -65 -75 -85 95 105 115 125 135 145 155 165 T
c
c The following Segment Divisor card is needed to get 1/sr for the n-spectra
sd11  0.214094347  $ 2pi(cos0 -cos15)
      0.374591188  $ 2pi(cos15 - cos25); 20 deg
      0.547615682  $ 2pi(cos25 - cos35)
      0.70400115   $ 2pi(cos35 - cos45); 40 deg
      0.8389959    $ 2pi(cos45 - cos55)
      0.948498184  $ 2pi(cos55 - cos65); 60 deg
      1.029180831  $ 2pi(cos65 - cos75)
      1.078592339  $ 2pi(cos75 - cos85); 80 deg
      1.095231365  $ 2pi(cos85 - cos95)
      1.078592339  $ 2pi(cos95 - cos105); 100 deg
      1.029180831  $ 2pi(cos105 - cos115)
      0.948498184  $ 2pi(cos115 - cos125); 120 deg
      0.8389959    $ 2pi(cos125 - cos135)
      0.70400115   $ 2pi(cos135 - cos145); 140 deg
      0.547615682  $ 2pi(cos145 - cos155)
      0.374591188  $ 2pi(cos155 - cos165); 160 deg
      0.214094347  $ 2pi(cos165 - cos180)
```

```
      12.56637061  $ 4pi
c
c The following Segment Divisor card is needed to get 1/sr for the p-spectra
sd21  0.214094347  $ 2pi(cos0 -cos15)
      0.374591188  $ 2pi(cos15 - cos25); 20 deg
      0.547615682  $ 2pi(cos25 - cos35)
      0.70400115   $ 2pi(cos35 - cos45); 40 deg
      0.8389959    $ 2pi(cos45 - cos55)
      0.948498184  $ 2pi(cos55 - cos65); 60 deg
      1.029180831  $ 2pi(cos65 - cos75)
      1.078592339  $ 2pi(cos75 - cos85); 80 deg
      1.095231365  $ 2pi(cos85 - cos95)
      1.078592339  $ 2pi(cos95 - cos105); 100 deg
      1.029180831  $ 2pi(cos105 - cos115)
      0.948498184  $ 2pi(cos115 - cos125); 120 deg
      0.8389959    $ 2pi(cos125 - cos135)
      0.70400115   $ 2pi(cos135 - cos145); 140 deg
      0.547615682  $ 2pi(cos145 - cos155)
      0.374591188  $ 2pi(cos155 - cos165); 160 deg
      0.214094347  $ 2pi(cos165 - cos180)
      12.56637061  $ 4pi
c
c The following Segment Divisor card is needed to get 1/sr for the d-spectra
sd31  0.214094347  $ 2pi(cos0 -cos15)
      0.374591188  $ 2pi(cos15 - cos25); 20 deg
      0.547615682  $ 2pi(cos25 - cos35)
      0.70400115   $ 2pi(cos35 - cos45); 40 deg
      0.8389959    $ 2pi(cos45 - cos55)
      0.948498184  $ 2pi(cos55 - cos65); 60 deg
      1.029180831  $ 2pi(cos65 - cos75)
      1.078592339  $ 2pi(cos75 - cos85); 80 deg
      1.095231365  $ 2pi(cos85 - cos95)
      1.078592339  $ 2pi(cos95 - cos105); 100 deg
      1.029180831  $ 2pi(cos105 - cos115)
      0.948498184  $ 2pi(cos115 - cos125); 120 deg
      0.8389959    $ 2pi(cos125 - cos135)
      0.70400115   $ 2pi(cos135 - cos145); 140 deg
      0.547615682  $ 2pi(cos145 - cos155)
      0.374591188  $ 2pi(cos155 - cos165); 160 deg
      0.214094347  $ 2pi(cos165 - cos180)
      12.56637061  $ 4pi
c
c The following Segment Divisor card is needed to get 1/sr for the t-spectra
sd41  0.214094347  $ 2pi(cos0 -cos15)
      0.374591188  $ 2pi(cos15 - cos25); 20 deg
      0.547615682  $ 2pi(cos25 - cos35)
      0.70400115   $ 2pi(cos35 - cos45); 40 deg
```

```
      0.8389959    $ 2pi(cos45 - cos55)
      0.948498184  $ 2pi(cos55 - cos65); 60 deg
      1.029180831  $ 2pi(cos65 - cos75)
      1.078592339  $ 2pi(cos75 - cos85); 80 deg
      1.095231365  $ 2pi(cos85 - cos95)
      1.078592339  $ 2pi(cos95 - cos105); 100 deg
      1.029180831  $ 2pi(cos105 - cos115)
      0.948498184  $ 2pi(cos115 - cos125); 120 deg
      0.8389959    $ 2pi(cos125 - cos135)
      0.70400115   $ 2pi(cos135 - cos145); 140 deg
      0.547615682  $ 2pi(cos145 - cos155)
      0.374591188  $ 2pi(cos155 - cos165); 160 deg
      0.214094347  $ 2pi(cos165 - cos180)
      12.56637061  $ 4pi
c
c The following Segment Divisor card is needed to get 1/sr for the He3-spectra
sd51  0.214094347  $ 2pi(cos0 -cos15)
      0.374591188  $ 2pi(cos15 - cos25); 20 deg
      0.547615682  $ 2pi(cos25 - cos35)
      0.70400115   $ 2pi(cos35 - cos45); 40 deg
      0.8389959    $ 2pi(cos45 - cos55)
      0.948498184  $ 2pi(cos55 - cos65); 60 deg
      1.029180831  $ 2pi(cos65 - cos75)
      1.078592339  $ 2pi(cos75 - cos85); 80 deg
      1.095231365  $ 2pi(cos85 - cos95)
      1.078592339  $ 2pi(cos95 - cos105); 100 deg
      1.029180831  $ 2pi(cos105 - cos115)
      0.948498184  $ 2pi(cos115 - cos125); 120 deg
      0.8389959    $ 2pi(cos125 - cos135)
      0.70400115   $ 2pi(cos135 - cos145); 140 deg
      0.547615682  $ 2pi(cos145 - cos155)
      0.374591188  $ 2pi(cos155 - cos165); 160 deg
      0.214094347  $ 2pi(cos165 - cos180)
      12.56637061  $ 4pi
c
c The following Segment Divisor card is needed to get 1/sr for the He4-spectra
sd61  0.214094347  $ 2pi(cos0 -cos15)
      0.374591188  $ 2pi(cos15 - cos25); 20 deg
      0.547615682  $ 2pi(cos25 - cos35)
      0.70400115   $ 2pi(cos35 - cos45); 40 deg
      0.8389959    $ 2pi(cos45 - cos55)
      0.948498184  $ 2pi(cos55 - cos65); 60 deg
      1.029180831  $ 2pi(cos65 - cos75)
      1.078592339  $ 2pi(cos75 - cos85); 80 deg
      1.095231365  $ 2pi(cos85 - cos95)
      1.078592339  $ 2pi(cos95 - cos105); 100 deg
      1.029180831  $ 2pi(cos105 - cos115)
```

```
      0.948498184  $ 2pi(cos115 - cos125); 120 deg
      0.8389959    $ 2pi(cos125 - cos135)
      0.70400115   $ 2pi(cos135 - cos145); 140 deg
      0.547615682  $ 2pi(cos145 - cos155)
      0.374591188  $ 2pi(cos155 - cos165); 160 deg
      0.214094347  $ 2pi(cos165 - cos180)
      12.56637061  $ 4pi
c
c     Boundaries of the proton energy bins: 0-5 MeV; 5-10 MeV, ...
c     tabulated exactly as used by CEM03.03 as stand alone code
e0    5     10    15    20    25    30    35    40    45    50
      55    60    65    70    75    80    85    90    95    100
      105   110   115   120   125   130   135   140   145   150
      155   160   165   170   175   180   185   190   195   200
c
em11 150.478 39r $ multiply to sig_inelastic = 752.39 mb, as predicted by
c                 CEM03.03noGPL in n175Fe.res of 01/07/2011, then divided by 5
c                 (the value of each energy bin in MeV). This is needed
c                 to get the spectra in [mb/sr/MeV]; we do so for all 40 E-bins
c                 of n-spectra
c
em21 150.478 39r $ the same as above, but for p-spectra
c
em31 150.478 39r $ the same as above, but for d-spectra
c
em41 150.478 39r $ the same as above, but for t-spectra
c
em51 150.478 39r $ the same as above, but for He3-spectra
c
em61 150.478 39r $ the same as above, but for He4-spectra
c
dbcn  20j  0  5j  -1  j  1  2j  0  1  $ needed to tally pi+ separately of pi-
```

[4]He spectra calculated by MCNP6 with CEM03.03 using the **noact=-2** option for the 8th parameter of the LCA card at 20, 40, 60, 80, 100, 120, 140, and 160 (±5) degrees are tabulated in units of [mb/sr/MeV] in the MCNP6 output file **n175Fe.o** as tally 61, respectively in the "segments":
1) segment: 15 -25
2) segment: 15 25 35 -45
3) segment: 15 25 35 45 55 -65
4) segment: 15 25 35 45 55 65 75 -85
5) segment: 15 25 35 45 55 65 75 85 -95 105
6) segment: 15 25 35 45 55 65 75 85 -95 -105 -115 125
7) segment: 15 25 35 45 55 65 75 85 -95 -105 -115 -125 -135 145
8) segment: 15 25 35 45 55 65 75 85 -95 -105 -115 -125 -135 -145 -155 165.

The output file is provided in subdirectory **/VALIDATION_CEM/Templates/LINUX/**.

As described above for the test-problem #6, to get the units of [mb] needed for the normalization of the calculated spectra to the total reaction cross section, we would have to use the Energy Multiplier card **EM61** in our input file with the value 752.39 on it for all the 40 energy bins of our tally **F61** for ^{4}He: 752.39 is the value of the total inelastic (reaction) cross section in [mb] as predicted by CEM03.03 used for this reaction as a stand alone code. However, to put the MCNP6 calculated spectra $d^2\sigma/dT/d\Omega$ in units of [1/MeV], we divide the tables from the MCNP6 output file for every "segment" described above by the corresponding values of the energy bins. We have chosen here for all energy bins a value of 5 MeV. After that, we can use on the **EM61** card a value of 752.39/5. = 150.47 (i.e., already divided by 5 [MeV]) for all 40 energy bins of our tally **F61**, so that no a further division is needed in this particular case.

In a similar manner, to get the units of [1/sr] for the calculated spectra, we use in our input file the Segment Divisor card **SD61** with values of the solid angles for each "segment" used to identify the needed angles of 20, 40, 60, 80, 100, 120, 140, and 160 ($\pm$5) degrees.

Note that in reality, to obtain some "extra" results, besides the ^{4}He spectra, we have calculated here also spectra of secondary neutrons (tally # 11), protons (tally # 21), deuterons (tally # 31), tritons (tally # 41), and ^{3}He (tally # 51) from this reaction. We had to use the corresponding **EM** and **SD** cards also for n, p, d, t, and ^{3}He, for the same reason and in the same manner as discussed above for ^{4}He.

To help plot the MCNP6 ^{4}He spectra with **xmgrace** (see file n175_Fe_He4.pdf), the MCNP6 results are copied to separate files named Fe_He4_20_6.dat, Fe_He4_40_6.dat, Fe_He4_60_6.dat, Fe_He4_80_6.dat, Fe_He4_100_6.dat, Fe_He4_120_6.dat, Fe_He4_140_6.dat, and Fe_He4_160_6.dat, for 20, 40, 60, 80, 100, 120, 140, and 160 degrees , respectively, provided in subdirectory **/VALIDATION_CEM/Experimental_data/n175Fe/** together with our results, experimental data, and final files with the figure for this test-problem.

Besides the MCNP6 results, for comparison, we show here also results by CEM03.03 used as a stand alone code; see files: Fe_He4_20_CEM.dat, Fe_He4_40_CEM.dat, Fe_He4_60_CEM.dat, Fe_He4_80_CEM.dat, Fe_He4_100_CEM.dat, Fe_He4_120_CEM.dat, Fe_He4_140_CEM.dat, and Fe_He4_160_CEM.dat, respectively.

The measurements for this problem have been performed at the Svedber Laboratory of the Uppsala University, Sweden by Dr. Riccardo Bevilacqua et al. The measured data are still under analysis and will be published in a future paper in Phys. Rev. C. Preliminary values of the measured ^{4}He spectra used here were presented at the ND2010 conference in Ref. [76] and were kindly provided us by Dr. Bevilacqua.

Experimental ^{4}He spectra $d^2\sigma/dT/d\Omega$ in units of [mb/sr/MeV] as functions of ^{4}He kinetic energy in [MeV] at 20, 40, 60, 80, 100, 120, 140, and 160 degrees are presented in the files XS_Fe_20_4He.dat, XS_Fe_40_4He.dat, XS_Fe_60_4He.dat, XS_Fe_80_4He.dat, XS_Fe_100_4He.dat, XS_Fe_120_4He.dat, XS_Fe_140_4He.dat, and XS_Fe_160_4He.dat, respectively, in the subdirectory **/VALIDATION_CEM/Experimental_data/n175Fe/**.

The file n175_Fe_He4.fig is a template for plotting the spectra with xmgrace. The pdf file for the figure with final results for this problem is n175_Fe_He4.pdf. It is shown below in Fig. 17.

From Fig. 17, we see very good agreement between the MCNP6 results obtained using the **GENXS** option with the CEM03.03 event generator and the calculations by CEM03.03 used as a stand alone code, for all ^{4}He spectra from this neutron-induced reaction. We observe also reasonably good agreement of our results with the experimental data.

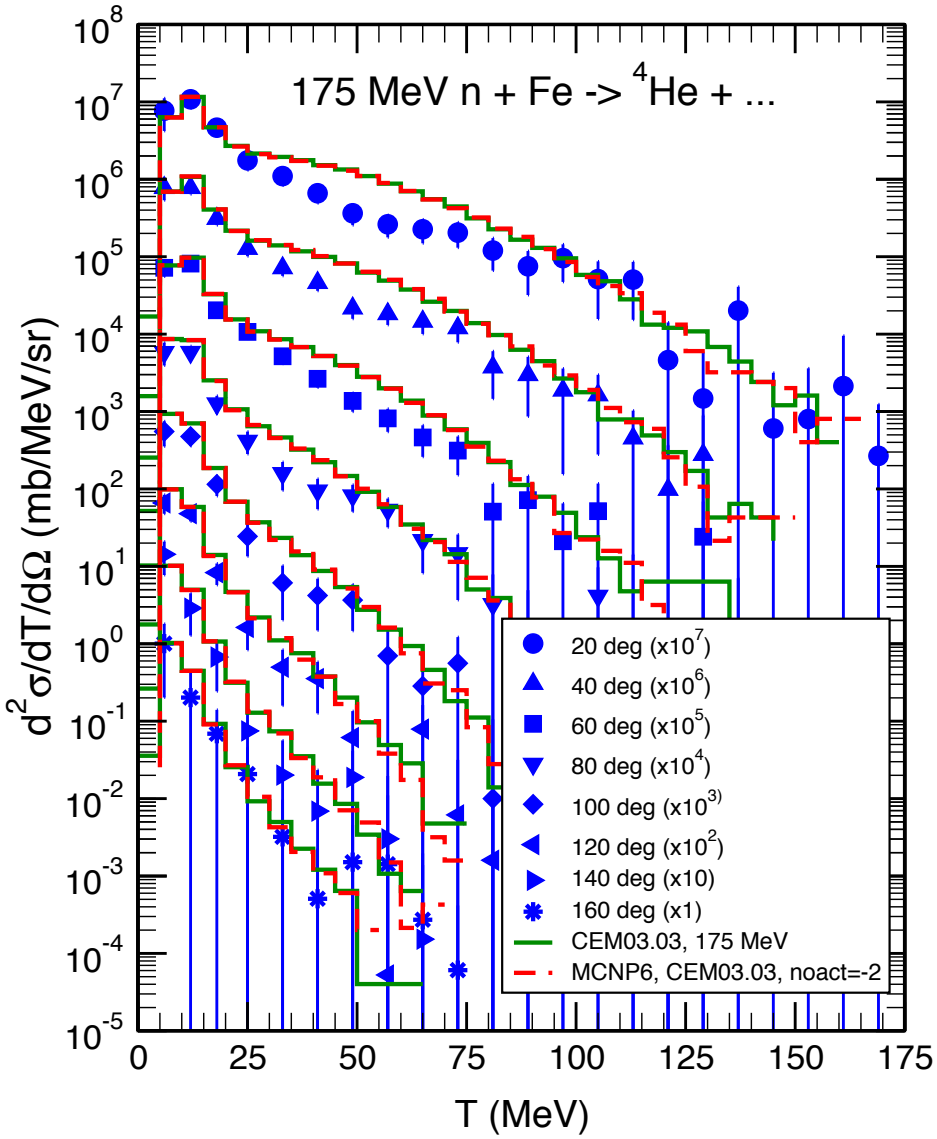

Figure 17: Experimental [76] double-differential spectra of ^{4}He at 20, 40, 60, 80, 100, 120, 140, and 160 degrees from interactions of 175 MeV Quasi-Monoenergetic Neutrons (QMN) with a thin Fe target compared with calculations for a monoenergetic beam of 175 MeV neutrons by CEM03.03 [6] used as a stand alone code and by the MCNP6 transport code using the CEM03.03 event-generator with the **noact=-2** option, as indicated.

3.15. Test-problem #15: pip1500Fe_n with inxcp1

This problem is to test the applicability of MCNP6 using the CEM03.03 event generator to calculate a new type of reaction which is of interest for many different applications at energies above the pion production threshold but was not addressed so far in our Primer, namely, reactions induced by pions.

To be specific, this test calculates with MCNP6 using CEM03.03 the neutron spectra at 30, 90, and 150 degrees from interactions of 1.5 GeV positive pions with Fe. It compares the MCNP6 results with experimental data and with results by CEM03.03 event-generator used as a stand alone code.

We calculate this test-problem using the GENXS option of MCNP6. As we have presented a detailed description of the use of GENXS option to calculate particle spectra from thin targets in test-problem #5, we do not need to discuss in detail here the input and output files for this case. Therefore, we limit ourselves below to only providing the text of the input files (let us recall here again that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output files.

The main MCNP6 input file for this test-problem is **pip1500Fe_n**. Its auxiliary companion file requires by the GENXS option is **inxcp1**. Both of them are presented in the subdirectory **/VALIDATION_CEM/Inputs/** and are also shown below.

pip1500Fe_n:

```
Comparison Test: pip+Fe56 at 1.5 GeV
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c -------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c -------------------------------------------------------------
  m1   26056 1.0
  sdef erg = 1500 par = / dir = 1 pos = 0 0 0 vec 0 0 1
  imp:/ 1 1 0
  phys:/ 2000
  mode   /
  tropt genxs inxcp1  nreact on  nescat off
c -------------------------------------------------------------
  print 40 110 95
  nps 1000000
  prdmp 2j -1
```

inxcp1:

```
Comparison Test: pip+Fe56 at 1.5 GeV
1 1 1 /
Cross Section Edit
34 -7 9 /
1 2 3 4 5 6 7 8 9 10 20 30 40 50 60 70 80 90 100 200 300
400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 /
155. 145. 95. 85. 35. 25. 0. /
1 5 6 7 8 21 22 23 24 /
```

Neutron spectra calculated by MCNP6 using CEM03.03 with the GENXS option at 150, 90, and 30 (±5.0) degrees are tabulated in units of [b/sr/MeV] in the 2nd, 4th, and 6th pairs of columns of the first part of the **neutron production cross section** table of the MCNP6 output file **pip1500Fe_n.o** (after the neutron energy tabulated in the 1st column); the angle-integrated energy-spectrum of all neutrons, is also printed, in the second part of the same table, as well as in the MCTAL **pip1500Fe_n.m**, presented in the Templates subdirectory **/VALIDATION_CEM/Templates/LINUX/**. Note that the GENXS method requires a second input file; we call it as **inxcp1** for this test-problem. To help plotting these spectra with **xmgrace** (see file pip1500Fe_sf4.pdf), the MCNP6 results are copied to separate files 30_GENXS.dat, 90_GENXS.dat, and 150_GENXS.dat, respectively, provided in the subdirectory **/VALIDATION_CEM/Experimental_data/pip1500Fe/** together with our other results, experimental data, and final files with the figure for this test-problem.

The experimental neutron spectra for this problem were measured using the Time-of-Flight (TOF) method at KEK, Japan and are published in the paper [77]; tabulated values of the measured spectra were received from the authors.

Experimental neutron spectra $d^2\sigma/dT/d\Omega$ in units of [mb/sr/MeV] as functions of neutron kinetic energy in [MeV] at 30, 90, and 150 degrees are presented in the files 30.dat, 90.dat, and 150.dat, respectively, in the subdirectory **/VALIDATION_CEM/Experimental_data/pip1500Fe/**.

Besides the MCNP6 results, for comparison, we show here also results by CEM03.03 used as a stand alone code; see files: 30CEM.dat, 90CEM.dat, and 150CEM.dat, respectively.

The file pip1500Fe_sf4.fig is a template for plotting the spectra with **xmgrace**. The pdf file for the figure is pip1500Fe_sf4.pdf. It is shown below in Fig. 18.

From Fig. 18, we see very good agreement between the MCNP6 results obtained using the **GENXS** option with the CEM03.03 event generator and the calculations by CEM03.03 used as a stand alone code, for all neutron spectra from this pion-induced reaction. We observe also reasonably good agreement of our results with the experimental data.

3.16. Test-problem #16: A) bg4.5GeV_Nb_30CEM; B) bg4.5GeV_Nb_30CEM_0 (both with inxs022)

This MCNP6 problem tests a very recent extension by Dick Prael of MCNP6 using the CEM03.03 event generator to describe reactions induced by bremsstrahlung photons on thin targets. This capability of MCNP6 is needed to test the CEM03.03 and LAQGSM03.03 event-generators able to describe this type of reaction. Such reactions are of interest to several astrophysical and space applications, as well as for the Continuous Electron Beam Accelerator Facility (CEBAF) in Newport News, VA, upgraded recently to be able to accelerate electron beams to energies up to 12 GeV.

This test calculates with MCNP6 using CEM03.03 the product yield of nuclei from interaction of bremsstrahlung photons with a maximum energy of $E_0 = 4.5$ GeV with a thin ^{93}Nb target. It is to compare the MCNP6 mass-distribution of products with available experimental data and with results by the CEM03.03 event generator used as a stand alone code.

The experimental data for this problem were measured at the Yerevan electron synchrotron of the Yerevan Physics Institute, Armenia, former USSR and are published in the paper [78].

Note that all the experimental characteristics for reactions induced by bremsstrahlung photons are usually normalized per "equivalent quanta", $Q =< E > /E_0$, where $< E >$ is the mean energy of the bremsstrahlung photons and E_0 is the "end-point" or the maximum energy

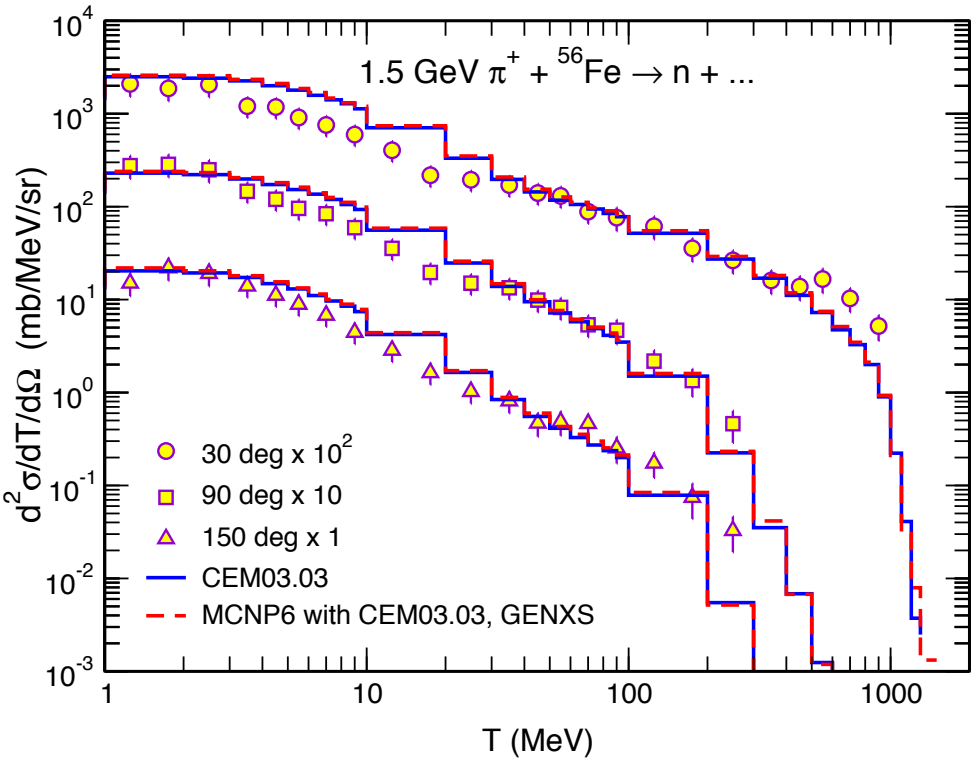

Figure 18: Experimental [77] double-differential spectra of neutrons at 30, 90, and 150 degrees from interactions of 1.5 GeV π^+ with a thin ^{56}Fe target compared with calculations by CEM03.03 [6] used as a stand alone code and with results by MCNP6 using the CEM03.03 event-generator with the GENXS option, as indicated.

of the bremsstrahlung photons.

Experimental cross section of the products published in Ref. [78] are presented in units of [mb/Q] as a function of the mass number of the measured ion in the file exp.dat in the subdirectory **/VALIDATION_CEM/Experimental_data/bg4.5GeV_Nb/** together with our results and final files with the figure for this test-problem.

Note that only a part of all products were measured in this experiment, while we compare these data with the mass distribution of the sum of all products as calculated by MCNP6 and by CEM03.03 used as a stand alone code. This is why we should expect that at least some of the experimental points should be below the theoretical A-distribution of all products.

We calculate with MCNP6 these spectra using the GENXS option in two different ways: using the value of **DBCN(29)** equal to **1** and to **0**. As we have presented a detailed description of the use of GENXS option to calculate yields of products from thin targets in test-problem #1, we do not need to discuss in detail the input and output files for this case. Therefore, we limit ourselves below to only providing the text of the input files (let us recall here again that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output files.

The main MCNP6 inputs files for the cases of **DBCN(29)** equal to **1** and to **0** are **bg4.5GeV_Nb_30CEM** and **bg4.5GeV_Nb_30CEM_0**, respectively. As companions to these, we use the same auxiliary MCNP6 input file **inxs022** for the cases of **DBCN(29)** equal to **1** and to **0**. All these input files are presented in the subdirectory **/VALIDA-**

TION_LAQGSM/Inputs/ and are also shown below.

bg4.5GeV_Nb_30CEM:

```
4.5GeV max bremstrahlung on Nb93 cross section calculation
c ---------------------------------------------------------------
c Uses CEM and dbcn(29)/=0
c ---------------------------------------------------------------
c Cells
c ---------------------------------------------------------------
11  1  -18.7  -40
31  0           40

c ---------------------------------------------------------------
c Surfaces
c ---------------------------------------------------------------
40  so  1.

c ---------------------------------------------------------------
c Materials
c ---------------------------------------------------------------
m1     41093 1
c ---------------------------------------------------------------
c Source
c ---------------------------------------------------------------
sdef   erg=4500 par=p vec=1 0 0 dir=1
c ---------------------------------------------------------------
c Options
c ---------------------------------------------------------------
imp:p 1 0
mode p
lca    7j -1 1 $ First interaction only
mx1:p    model
phys:p 3j 1 $ Turn on photonuclear
c ---------------------------------------------------------------
c nps    1000
nps    1000000
prdmp  1000000 100000 1 2
tropt  genxs inxs022
dbcn   28j 1 2j 1 $ For MCNP6, E_min=30 MeV (default)
c dbcn   28j 1 2j 1 4j 10 $ For MCNP6, E_min=10 MeV (DBCN(37)=10)
```

inxs022:

```
4.5 GeV max bremstrahlung on Nb93 cross section calculation
1 1 1
Uses CEM and dbcn(29)/=1
```

```
0,0,11,1.0/
5,1,21,22,23,24,2,6,7,8,-1/
```

bg4.5GeV_Nb_30CEM_0:

```
4.5 GeV max bremstrahlung on Nb93 cross section calculation
c ------------------------------------------------------------
c Uses CEM and dbcn(29) = 0
c ------------------------------------------------------------
c Cells
c ------------------------------------------------------------
11  1  -18.7  -40
31  0           40

c ------------------------------------------------------------
c Surfaces
c ------------------------------------------------------------
40  so  1.

c ------------------------------------------------------------
c Materials
c ------------------------------------------------------------
m1     41093 1
c ------------------------------------------------------------
c Source
c ------------------------------------------------------------
sdef   erg=4500 par=p vec=1 0 0 dir=1
c ------------------------------------------------------------
c Options
c ------------------------------------------------------------
imp:p 1 0
mode p
lca    7j -1 1 $ First interaction only
mx1:p    model
phys:p 3j 1 $ Turn on photonuclear
c ------------------------------------------------------------
c nps    1000
nps    1000000
prdmp  1000000 100000 1 2
tropt  nreact on nescat off genxs inxs021
C tropt  genxs inxs022
dbcn   31j 1 $ For MCNP6, E_min=30 MeV (default)
c dbcn   28j 1 2j 1 4j 10 $ For MCNP6, E_min=10 MeV (DBCN(37)=10)
```

The main difference of the current MCNP6 input files using the GENXS option for reactions induced by bremsstrahlung gammas from all the other examples we provided above is in the **DBCN** card. Let us address this point in detail here, as it is a new MCNP6 feature introduced

very recently by Dick Prael and is not documented anywhere yet. As we can see from our input files, the last card is **DBCN** (let us recall that the most detailed description of the MCNP6 **DBCN** input card is presented in the recent document by Grady Hughes [58], but this paper was written by Dr. Hughes before Dr. Prael introduced the very recent bremsstrahlung capability in MCNP6 using GENXS, therefore it was not described in [58]). So, the last two cards of the input file **bg4.5GeV_Nb_30CEM** are:

```
dbcn   28j 1 2j 1 $ For MCNP6, E_min=30 MeV (default)
c dbcn   28j 1 2j 1 4j 10 $ For MCNP6, E_min=10 MeV (DBCN(37)=10) .
```

On the **DBCN** card we have **1** for its 32nd parameter. The use of a **non-zero** value for the 32nd parameter of the **DBCN** card is the main instruction for MCNP6 **to calculate a reaction induced by bremsstrahlung gammas**. The maximum value of the energies of bremsstrahlung gammas, E^{max}, or, as it is often noted in the literature, E_0, is defined on the **SDEF** card:

```
sdef   erg=4500 par=p vec=1 0 0 dir=1 .
```

We see that is is equal to 4500 MeV, for this test-problem. The minimum energy for bremsstrahlung gammas is set in MCNP6 by default to be equal to $E_{min} = 30$ MeV (as is in our test-problem). But users can change the value of the E_{min}, providing the needed value (in MeV) as the value for the 37th parameter on the **DBCN** card. In our input file, we have a commented **DBCN** card where we chose the values of the minimum energy of bremsstrahlung gammas to be equal to 10 MeV: To calculate with this option, MCNP6 users need only to comment the first **DBCN** card in our input file and to uncomment the second one.

Finally, let us mention that the current version of MCNP6 with GENXS for bremsstrahlung induced reactions **allows only one isotope as the material of the problem**, in contrast to reactions induced by other types of projectiles, where we can have a complex material of several isotopes (see, *e.g.*, test-problem #10, where we use the GENXS option for a reaction induced by protons on a ^{nat}Ti target composed of 5 different isotopes).

The MCNP6 output files for cases with **DBCN(29)** equal to **1** and **0** are **bg4.5GeV_Nb_30CEM.o** and **bg4.5GeV_Nb_30CEM_0.o**, respectively, both presented in the Templates subdirectory **/VALIDATION_LAQGSM/Templates/LINUX/**; also presented are the MCTAL files for both cases, **bg4.5GeV_Nb_30CEM.m** and **bg4.5GeV_Nb_30CEM_0.m**. The mass distribution of all products is tabulated in units of barns in these output files in the table entitled "Summary by mass number:", located by the end of the output files.

Note that the MCNP6 results for reactions induced by bremsstrahlung photons are not normalized per "equivalent quanta". This is, in order to compare our MCNP6 results with the measured spectra we need to estimate separately the value of the "equivalent quanta", $Q =< E > /E_0$, or to use its value from other calculations. We have calculated this problem also with CEM03.03 used as a stand alone code, which provides the value of $Q = 0.1659986$ in its output. Here, while plotting our figure, we normalize the MCNP6 results to the value of the "equivalent quanta", $Q = 0.1659986$, as calculated by CEM03.03 for this reaction for bremsstrahlung photons with energies between $E_{min} = 30$ MeV and $E^{max} = 4500$ MeV.

To help plotting the MCNP6 results with **xmgrace** (see file bg4_5Nb_A_CEM_cor.pdf), the MCNP6 A-distributions of all products for cases with **DBCN(29)** equal to **1** and **0** are copied from the original output files in the separate files GENXS_CEM_non0_cor.dat and GENXS_CEM_=0.dat, respectively, provided in the subdirectory

/VALIDATION_CEM/Experimental_data/bg4.5GeV_Nb/. Let us note one more time that while plotting our figure, we have to divide the MCNP6 results by the value of the "equivalent quanta", $Q = 0.1659986$, as calculated by CEM03.03 for this reaction.

Besides the MCNP6 results, for comparison, we show here also our calculation by CEM03.03 used as a stand alone code (see file A_CEM.dat).

The file bg4_5Nb_A_CEM_cor.fig is a template for plotting our results with **xmgrace**. The pdf files of the figure is: bg4_5Nb_A_CEM_cor.pdf. Our final results for this test-problem are shown below in Fig. 19.

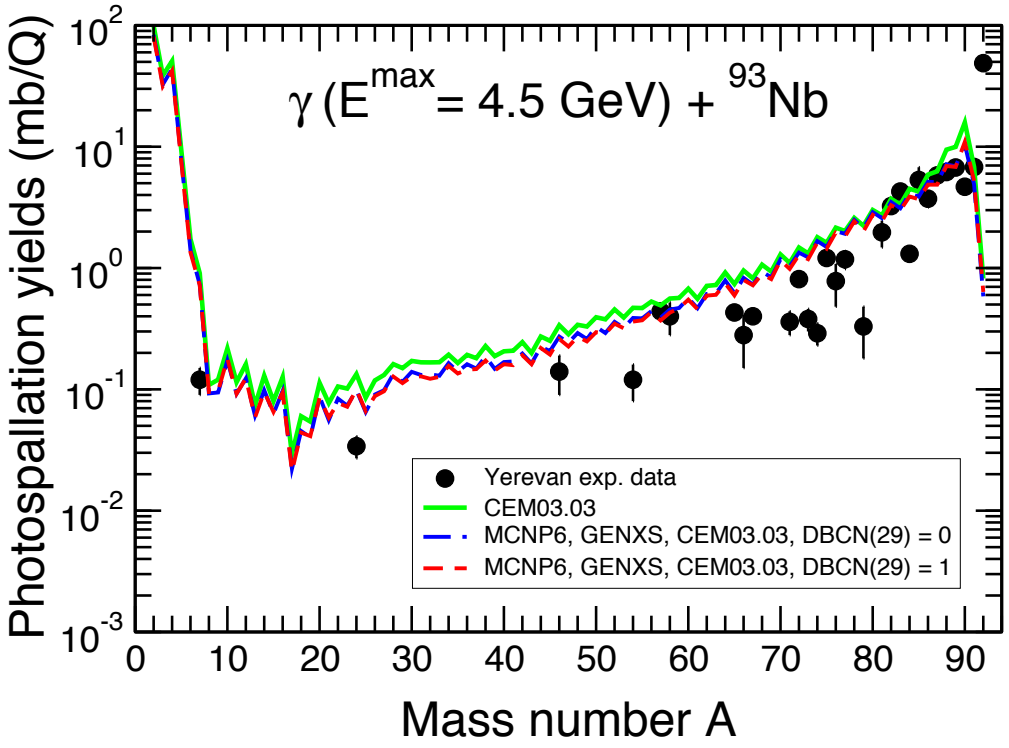

Figure 19: Comparison of measured [78] mass distribution of the nuclides produced by $E^{max} = 4.5$ GeV bremsstrahlung photons on ^{93}Nb with results by CEM03.03 used as a stand alone code and with calculations by MCNP6 using CEM03.03 with the GENXS option in two different ways: using for DBCN(29) the values of 0 and 1, as indicated.

From Fig. 19, we see very good agreement between the MCNP6 results obtained using the **GENXS** option for both cases of **DBCN(29)** equal to **1** and **0** with the calculations by CEM03.03 used as a stand alone code. We observe also reasonably good agreement of our results with the experimental data.

3.17. Test-problem #17: bg4.5GeVC_pi_CEM with inxs026

This MCNP6 problem is to test a very recent extension by Dick Prael of MCNP6 using the CEM03.03 event generator to describe double-differential spectra of particles produced in reactions induced by bremsstrahlung photons on thin targets. This capability of MCNP6 is needed to test the CEM03.03 and LAQGSM03.03 event-generators for this type of reaction.

Such reactions are of interest to several astrophysical and space applications, as well as for the Continuous Electron Beam Accelerator Facility (CEBAF) in Newport News, VA, upgraded recently to be able to accelerate electron beams to energies up to 12 GeV. In a way, this test-problem is a continuation of the previous test-problem #16, where MCNP6 with CEM03.03 was V&V'ed on a bremsstrahlung-induced reaction to study product yields, while here we investigate spectra of secondary particles.

This test calculates with MCNP6 using CEM03.03 spectra of protons at 30, 60, 90, 120, and 160 degrees from interactions of bremsstrahlung photons with energies from E_{min} = 30 MeV to E_0 = 4.5 GeV with a thin ^{12}C target. It compares the MCNP6 results with available experimental data and with results by the CEM03.03 event generator used as a stand alone code. Note that, to the best of our knowledge, the tested proton spectra at E_0 = 4.5 GeV represent actually examples of experimental proton spectra from reactions induced by bremsstrahlung gammas on nuclei with the highest energy as available in the literature by now (July 2011). That is, the current problem tests MCNP6 against measured proton spectra from reactions induced by bremsstrahlung gammas on nuclei with the highest maximum energy published so far in the literature.

The experimental data for this problem were measured at the Yerevan electron synchrotron of the Yerevan Physics Institute, Armenia, former USSR. The proton spectra are published in the paper [79].

Note that all the experimental characteristics for reactions induced by bremsstrahlung photons are usually normalized per "equivalent quanta", $Q =< E > /E_0$, where $< E >$ is the mean energy of the bremsstrahlung photons and E_0 is the "end-point" or the maximum energy of the bremsstrahlung photons E^{max}.

Experimental double-differential spectra of protons $d^2\sigma/dT/d\Omega/Q$ at 30, 60, 90, 120, and 160 degrees are presented in units of [μb/MeV/sr/Q] in the files p30e.dat, p60e.dat, p90e.dat, p120e.dat, and p160e.dat, respectively, in the subdirectory
/VALIDATION_CEM/Experimental_data/bg4.5GeV_C_p/ together with our results and final files with the figure for this test-problem.

We calculate with MCNP6 these spectra using the GENXS option. As we have presented a detailed description of the use of the GENXS option to calculate particle spectra from thin targets in test-problem #5, we do not need to discuss in detail the input and output files for this case. Therefore, we limit ourselves below to only providing the text of the input files (let us recall here again that the GENXS option of MCNP6 requires a second, auxiliary input file in addition to the main MCNP6 input file), as well as describing where to find the results in the MCNP6 output files.

The main MCNP6 input file for this test-problem is **bg4.5C_pi_CEM**. Its auxiliary companion required by the GENXS option is **inxs026**. Both of them are presented in the subdirectory **/VALIDATION_CEM/Inputs/** and are also shown below.

bg4.5GeVC_pi_CEM:

```
4.5 GeV max bremstrahlung on C12 particle calculation
c ------------------------------------------------------------
c Uses CEM and dbcn(29)/=0
c ------------------------------------------------------------
c Cells
c ------------------------------------------------------------
```

```
11  1  -18.7  -40
31  0           40

c ------------------------------------------------------------------
c Surfaces
c ------------------------------------------------------------------
40  so  1.

c ------------------------------------------------------------------
c Materials
c ------------------------------------------------------------------
m1     6012 1
c ------------------------------------------------------------------
c Source
c ------------------------------------------------------------------
sdef   erg=4500 par=p vec=1 0 0 dir=1
c ------------------------------------------------------------------
c Options
c ------------------------------------------------------------------
imp:p 1 0
mode p
lca    7j -1 1 $ First interaction only
mx1:p    model
phys:p 3j 1 $ Turn on photonuclear
c ------------------------------------------------------------------
c nps    1000
nps    1000000
prdmp  1000000 100000 1 2
tropt  genxs inxs026
dbcn   28j 1 2j 1 $ For MCNP6, E_min=30 MeV (default)
c dbcn   28j 1 2j 1 4j 10 $ For MCNP6, E_min=10 MeV (DBCN(37)=10)
```

inxs026:

```
4.5 GeV max bremstrahlung on C12 particle spectra calculation
1 0 1
Uses CEM and dbcn(29)/=1
150, -17, 4, 1000000.0/
   1.    3.    5.    7.    9.   11.   13.   15.   17.   19.
  22.   27.   32.   37.   42.   47.   52.   57.   62.   67.
  72.    77.    82.    87.    92.    97.   105.   125.   135.   145.
 155.   165.   175.   185.   195.   205.   215.   225.   235.   245.
 255.   265.   275.   285.   295.   305.   315.   325.   335.   345.
 355.   365.   375.   385.   395.   405.   415.   425.   435.   445.
 455.   465.   475.   485.   495.   505.   515.   525.   535.   545.
 555.   565.   575.   585.   595.   605.   615.   625.   635.   645.
 655.   665.   675.   685.   695.   705.   715.   725.   735.   745.
```

```
 755.   765.   775.   785.   795.   805.   815.   825.   835.   845.
 855.   865.   875.   885.   895.   905.   915.   925.   935.   945.
 955.   965.   975.   985.   995.  1025.  1075.  1125.  1175.  1225.
1275.  1325.  1375.  1425.  1475.  1525.  1575.  1625.  1675.  1725.
1775.  1825.  1875.  1925.  1975.  2025.  2075.  2125.  2175.  2225. /
165. 155. 145. 135. 125. 115. 95. 85. 75. 65. 55. 51. 41. 35. 25. 15. 0./
5, 6, 7, 21/
```

The main difference of the current MCNP6 input file using the GENXS option for reactions induced by bremsstrahlung gammas from all the other examples we provided above, except the previous test-problem # 16, is in the **DBCN** card. Let us address this point here again (though we discussed it already in test-problem # 16), as it is a new MCNP6 feature introduced very recently by Dick Prael and it is not documented yet. As we can see from our input file, the last card is **DBCN** (let us recall again that the most detailed description of the MCNP6 **DBCN** input card is presented in the recent document by Grady Hughes [58], but this paper was written by Dr. Hughes before Dr. Prael introduced the very recent bremsstrahlung capability in MCNP6 using GENXS; therefore, it was not described in [58]). So, the last two cards of the current input file **bg4.5GeVC_pi_CEM** are:

```
dbcn   28j 1 2j 1 $ For MCNP6, E_min=30 MeV (default)
c dbcn   28j 1 2j 1 4j 10 $ For MCNP6, E_min=10 MeV (DBCN(37)=10) .
```

On the **DBCN** card we have **1** for its 32nd parameter. The use of a **non-zero** value for the 32nd parameter of the **DBCN** card is the main instruction for MCNP6 **to calculate a reaction induced by bremsstrahlung gammas**. The maximum value of the energies of bremsstrahlung gammas, E^{max}, or, as it is often noted in the literature, E_0, is defined on the **SDEF** card:

```
sdef   erg=4500 par=p vec=1 0 0 dir=1 .
```

We see that is is equal to 4500 MeV, for this test-problem. The minimum energy for bremsstrahlung gammas is set in MCNP6 by default to be equal to $E_{min} = 30$ MeV (as is in our test-problem). But users can change the value of the E_{min}, providing the needed value (in MeV) as the value for the 37th parameter on the **DBCN** card. In our input file, we have a commented **DBCN** card where we chose the values of the minimum energy of bremsstrahlung gammas to be equal to 10 MeV: To calculate with this option, MCNP6 users need only to comment the first **DBCN** card in our input file and to uncomment the second one.

Finally, let us mention that the current version of MCNP6 with GENXS for bremsstrahlung induced reactions **allows only one isotope as the material of the problem**, in contrast to reactions induced by other types of projectiles, where we can have a complex material of several isotopes (see, *e.g.*, test-problem #10, where we use the GENXS option for a reaction induced by protons on a ^{nat}Ti target composed of 5 different isotopes).

Proton double-differential spectra calculated by MCNP6 using CEM03.03 with the GENXS option at 160, and 120 ($\pm$ 5) degrees are tabulated in units of [μb/sr/MeV] in the 2nd and 6th pairs of columns of the first part of the "proton production cross section" table of the MCNP6 output file **bg4.5C_pi_CEM.o** (after the proton energy tabulated in the 1st column); for 90 and 60 degrees, in the 1st and 4th pairs of columns of the second part of the same table, following the proton energy tabulated in the 1st column; and for 30 degrees, in the 1st pair of columns of the third part of the same table. We present the MCNP6 output file in the

subdirectory
/VALIDATION_CEM/Templates/LINUX/.

Let us mention here one more little detail, which makes this example a little different from all other previous test-problems of our Primer: We got the units of μb for the proton double-differential spectra $d^2\sigma/dT/d\Omega$ [μb/sr/MeV] in the MCNP6 output file due to the 4th parameter (entry) on the 4th line of our auxiliary INXC input file **inxs026**. By default, all MCNP6 results would be provided in barns, **i.e.**, without using **1000000.0** for the 4th parameter (entry) on the 4th line of our auxiliary INXC input file **inxs026**, we would get here our spectra in units of [b/sr/MeV]; this **1000000.0** multiples all our results by 10^6, converting the [b] to [μb] in the calculated proton spectra, just as the experimental spectra were published.

Finally, let us note that the MCNP6 results for reactions induced by bremsstrahlung photons are not normalized per "equivalent quanta". That is, in order to compare our MCNP6 results with the measured spectra we need to estimate separately the value of the "equivalent quanta", $Q =< E > /E_0$, or to use its value from other calculations. We have calculated our spectra also with the CEM03.03 used as a stand alone code; it provides the value of Q in its output file. Here, while plotting our figures, we divide the MCNP6 results by the value of the "equivalent quanta", $Q = 0.1341099$, as calculated by CEM03.03 for this reaction for bremsstrahlung photons with energies between $E_{min} = 30$ MeV and $E_{max} = (= E_0) = 4500$ MeV.

To help plotting the MCNP6 proton spectra with **xmgrace** (see file gb4_5C_p_CEM.pdf), the MCNP6 double-differential spectra are copied from the original MCNP6 output file in separate files p30_M6CEM.dat, p60_M6CEM.dat, p90_M6CEM.dat, p120_M6CEM.dat, and p160_M6CEM.dat, respectively, provided in the subdirectory
/VALIDATION_CEM/Experimental_data/bg4.5GeV_Nb/.

Let us recall one more time that while plotting our figures, we normalize the MCNP6 results to, i.e., we divide by the value of the "equivalent quanta", $Q = 0.1341099$, as calculated by CEM03.03 for this reaction.

Besides the MCNP6 results, for comparison, we show also calculations by CEM03.03 used as a stand alone code. Spectra of protons by CEM03.03 used as a stand alone code at 30, 60, 90, 120, and 160 degrees are presented here in the files: p30c.dat, p60c.dat, p90c.dat, p120c.dat, and p160c.dat, respectively.

The file gb4_5C_p_CEM.fig is a template for plotting the proton spectra with **xmgrace**. The pdf files of the figure with these spectra is gb4_5C_p_CEM.pdf. It is shown below in Fig. 20.

From Fig. 20, we see good agreement between the MCNP6 results obtained using the **GENXS** option with the CEM03.03 event generator and the calculations by CEM03.03 used as a stand alone code, for all proton spectra from this reaction induced by bremsstrahlung photons. A little smaller absolute values on the MCNP6 spectra in comparison with the results by CEM03.03 used as a stand alone code is due to different approximations for the normalization of the total photonuclear cross sections used by MCNP6 and by CEM03.03 used as a stand alone code. We observe also very good agreement of our results with the experimental data.

3.18. Test-problem #18: n1000Bi_CEM with inxs96

This problem is to test how MCNP6 with the CEM03.03 event-generator describes neutron-induced fission cross section of subactinide nuclei.

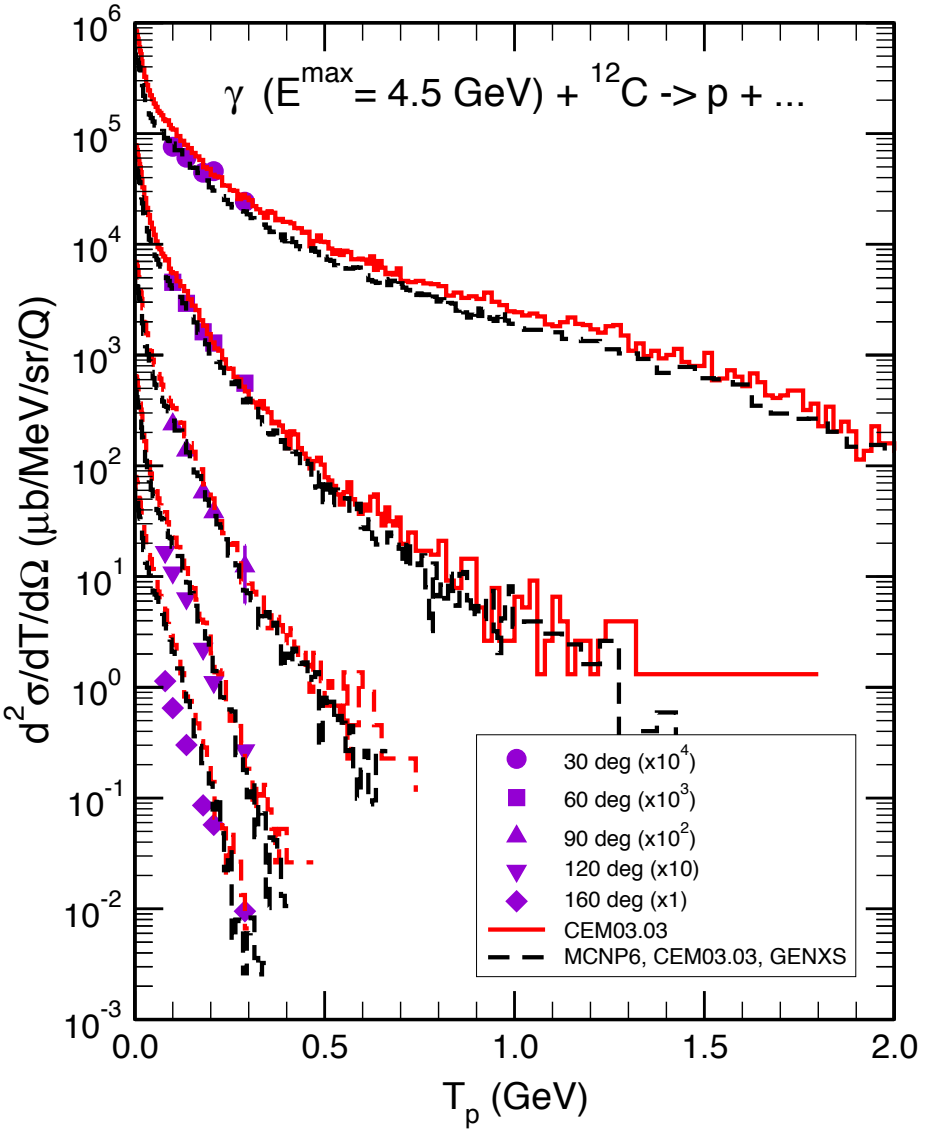

Figure 20: Experimental [79] double-differential spectra of protons at 30, 60, 90, 120, and 150 degrees from interactions of $E^{max} = 4.5$ GeV bremsstrahlung photons with ^{12}C compared with results by CEM03.03 used as a stand alone code and with MCNP6 calculation using CEM03.03 and the GENXS option, as indicated.

To be exact, this test-problem calculates with MCNP6, using CEM03.03, neutron-induced fission cross section of ^{209}Bi at energies from 20 MeV to 1 GeV and compares the results with predictions by CEM03.03 used as stand alone code and with available experimental data. Such reactions are of interest for different current applications, for instance, at Accelerator Driven Systems (ADS), as ^{209}Bi is considered as one of the main possible materials of the spallation targets. Another application of ^{209}Bi is in neutron fluence monitors.

For this problem, we use two sets of experimental data: 1) The fission cross section measured very recently by the n_TOF Collaboration (www.cern.ch/ntof) at the neutron Time-Of-Flight (n_TOF) facility at CERN and published in the paper [80]; numerical values of fission cross sections from this paper are presented here in the file n_TOF_PRC.dat of the subdirectory **/VALIDATION_CEM/Experimental_data/nBi_fiss/**. 2) The data measured several years ago at the spallation neutron source of PNPI, Gatchina, Russia by the Group of A. V. Fomichev

from the V. G. Khlopin Radium Institute, St.-Petersburg, Russia and published in the paper [81]; experimental data measured by the Group of Alexander Fomichev are presented in the file Fomichev.data, in the same subdirectory, together with our results and files for the final figure of this test-problem.

The easiest way to calculate an "excitation function" of a fission cross section with MCNP6 is to use the GENXS option for a single incident energy of neutrons; then, to perform as many calculations as needed changing only the neutron energy on the **SDEF** card of the MCNP6 input. As all inputs at different neutron energies are exactly the same, with the only difference in the neutron energy on the **SDEF** card, we present here only one example of MCNP6 input at output, at $T_n = 1$ GeV. The input file for this example is **n1000Bi_CEM**. Let us recall that the GENXS option of MCNP6 requires a second, auxiliary, input file. For this example, it is **inxs96**. Both of them are presented in the subdirectory **/VALIDATION_CEM/Inputs/** and are also shown below.

n1000Bi_CEM:

```
MCNP6 test: n + Bi -> fission cross section by CEM03.03 at 1000 MeV, nevtype=66
C To evaluate how MCNP6 with CEM describes preactinide fission cross sections
  1  1  1.0   -1 2 -3
  2  0        -4 (1:-2:3)
  3  0         4

c ------------------------------------------------------------
  1  cz  4.0
  2  pz  -1.0
  3  pz  1.0
  4  so  50.0

c ------------------------------------------------------------
  m1 83209 1.0
  sdef erg = 1000 par = n dir = 1 pos = 0 0 0 vec 0 0 1
  imp:n 1 1 0
  phys:n 1010
  mode   n
LCA  8j 1    $ use CEM03.03, nevtype = 66                    !!!
  tropt genxs inxs96  nreact on  nescat off
c ------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 100000
  prdmp 2j -1
```

inxs96:

```
MCNP6 test: n + Bi -> fission cross section by CEM03.03 at 800 MeV, nevtype=66
0 0 1 /
Cross Section Edit
```

```
0 0 0 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
1 5 6 7 8 21 22 23 24 /
```

The output file for this example is **n1000Bi_CEM.o**, presented in the subdirectory **/VALIDATION_CEM/Templates/LINUX/**. The fission cross section is printed in the output file in barns, two lines before the table with residual nuclei yields, as shown below.

```
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
                    nonelastic cross section   =  1.90610E+00 0.0000
                         fission cross section =  1.47094E-01 0.0109
                         fission/nonelastic    =  7.71700E-02

                    elastic cross section      =  0.00000E+00 0.0000


1 Distribution of residual nuclei:
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```

For comparison, we present in the file CEM0303.dat of the subdirectory **/VALIDATION_CEM/Experimental_data/nBi_fiss/** results by CEM03.03 used as a stand alone code.

The file nBi_fiss-xsecPRC.fig is a template for plotting with **xmgrace** the fission cross section n(Bi,f) for all incident energies of neutrons we calculated here. The pdf file for the figure is nBi_fiss-xsecPRC.pdf. It is shown below in Fig. 21.

From Fig. 21, we see good agreement between the MCNP6 results obtained using the **GENXS** option with the CEM03.03 event generator and the calculations by CEM03.03 used as a stand alone code, for the neutron-induced fission cross section of ^{209}Bi in a large range of incident energy, from threshold to 1 GeV. A little difference in the values on the MCNP6 fission cross section at some energies in comparison with the results by CEM03.03 used as a stand alone code is due to different approximations for the normalization of the total reaction (inelastic) cross sections used by MCNP6 and by CEM03.03 used as a stand alone code. We observe also good agreement of our results with both experimental sets of measured data.

4. Conclusion

MCNP6, the latest and most advanced LANL Monte Carlo transport code representing a recent merger of MCNP5 and MCNPX, has been validated and verified against a variety of intermediate and high-energy experimental data and against calculations by different versions of MCNPX and results by several other codes. In the present primer, we show 18 examples of test-problems for MCNP6 using mostly the latest modifications of the Cascade-Exciton Model (CEM) event-generator, CEM03.03. Other 18 text-problems for the MCNP6 with the Los Alamos version of the Quark-Gluon String Model (LAQGSM) event-generator LAQGSM03.03 are presented in a separate, second primer of this series [5].

We found that MCNP6 describes reasonably well various reactions induced by particles (and heavy-ions, as can be seen in Refs. [5, 20]) at incident energies from 18 MeV to about 1 TeV/nucleon measured on both thin and thick targets and agrees very well with similar results

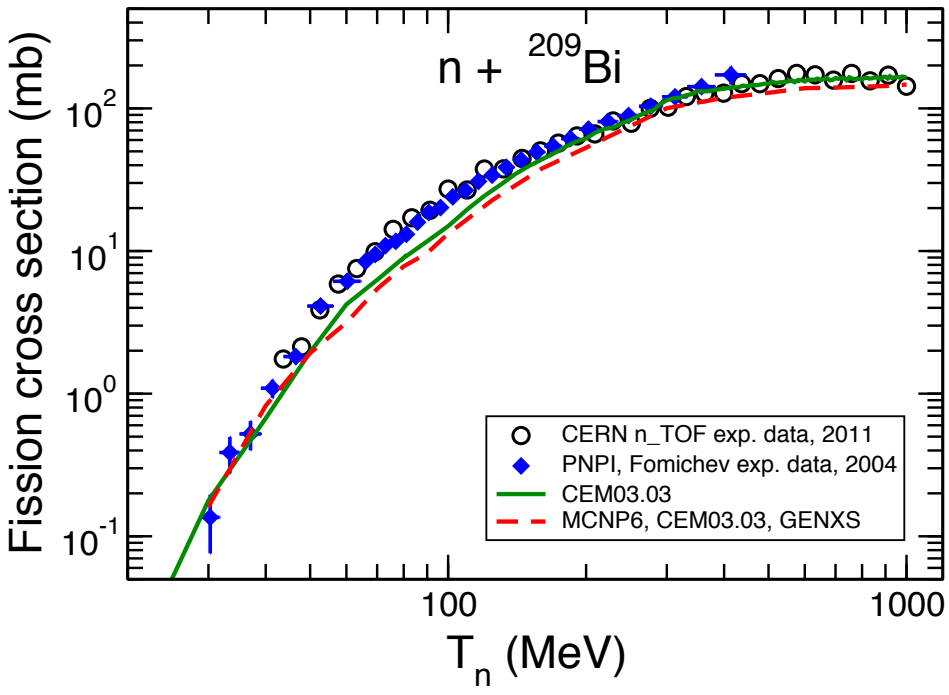

Figure 21: Experimental [80, 81] neutron-induced fission cross section of ^{209}Bi compared with results by CEM03.03 used as a stand alone code and with MCNP6 calculations using CEM03.03 and the GENXS option, as indicated.

obtained with MCNPX and calculations by other codes. Most of several computational bugs and more serious physics problems observed in MCNP6/X during our V&V have been fixed. We continue our work to solve all the known problems before the official distribution of MCNP6 to the public via RSICC at Oak Ridge, TN, USA planned for the year 2011. From the results presented here as well as in Refs. [5, 20], we can conclude that MCNP6 is a reliable and useful Monte Carlo transport code for different applications involving reactions induced by almost all types of elementary particles and heavy-ions, in a very broad range of incident energies. We hope that the current primer will help future users of MCNP6 construct their input files and better understand the final MCNP6 results for their applications at intermediate and high energies.

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