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V&V of MCNP 6.1.1 Beta Against Intermediate and High-Energy Experimental Data

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Abstract

This report presents a set of validation and verification (V&V) MCNP 6.1.1 beta results calculated in parallel, with MPI, obtained using its event generators at intermediate and high-energies compared against various experimental data. It also contains several examples of results using the models at energies below 150 MeV, down to 10 MeV, where data libraries are normally used. This report can be considered as the forth part of a set of MCNP6 Testing Primers, after its first, LA-UR-11-05129, and second, LA-UR-11-05627, and third, LA-UR-26944, publications, but is devoted to V&V with the latest, 1.1 beta version of MCNP6. The MCNP6 test-problems discussed here are presented in the **/VALIDATION_CEM/** and **/VALIDATION_LAQGSM/** subdirectories in the MCNP6 **/Testing/** directory. 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. Several technical "bugs" in MCNP 6.1.1 beta were discovered during our current V&V of MCNP6 while running it in parallel with MPI using its event generators. These "bugs" are to be fixed in the following version of MCNP6. Our results show that MCNP 6.1.1 beta using its CEM03.03, LAQGSM03.03, Bertini, and INCL+ABLA, event generators describes, as a rule, reasonably well different intermediate- and high-energy measured data. This primer isn't meant to be read from cover to cover. Readers may skip some sections and go directly to any test problem in which they are interested.

September 2014

Contents

1. Introduction

During the past several years, a major effort has been undertaken at the Los Alamos National Laboratory (LANL) to develop the transport code MCNP6 [1, 2], the latest and most advanced LANL Monte Carlo transport code produced by the XCP-3 and NEN-5 LANL Groups.

This report presents a set of Validation and Verification (V&V) test problems calculated in parallel, with MPI, with the latest version of MCNP6, MCNP 6.1.1 beta [3], using its event generators at intermediate and high-energies. It also contains several examples of results using the event generators at energies below 150 MeV, down to 10 MeV, where data libraries are normally used.

This report can be considered as the forth part of a set of MCNP6 Testing Primers at intermediate and high energies, after its first [4], second [5], and third [6], publications. It is devoted to V&V only of the latest, 1.1 beta version, of MCNP6 [3]. Part of the results presented here were discussed in more detail in our recent paper [7]. True, in Ref. [7], this was done mostly from a physical point of view, without addressing any MCNP6 input and output files and running of MCNP6 with MPI.

The MCNP6 test problems discussed here are presented in the **/VALIDATION_CEM/** and **/VALIDATION_LAQGSM/** subdirectories in the MCNP6 **/Testing/** directory.

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. Several technical "bugs" in MCNP 6.1.1 beta were discovered during our current V&V of MCNP6, while running it in parallel with MPI using its event generators. These "bugs" are to be fixed in the following version of MCNP6. Our results show that MCNP 6.1.1 beta using its CEM03.03, LAQGSM03.03, Bertini, and INCL+ABLA, event generators describes, as a rule, reasonably well different intermediate- and high-energy measured data.

2. Testing CEM, Bertini, and INCL+ABLA

All the test problems discussed in this Section are presented in the **VALIDATION_CEM** subdirectory in the basic **/MCNP6/Testing/** directory.

2.1. p + ^{14}N Excitation Functions

This MCNP6 problem is to test the applicability of MCNP6 using the CEM03.03 event generator to describe excitation functions from the fragmentation of ^{14}N bombarded with protons from 10 MeV up to 5 GeV and to compare the results with available experimental data and with calculations by CEM03.03 used as a stand-alone code [8, 9] with two modifications of its Fermi break-up model, as described in Ref. [7].

Fragmentation reactions induced by protons and light nuclei of energies around 1 GeV/nucleon and below on light target nuclei are involved in different applications, like cosmic-ray-induced single event upsets (SEUs), radiation protection, and cancer therapy with proton and ion beams, among others. It is impossible to measure all nuclear data needed for such applications; therefore, Monte Carlo transport codes are normally used to simulate impacts associated with fragmentation reactions. It is important that available transport codes simulate such reactions as well as possible.

Note that prediction of cross sections of arbitrary products as functions of the incident energy of the projectiles initiating the reactions, i.e., of excitation functions, is one of the most difficult tasks for any theoretical model/code.

Experimental data for this test problem were published by many authors in different publications; detailed references to all measured data we use here can be found in our recent paper [7].

We calculated the reactions studied in this test problem with MCNP6, using its GENXS option [10], in parallel, with MPI, using 8 nodes, 64 processors, on the "Moonlight" LANL supercomputer, for the incident proton energies of 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 2000, 3000, 4000, and 5000 MeV. As the MCNP6 input files at all these incident energies differ only in their SDEF card, in the value of the input parameter ERG (i.e., the proton incident energy, in MeV), we present here only one example of the MCNP6 input and output files, at 1000 MeV. The main MCNP6 input file at 1000 MeV is p1000_N14.CEM. For the second input files required by the GENXS option we use the same file, inxc96, at all incident energies listed above. Both p1000_N14.CEM and inxc96 input files are presented in subdirectory */VALIDATION_CEM/Inputs/.

Below, we provide both p1000_N14.CEM and inxc96 MCNP6 input files used for this test problem.

p1000_N14.CEM:

```
MCNP6 test: p + N14 by CEM03.03 at 1000 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   07014 1.0
  sdef erg = 1000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 5001
  mode   h
LCA  8j 1    $ use CEM03.03, nevtype = 66                 !!!
  tropt genxs inxc96  nreact on  nescat off
c -------------------------------------------------------------
  print 40 110 95
c  nps 10000
  nps 1000000
c  prdmp 2j -1
```

inxc96:

```
MCNP6 test: p + Ta181 by CEM03.03, nevtype=66
0 0 1 /
Cross Section Edit
0 0 9 /
1 5 6 7 8 21 22 23 24 /
```

In the current test problem, we compare the MCNP6 results for the p+^{14}N reaction with available data and with calculations by CEM03.03 used as a stand alone code for the total inelastic cross section and for excitation functions for the production of ^{14}O, ^{13}N, ^{12}N, ^{13}C, ^{12}C, ^{11}C, ^{10}C, ^{11}B, ^{10}B, ^{10}Be, ^{9}Be, ^{7}Be, ^{9}Li, ^{8}Li, and t. The MCNP6 cross sections for the production of different isotopes are printed (in barns) in the corresponding portion of the table entitled "Distribution of residual nuclei" of the output file p1000_N14.CEM.mpi.o presented in the subdirectory */VALIDATION_CEM/Templates/LINUX/. The total inelastic cross section calculated by MCNP6 is printed in its output file just several lines higher, in the table entitled "nonelastic cross section". To help plotting all these results with xmgrace, we copy the MCNP6 values obtained at different incident proton energies into separate files.

To save space, we do not show here explicitly files with MCNP6 results for the total p+^{14}N inelastic cross sections and for the production of ^{14}O, ^{13}N, ^{12}N, ^{13}C, ^{12}C, ^{11}C, ^{10}C, ^{11}B, ^{10}B, ^{10}Be, ^{9}Be, ^{7}Be, ^{9}Li, ^{8}Li, and t, as their values are included in the provided templates for the xmgrace figures we use to plot our results. Templates to plot with xmgrace the total p+^{14}N inelastic cross sections and cross sections for the production of ^{14}O, ^{13}N, ^{12}N, ^{13}C, ^{12}C, ^{11}C, ^{10}C, ^{11}B, ^{10}B, ^{10}Be, ^{9}Be, ^{7}Be, ^{9}Li, ^{8}Li, and t are presented in files sig_in.fig, and O14.fig, N13.fig, N12.fig, C13.fig, C12.fig, C11.fig, C10.fig, B11.fig, B10.fig, Be10.fig, Be9.fig, Be7.fig, Li9.fig, Li8.fig, and t.fig, respectively, all shown in subdirectory */VALIDATION_CEM/Experimental_data/pN14/. These xmgrace files contain also all the experimental data as well as the results by CEM03.03 used as a stand alone code. Useful details and discussion of all these data and calculation results can be found in the listed above Ref. [7].

Postscript files generated by xmgrace for all our plots were generated in files with similar names, simply using in their names extensions "ps" instead of "fig".

To ease an overview of all our results, we provide two summary files pN14_1.pdf and pN14_2.pdf which show cross sections for all products studied here (see Figs. 1 and 2). These summary pdf files were produced with the LaTeX files pN14_1.tex and pN14_2.tex using the listed above postscript files as input.

The first thing to note is that the total reaction cross sections simulated with MCNP6 and shown in the upper-left plot in Fig. 1 with small solid circles agree well with the available experimental data (symbols) and with calculations by CEM03.03 used as a stand-alone code (solid line). There is a difference between the models, especially in the regions of incident proton energies $T_p = 50 - 100$ MeV and $T_p \geq 2$ GeV. To be expected, since MCNP6 and CEM03.03 use very similar, but slightly different approximations for the total proton-nucleus reaction cross sections (see details and references in [1, 8, 9]). These little differences in the total reaction cross sections will produce, respectively, similar differences in all excitation functions simulated with MCNP6 and CEM03.03.

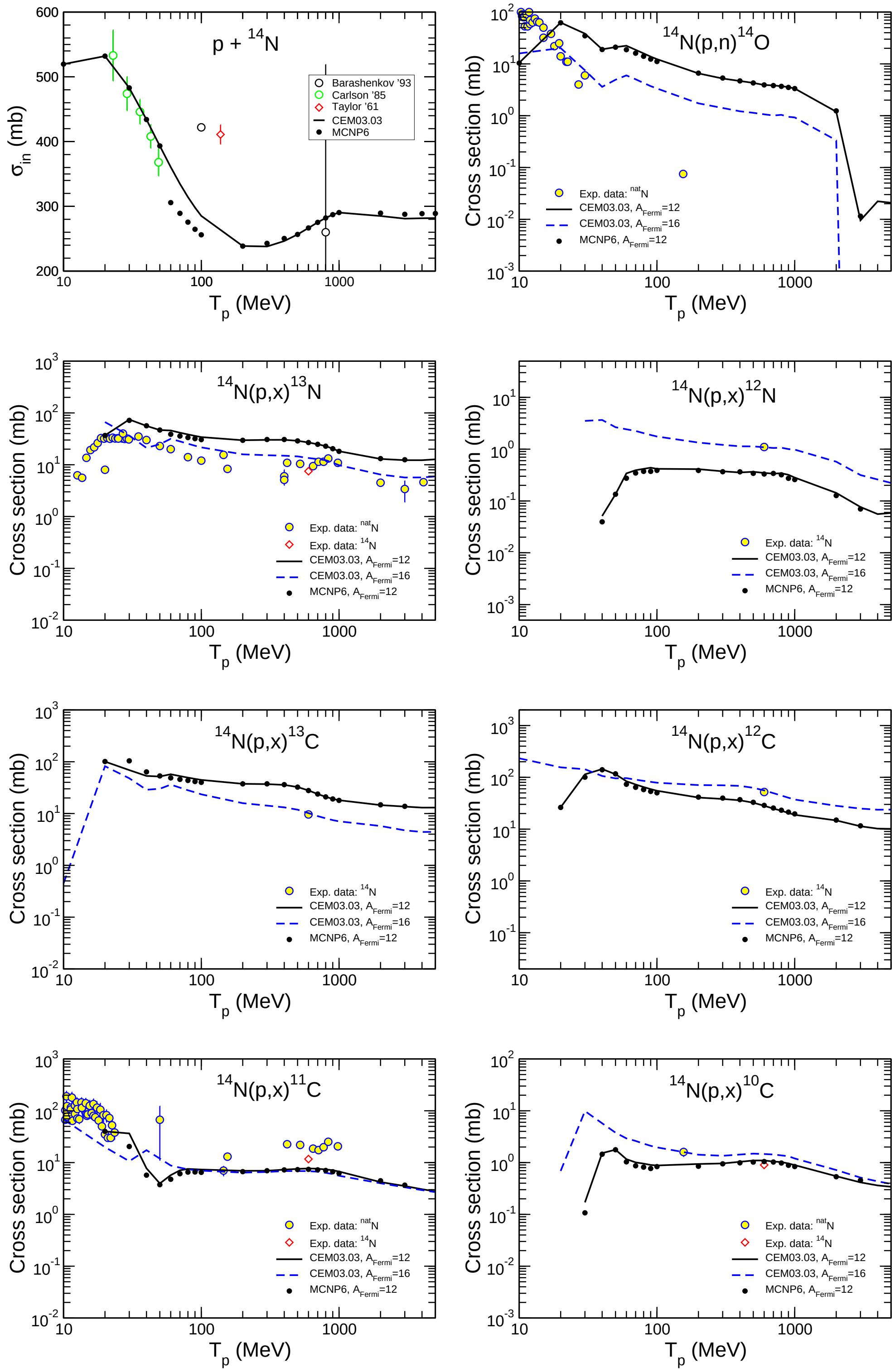


Figure 1: Total inelastic cross sections and excitation functions for the production of ^{14}O, ^{13}N, ^{12}N, ^{13}C, ^{12}C, ^{11}C, and ^{10}C from p + ^{14}N calculated with CEM03.03 using the "standard" version of the Fermi break-up model ($A_{Fermi} = 12$; solid black lines; see details in Ref. [7]) and with a cut-off value of 16 for A_{Fermi} (dashed blue lines), as well as with MCNP6 using CEM03.03 ($A_{Fermi} = 12$; small solid black circles) compared with experimental data. Experimental data for inelastic cross sections are from Refs. [11]-[13], while the data for excitation functions are from the T16 Lib compilation [14].

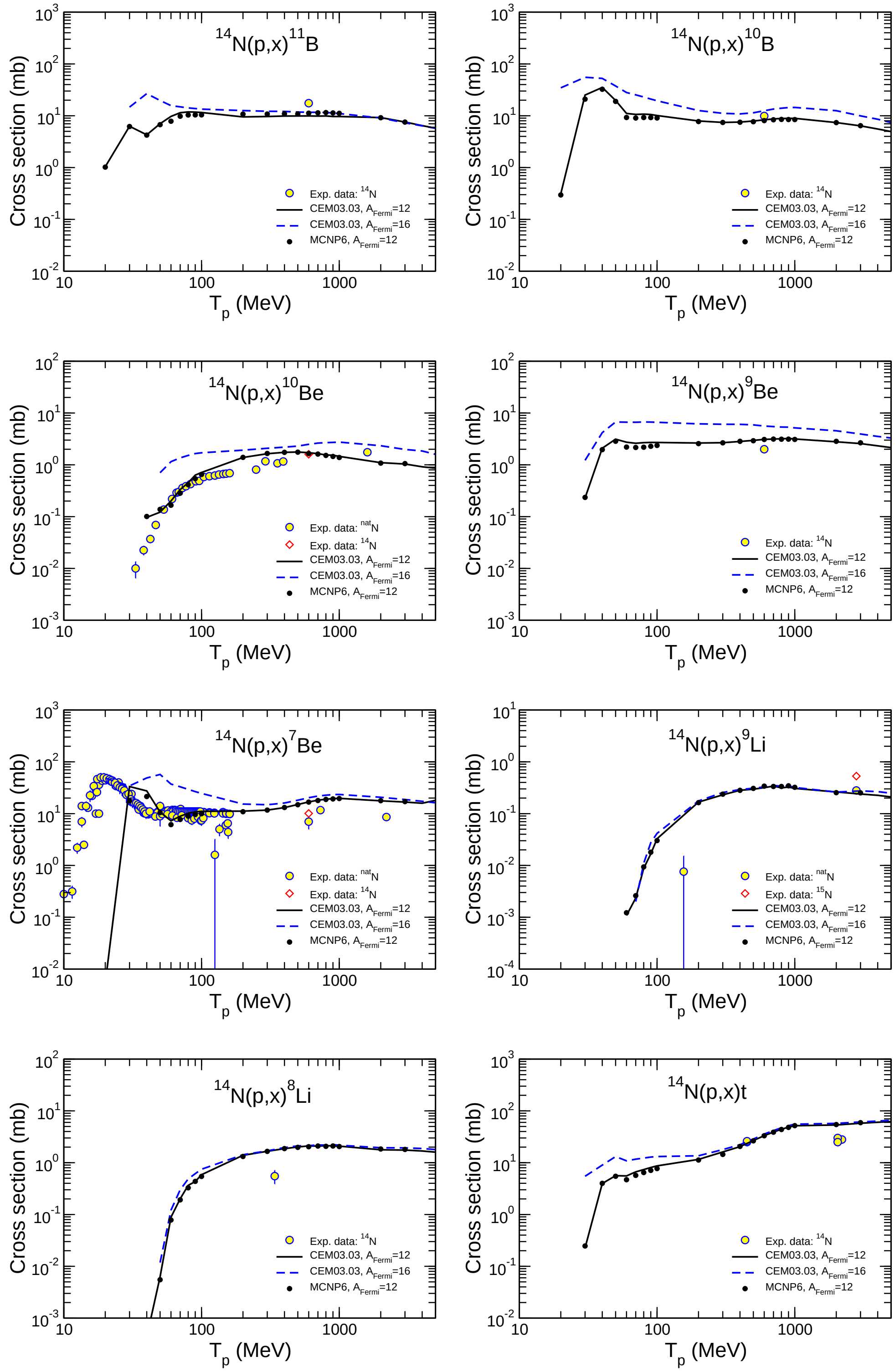


Figure 2: Excitation functions for the production of ^{11}B, ^{10}B, ^{10}Be, ^{9}Be, ^{7}Be, ^{9}Li, ^{8}Li, and t from p + ^{14}N calculated with CEM03.03 using the "standard" version of the Fermi breakup model ($A_{Fermi} = 12$; solid black lines) and with a cut-off value of 16 for A_{Fermi} (dashed blue lines), as well as with MCNP6 using CEM03.03 ($A_{Fermi} = 12$; small solid black circles) compared with experimental data. Experimental data are from the T16 Lib compilation [14].

The total reaction cross sections are based on systematics (see details and references in [1, 8]), therefore they do not depend on the value of A_{Fermi} we use in our calculations (see details about A_{Fermi} in Ref. [7]). However, we performed calculations of all excitation functions shown in Figs. 1 and 2 with CEM03.03 used as a stand-alone code with its "default value" $A_{Fermi} = 12$, as well as with a modification of the code using $A_{Fermi} = 16$, which in case of these p + ^{14}N reactions, actually corresponds to $A_{Fermi} = 14$: We cannot get a mass number A = 16 from p + ^{14}N interactions, and even a nucleus with $A = 15$ would not be produced by the INC of CEM03.03 at these intermediate energies.

First, from the results presented in Figs. 1 and 2, we see a very good agreement between the excitation functions simulated by MCNP6 using CEM03.03 and calculations by CEM03.03 used as a stand-alone code. We also can see a reasonable agreement with most of the available experimental data. This fact shows no problems with the implementation of CEM03.03 in MCNP6 or with the simulations of these reactions by either code.

Second, we'd like to explicitly inform the readers that we do not worry too much about some observed discrepancies between some calculated excitation functions and measured data at low energies, below 20 MeV. As default, MCNP6 uses data libraries at such low energies and never uses CEM03.03 or its other event generators, if data libraries are available (MCNP6 has proton-induced data libraries for the reactions studied here). By contrast, CEM uses its INC to simulate the first stage of nuclear reactions, and the INC is not supposed to work properly at such low energies (see details in [1, 8]).

Third, results calculated both with $A_{Fermi} = 12$ and 16 agree reasonably well with available data, taking into account that all calculations, at all energies and for all reactions were done with the fixed version of our codes, without any tuning or changing of any parameters. However, in some cases, we can observe significant differences between excitation functions calculated with $A_{Fermi} = 12$ and 16.

For this particular reaction, the excitation functions for the production of ^{14}O, ^{13}N, ^{12}N, ^{13}C, ^{12}C, and ^{10}C calculated with $A_{Fermi} = 16$ (that for our p + ^{14}N reaction is the same as $A_{Fermi} = 14$, which from a physical point of view means that we use only Fermi breakup after INC and never use preequilibrium and/or evaporation models to calculate this reaction) agree better with available experimental data than results obtained with $A_{Fermi} = 12$. On the other hand, excitation functions for the production of ^{9}Be and ^{7}Be are reproduced better with $A_{Fermi} = 12$.

2.2. p + ^{16}O Excitation Functions

This MCNP6 problem is to test the applicability of MCNP6 using the CEM03.03 event generator to describe excitation functions from the fragmentation of ^{16}O bombarded with protons from 10 MeV up to 5 GeV and to compare the results with available experimental data and with calculations by CEM03.03 used as a stand-alone code with three modifications of its Fermi break-up model, as described in Ref. [7]. This test problem is somehow similar to the previous problem, # 24. But it is for another target nucleus, studies excitation functions of many final products not covered by problem #24, and involves an additional modification of the Fermi break-up model of CEM.

Fragmentation reactions induced by protons and light nuclei of energies around 1 GeV/nucleon and below on light target nuclei are involved in different applications, like cosmic-ray-induced single event upsets (SEUs), radiation protection, and cancer therapy with proton and ion beams, among others. It is impossible to measure all nuclear data needed for such applications;

therefore, Monte Carlo transport codes are usually used to simulate impacts associated with fragmentation reactions. It is important that available transport codes simulate such reactions as well as possible.

Note that prediction of cross sections of arbitrary products as functions of the incident energy of the projectiles initiating the reactions, i.e., of excitation functions, is one of the most difficult tasks for any theoretical model/code.

Experimental data for this test problem were published by many authors in different publications; detailed references to all measured data we use here can be found in the paper [7] and references therein.

We calculated the reactions studied in this test problem with MCNP6, using its GENXS option, in parallel, with MPI, using 8 nodes, 64 processors, on the "Moonlight" LANL supercomputer, for the incident proton energies of 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 2000, 3000, 4000, and 5000 MeV. As the MCNP6 input files at all these incident energies differ only in their SDEF card, in the value of the input parameter ERG (i.e., the proton incident energy, in MeV), we present here only one example of the MCNP6 input and output files, at 1000 MeV. The main MCNP6 input file at 1000 MeV is p1000_O16.CEM. For the second input files required by the GENXS option we use the same file, inxc96, at all incident energies listed above. Our p1000_O16.CEM and inxc96 input files are presented in subdirectory */VALIDATION_CEM/Inputs/.

Below, we provide both p1000_O16.CEM and inxc96 MCNP6 input files used for this test problem.

p1000_O16.CEM:

```
MCNP6 test: p + O16 by CEM03.03 at 1000 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   08016 1.0
  sdef erg = 1000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 5001
  mode   h
LCA  8j 1    $ use CEM03.03, nevtype = 66                  !!!
  tropt genxs inxc96  nreact on  nescat off
c ---------------------------------------------------------------
  print 40 110 95
c  nps 10000
  nps 1000000
```

```
c  prdmp 2j -1
```

inxc96:

```
MCNP6 test: p + Ta181 by CEM03.03, nevtype=66
0 0 1 /
Cross Section Edit
0 0 9 /
1 5 6 7 8 21 22 23 24 /
```

In the current test problem, we compare the MCNP6 results for the p+^{16}O reaction with available data and with calculations by CEM03.03 used as a stand alone code for the total inelastic cross section and for excitation functions for the production of ^{15}O, ^{14}O, ^{13}N, ^{14}C, ^{11}C, ^{10}C, ^{11}B, ^{10}B, ^{10}Be, ^{9}Be, ^{7}Be, ^{9}Li, ^{7}Li, ^{6}Li, and t. The MCNP6 cross sections for the production of different isotopes are printed (in barns) in the corresponding portion of the table entitled "Distribution of residual nuclei" of the output file p1000_O16.CEM.mpi.o presented in the subdirectory */VALIDATION_CEM/Templates/LINUX/. The total inelastic cross section calculated by MCNP6 is printed in its output file just several lines higher, in the table entitled "nonelastic cross section". To help plotting all these results with xmgrace, we copy the MCNP6 values obtained at different incident proton energies into separate files.

To save space, we do not show here explicitly files with MCNP6 results for the total p+^{16}O inelastic cross sections and for the production of ^{15}O, ^{14}O, ^{13}N, ^{14}C, ^{11}C, ^{10}C, ^{11}B, ^{10}B, ^{10}Be, ^{9}Be, ^{7}Be, ^{9}Li, ^{7}Li, ^{6}Li, and t, as their values are included in the provided templates for the xmgrace figures we use to plot our results. Templates to plot with xmgrace the total p+^{16}O inelastic cross sections and cross sections for the production of ^{15}O, ^{14}O, ^{13}N, ^{14}C, ^{11}C, ^{10}C, ^{11}B, ^{10}B, ^{10}Be, ^{9}Be, ^{7}Be, ^{9}Li, ^{7}Li, ^{6}Li, and t are presented in files sig_in.fig, and O15.fig, O14.fig, N13.fig, C14.fig, C11.fig, C10.fig, B11.fig, B10.fig, Be10.fig, Be9.fig, Be7.fig, Li9.fig, Li7.fig, Li6.fig, and t.fig, respectively, all shown in subdirectory */VALIDATION_CEM/Experimental_data/pO16/. These xmgrace files contain also all the experimental data as well as the results by CEM03.03 used as a stand alone code. Useful details and discussion of all these data and calculation results can be found in the listed above paper [7].

Postscript files generated by xmgrace for all our plots were generated in files with similar names, simply using in their names extensions "ps" instead of "fig".

To ease an overview of all our results, we provide two summary files pO16_1.pdf and pO16_2.pdf which shows cross sections for all products studied here (see Figs. 3 and 4). These summary pdf files were produced with the LaTeX files pO16_1.tex and pO16_2.tex using the listed above postscript files as input.

Note that most of the experimental data for these reactions were measured on ^{nat}O, with only a few data points obtained for ^{16}O; all our calculations were performed for ^{16}O. For these reactions, we performed three sets of calculations, using $A_{Fermi} = 12$, 14, and 16 in CEM03.03 (see details in Ref. [7]). The general agreement/disagreement of our results with available measured data for oxygen is very similar to what we showed above for p + ^{14}N, with the major difference that almost all products from oxygen are better predicted with $A_{Fermi} = 14$; production of ^{11}B is described a little better with $A_{Fermi} = 16$, while ^{9}Be and ^{7}Be are reproduced better with $A_{Fermi} = 12$, just as for nitrogen (see Figs. 1 and 2).

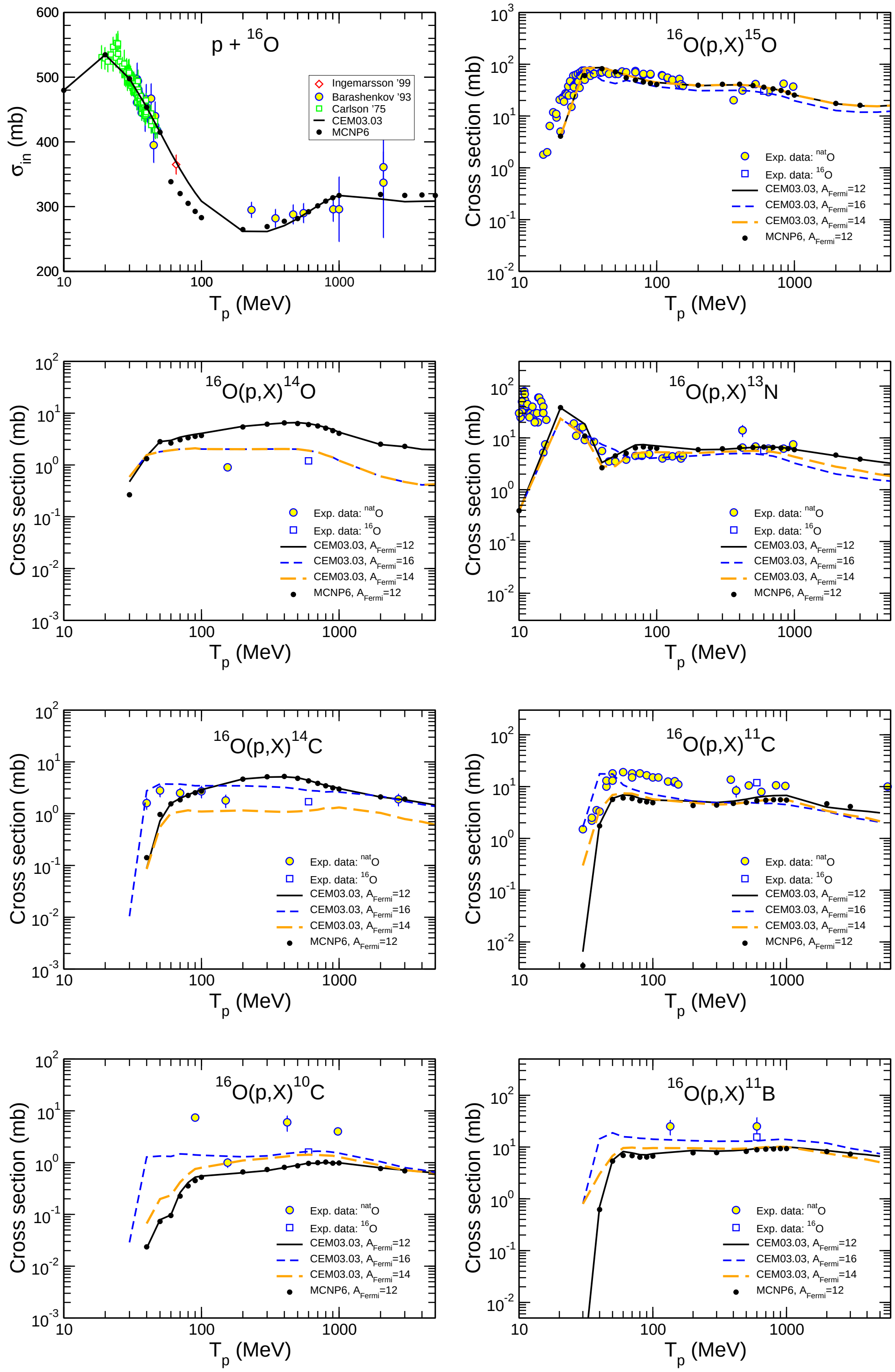


Figure 3: Total inelastic cross section and excitation functions for the production of ^{15}O, ^{14}O, ^{13}N, ^{14}C, ^{11}C, ^{10}C, and ^{11}B from p + ^{16}O calculated with CEM03.03 using the "standard" version of the Fermi break-up model (A_{Fermi} = 12; solid black lines) and with cup-off values for A_{Fermi} of 16 (dashed blue lines) and 14 (long-dashed orange lines), as well as with MCNP6 using CEM03.03 (A_{Fermi} = 12; small solid black circles) compared with experimental data. Experimental data for inelastic cross sections are from Refs. [11, 15, 16] while the data for excitation functions are from the T16 Lib compilation [14].

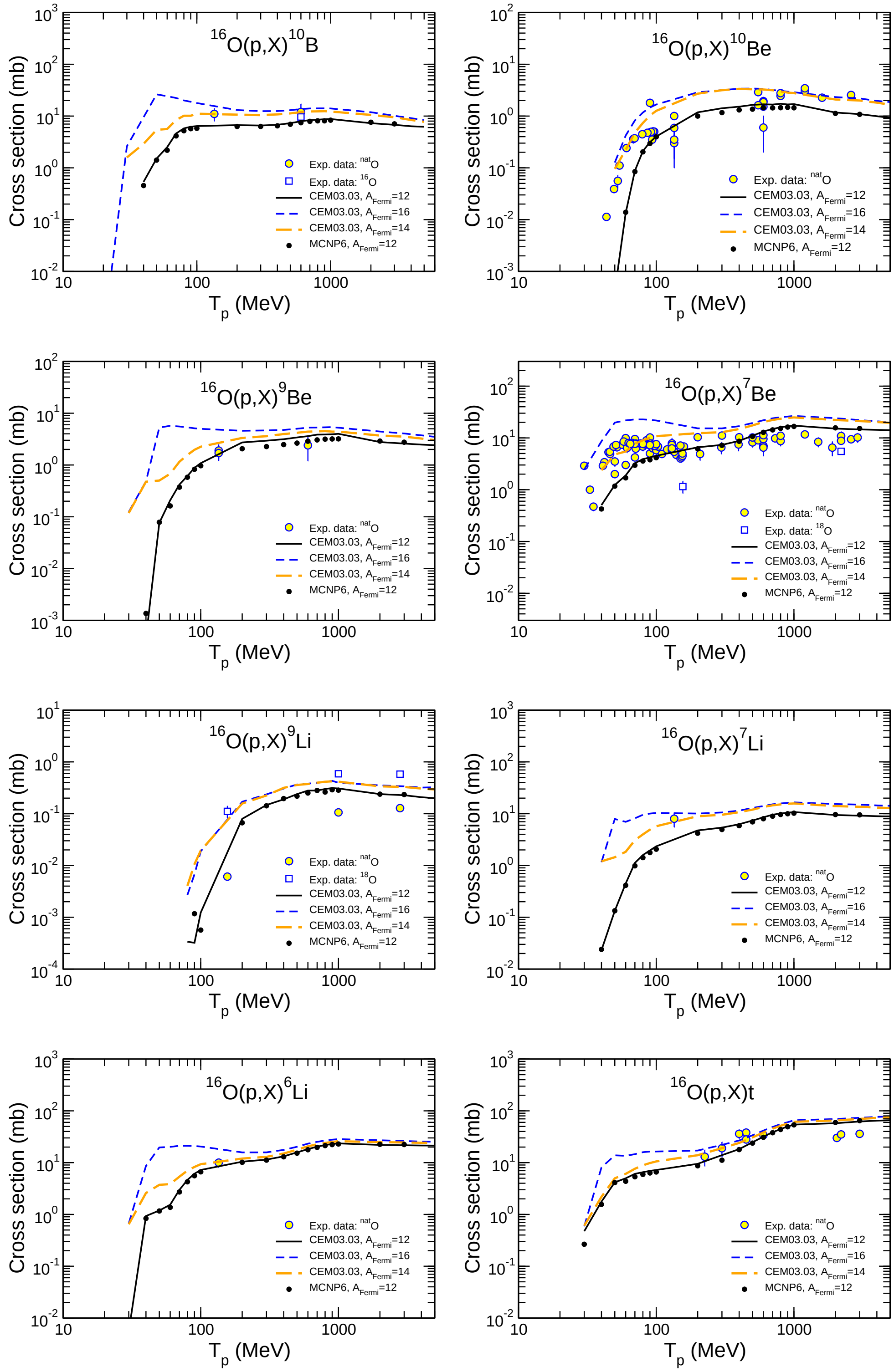


Figure 4: Excitation functions for the production of ^{10}B, ^{10}Be, ^{9}Be, ^{7}Be, ^{9}Li, ^{7}Li, ^{6}Li, and t from p + ^{16}O calculated with CEM03.03 using the "standard" version of the Fermi breakup model ($A_{Fermi} = 12$; solid black lines) and with cup-off values for A_{Fermi} of 16 (dashed blue lines) and 14 (long-dashed orange lines), as well as with MCNP6 using CEM03.03 ($A_{Fermi} = 12$; small solid black circles) compared with experimental data. Experimental data are from the T16 Lib compilation [14].

2.3. p + ^{27}Al Excitation Functions

This MCNP6 problem is to test the applicability of MCNP6 using the CEM03.03 event generator to describe excitation functions from the fragmentation of ^{27}Al bombarded with protons from 10 MeV up to 5 GeV and to compare the results with available experimental data and with calculations by CEM03.03 used as a stand-alone code with three modifications of its Fermi break-up model, as described in Ref. [7]. This test problem is somehow similar to the previous problems, #24 and 25. But it is for another target nucleus and includes excitation functions of several final products not covered by problems #24 and 25.

Fragmentation reactions induced by protons and light nuclei of energies around 1 GeV/nucleon and below on light target nuclei are involved in different applications, like cosmic-ray-induced single event upsets (SEUs), radiation protection, and cancer therapy with proton and ion beams, among others. It is impossible to measure all nuclear data needed for such applications; therefore, Monte Carlo transport codes are usually used to simulate impacts associated with fragmentation reactions. It is important that available transport codes simulate such reactions as well as possible.

Note that prediction of cross sections of arbitrary products as functions of the incident energy of the projectiles initiating the reactions, i.e., of excitation functions, is one of the most difficult tasks for any theoretical model/code.

Experimental data for this test problem were published by many authors in different publications; detailed references to all measured data we use here can be found in the paper [7]. and references therein.

We calculated the reactions studied in this test problem with MCNP6, using its GENXS option, in parallel, with MPI, using 8 nodes, 64 processors, on the “Moonlight” LANL supercomputer, for the incident proton energies of 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 2000, 3000, 4000, and 5000 MeV. As the MCNP6 input files at all these incident energies differ only in their SDEF card, in the value of the input parameter ERG (i.e., the proton incident energy, in MeV), we present here only one example of the MCNP6 input and output files, at 1000 MeV. The main MCNP6 input file at 1000 MeV is p1000_Al27.CEM. For the second input files required by the GENXS option we use the same file, inxc96, at all incident energies listed above. Our p1000_Al27.CEM and inxc96 input files are presented in subdirectory */VALIDATION_CEM/Inputs/.

Below, we provide both p1000_Al27.CEM and inxc96 MCNP6 input files used for this test problem.

p1000_Al27.CEM:

```
MCNP6 test: p + Al27 by CEM03.03 at 1000 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   13027 1.0
  sdef erg = 1000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 5001
  mode   h
LCA  8j 1    $ use CEM03.03, nevtype = 66                   !!!
  tropt genxs inxc96  nreact on  nescat off
c ----------------------------------------------------------------
  print 40 110 95
c  nps 10000
  nps 1000000
c  prdmp 2j -1
```

inxc96:

```
MCNP6 test: p + Ta181 by CEM03.03, nevtype=66
0 0 1 /
Cross Section Edit
0 0 9 /
1 5 6 7 8 21 22 23 24 /
```

In the current test problem, we compare the MCNP6 results for the p+^{27}Al reaction with available data and with calculations by CEM03.03 used as a stand alone code for the total inelastic cross section and for excitation functions for the production of ^{13}N, ^{11}C, ^{10}Be, ^{7}Be, ^{9}Li, ^{6}He, ^{4}He, ^{3}He, t, d, and p. The MCNP6 cross sections for the production of different isotopes are printed (in barns) in the corresponding portion of the table entitled "Distribution of residual nuclei" of the output file p1000_Al27.CEM.mpi.o presented in the subdirectory */VALIDATION_CEM/Templates/LINUX/. The total inelastic cross section calculated by MCNP6 is printed in its output file just several lines higher, in the table entitled "nonelastic cross section". To help plotting all these results with xmgrace, we copy the MCNP6 values obtained at different incident proton energies into separate files.

To save space, we do not show here explicitly files with MCNP6 results for the total p+^{27}Al inelastic cross sections and for the production of ^{13}N, ^{11}C, ^{10}Be, ^{7}Be, ^{9}Li, ^{6}He, ^{4}He, ^{3}He, t, d, and p, as their values are included in the provided templates for the xmgrace figures we use to plot our results. Templates to plot with xmgrace the total p+^{27}Al inelastic cross sections and cross sections for the production of ^{13}N, ^{11}C, ^{10}Be, ^{7}Be, ^{9}Li, ^{6}He, ^{4}He, ^{3}He, t, d, and p, are presented in files sigin.fig, and n13.fig, c11.fig, be10.fig, be7.fig, li9.fig, he6.fig, he4.fig, he3.fig, t.fig, d.fig, and p.fig, respectively, all shown in subdirectory */VALIDATION_CEM/Experimental_data/pAl27/. These xmgrace files contain also all the experimental data as well as the results by CEM03.03 used as a stand alone code. Useful details and discussion of all these data and calculation results can be found in the listed above paper [7].

Postscript files generated by xmgrace for all our plots were generated in files with similar names, simply using in their names extensions "eps" instead of "fig".

To ease an overview of all our results, we provide a summary file pAl27_1.pdf which shows cross sections for all products studied here (see Fig. 5). This summary pdf file was produced with the LaTeX file pAl_1.tex using the listed above postscript files as input.

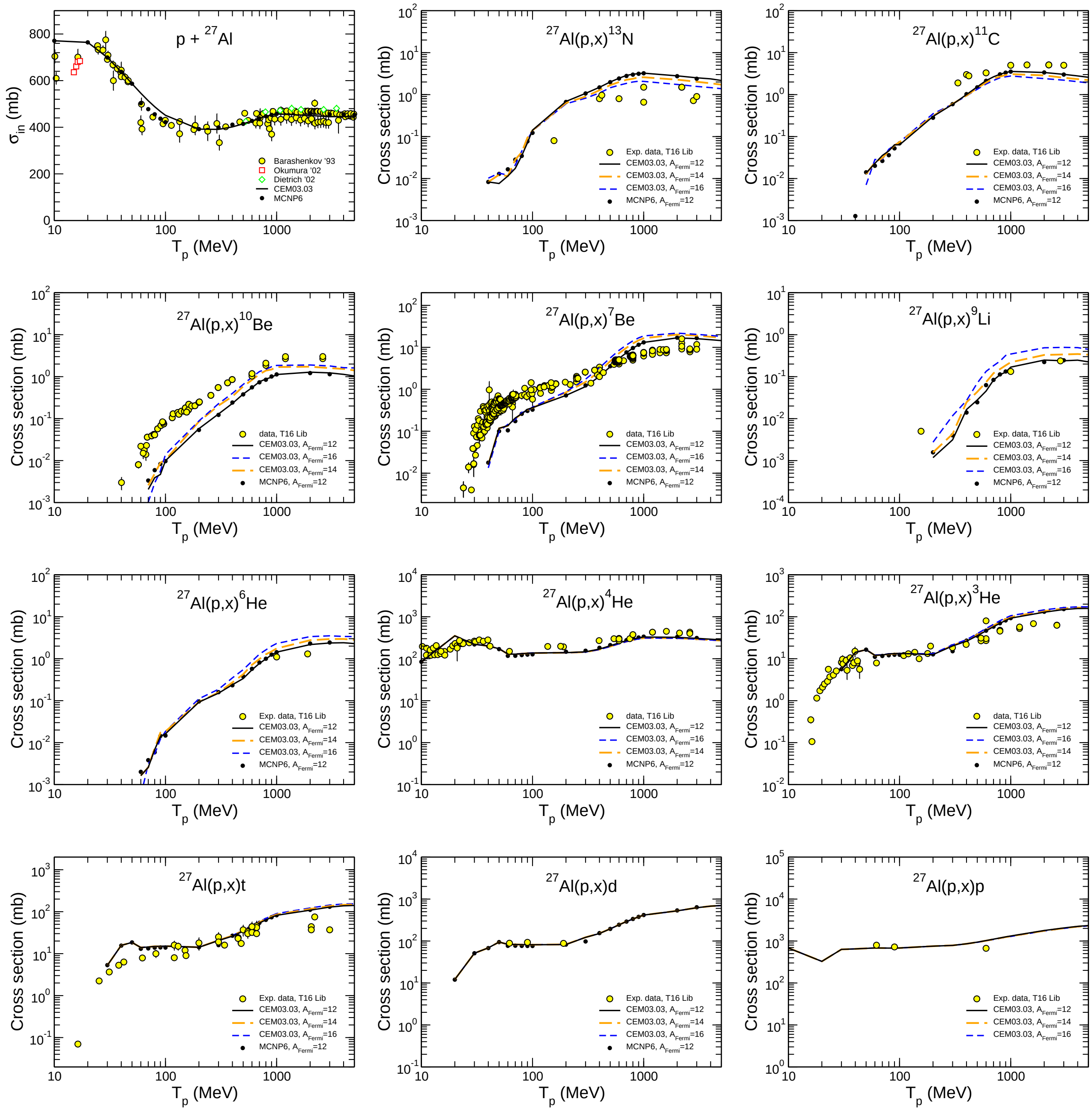


Figure 5: Total inelastic cross section and excitation functions for the production of ^{13}N, ^{11}C, ^{10}Be, ^{7}Be, ^{9}Li, ^{6}He, ^{4}He, ^{3}He, t, d, and p from p + ^{27}Al calculated with CEM03.03 using the "standard" version of the Fermi break-up model ($A_{Fermi} = 12$; solid black lines) and with cup-off values for A_{Fermi} of 16 (dashed blue lines) and 14 (long-dashed orange lines), as well as with MCNP6 using CEM03.03 ($A_{Fermi} = 12$; small solid black circles) compared with experimental data. Experimental data for inelastic cross sections are from Refs. [11, 17, 18], while the data for excitation functions are from the T16 Lib compilation [14].

Aluminum as a target is very interesting because it is used in many applications. From a theoretical point of view, p + ^{27}Al reactions are challenging because Al is relatively light, with significant contributions from the Fermi breakup models in our simulations. At the same time Al has mass number higher than the discussed above values of A_{Fermi} (see details in Ref. [7]), allowing some significant contribution to the calculated cross sections from preequilibrium and evaporation processes. On the whole, the agreement of the results with available measured data for Al is very similar to what we find for N and O. In many cases, we get a better description of the heavy fragments when we use $A_{Fermi} = 16$ or 14, and usually we predict a little better the light fragments using $A_{Fermi} = 12$. For comparison, for Al, we show also excitation functions for the production of all complex particles from d to ^{4}He, as well as of secondary protons, as we found experimental data available for them. Because the absolute values of the yields of light fragment production is much lower compared to the yields of complex particles, and especially of protons, the production cross sections of d, t, ^{3}He, ^{4}He, and especially of p, calculated with different values of A_{Fermi} are very close to each other. This is true also for the production of neutrons; although we do not have experimental data for neutron production for these reactions. Generally, emission of nucleons and complex particles are the most determinative in the calculation of spallation products (heavier residuals) from reactions on medium-mass nuclei, while LF yields are generally low, and their calculation does not affect significantly the final cross sections for these heavier products.

2.4. p + ^{28}Si Excitation Functions

This MCNP6 problem is to test the applicability of MCNP6 using the CEM03.03 event generator to describe excitation functions from the fragmentation of ^{28}Si bombarded with protons from 10 MeV up to 5 GeV and to compare the results with available experimental data and with calculations by CEM03.03 used as a stand-alone code with three modifications of its Fermi break-up model, as described in Ref. [7]. This test problem is somehow similar to the previous problem, #26. But it is for another target nucleus and includes excitation function of a final product not covered by the problem #26.

Fragmentation reactions induced by protons and light nuclei of energies around 1 GeV/nucleon and below on light target nuclei are involved in different applications, like cosmic-ray-induced single event upsets (SEUs), radiation protection, and cancer therapy with proton and ion beams, among others. It is impossible to measure all nuclear data needed for such applications; therefore, Monte Carlo transport codes are usually used to simulate impacts associated with fragmentation reactions. It is important that available transport codes simulate such reactions as well as possible.

Note that prediction of cross sections of arbitrary products as functions of the incident energy of the projectiles initiating the reactions, i.e., of excitation functions, is one of the most difficult tasks for any theoretical model/code.

Experimental data for this test problem were published by many authors in different publications; detailed references to all measured data we use here can be found in the paper [7] and references therein.

We calculated the reactions studied in this test problem with MCNP6, using its GENXS option, in parallel, with MPI, using 8 nodes, 64 processors, on the “Moonlight” LANL supercomputer, for the incident proton energies of 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 2000, 3000, 4000, and 5000 MeV. As the MCNP6 input files at all these incident energies differ only in their SDEF card, in the value of the input parameter ERG (i.e., the proton incident energy, in MeV), we present here only one example of the MCNP6 input and output files, at 1000 MeV. The main MCNP6 input file at 1000 MeV is p1000_Si28.CEM. For the second input file required by the GENXS option we use the same file, inxc96, at all incident energies listed above. Our p1000_Si28.CEM and inxc96 input files are presented in subdirectory */VALIDATION_CEM/Inputs/.

Below, we provide both p1000_Si28.CEM and inxc96 MCNP6 input files used for this test problem.

p1000_Si28.CEM:

```
MCNP6 test: p + Si28 by CEM03.03 at 1000 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   14028 1.0
  sdef erg = 1000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:h 1 1 0
  phys:h 5001
  mode   h
LCA  8j 1    $ use CEM03.03, nevtype = 66                  !!!
  tropt genxs inxc96  nreact on  nescat off
c ----------------------------------------------------------------
  print 40 110 95
c  nps 10000
  nps 1000000
c  prdmp 2j -1
```

inxc96:

```
MCNP6 test: p + Ta181 by CEM03.03, nevtype=66
0 0 1 /
Cross Section Edit
0 0 9 /
1 5 6 7 8 21 22 23 24 /
```

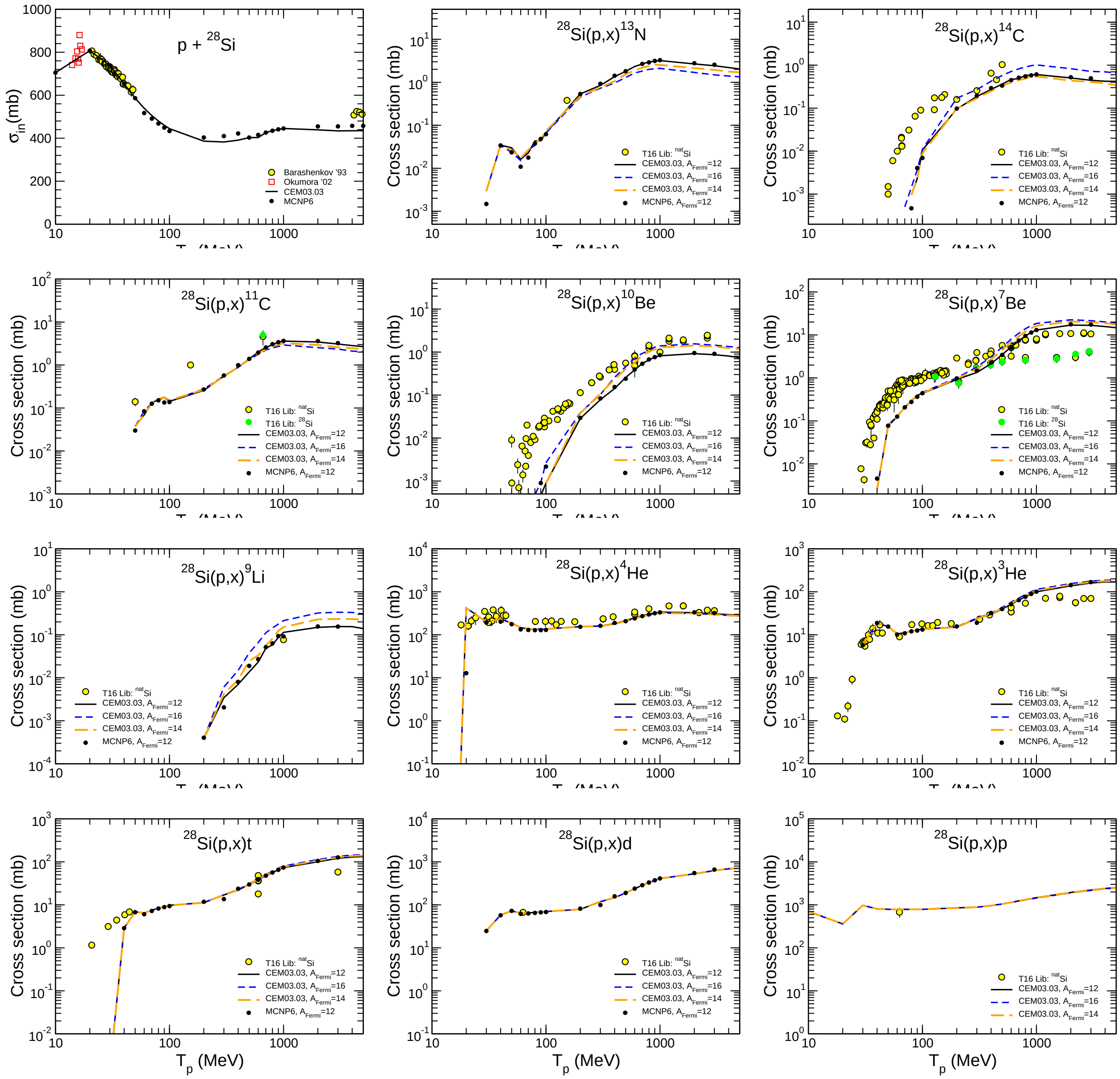


Figure 6: Total inelastic cross section and excitation functions for the production of ^{13}N, ^{14}C, ^{11}C, ^{10}Be, ^{7}Be, ^{9}Li, ^{4}He, ^{3}He, t, d, and p from p + ^{28}Si calculated with CEM03.03 using the "standard" version of the Fermi break-up model ($A_{Fermi} = 12$; solid black lines) and with cup-off values for A_{Fermi} of 16 (dashed blue lines) and 14 (long-dashed orange lines), as well as with MCNP6 using CEM03.03 ($A_{Fermi} = 12$; small solid black circles) compared with experimental data. Experimental data for inelastic cross sections are from Refs. [11, 17], while the data for excitation functions are from the T16 Lib compilation [14].

In the current test problem, we compare the MCNP6 results for the p+^{28}Si reaction with available data and with calculations by CEM03.03 used as a stand alone code for the total inelastic cross section and for excitation functions for the production of ^{13}N, ^{14}C, ^{11}C, ^{10}Be, ^{7}Be, ^{9}Li, ^{4}He, ^{3}He, t, d, and p. The MCNP6 cross sections for the production of different isotopes are printed (in barns) in the corresponding portion of the table entitled "Distribution of residual nuclei" of the output file p1000_Si28.CEM.mpi.o presented in the subdirectory */VALIDATION_CEM/Templates/LINUX/. The total inelastic cross section calculated by MCNP6 is printed in its output file just several lines higher, in the table entitled "nonelastic cross section". To help plotting all these results with xmgrace, we copy the MCNP6 values obtained at different incident proton energies into separate files.

To save space, we do not show here explicitly files with MCNP6 results for the total p+^{28}Si inelastic cross sections and for the production of ^{13}N, ^{14}C, ^{11}C, ^{10}Be, ^{7}Be, ^{9}Li, ^{4}He, ^{3}He, t, d, and p, as their values are included in the provided templates for the xmgrace figures we use to plot our results. Templates to plot with xmgrace the total p+^{28}Si inelastic cross sections and cross sections for the production of ^{13}N, ^{14}C, ^{11}C, ^{10}Be, ^{7}Be, ^{9}Li, ^{4}He, ^{3}He, t, d, and p, are presented in files sigin.fig, and n13.fig, c14.fig, c11.fig, be10.fig, be7.fig, li9.fig, he4.fig, he3.fig, t.fig, d.fig, and p.fig, respectively, all shown in subdirectory */VALIDATION_CEM/Experimental_data/pSi28/. These xmgrace files contain also all the experimental data as well as the results by CEM03.03 used as a stand alone code. Useful details and discussion of all these data and calculation results can be found in the listed above Ref. [7].

Postscript files generated by xmgrace for all our plots were generated in files with similar names, simply using in their names extensions "eps" instead of "fig".

To ease an overview of all our results, we provide a summary file pSi28.pdf which shows cross sections for all products studied here (see Fig. 6). This summary pdf file was produced with the LaTeX file pSi28.tex using the listed above postscript files as input.

All reactions on silicon were calculated for ^{28}Si, while most of the data were measured from ^{nat}Si (see details in legends of Fig. 6). Silicon as a target is very interesting because it is used in many applications. From a theoretical point of view, p + ^{28}Si reactions are challenging because Si is relatively light, with significant contributions from the Fermi breakup models in our simulations. At the same time Si has mass number higher than the discussed above values of A_{Fermi} (see details in Ref. [7]), allowing some significant contribution to the calculated characteristics from preequilibrium and evaporation processes. On the whole, the agreement of the results with available measured data for Si is very similar to what we find for Al, O, and N. In many cases, we get a better description of the heavy fragments when we use $A_{Fermi} = 16$ or 14, and usually we predict a little better the light fragments using $A_{Fermi} = 12$. For comparison, for Si, we show also excitation functions for the production of all complex particles from d to ^{4}He, as well as of secondary protons, as we found experimental data available for them. Because the absolute values of the yields of light fragment production is much lower compared to the yields of complex particles, and especially of protons, the production cross sections of d, t, ^{3}He, ^{4}He, and especially of p calculated with different values of A_{Fermi} are very close to each other. This is true also for the production of neutrons, although we do not have experimental data for neutron production for these reactions. Generally, emission of nucleons and complex particles are the most determinative in the calculation of spallation products (heavier residuals) from reactions on medium-mass nuclei, while LF yields are generally low, and their calculation does not affect significantly the final cross sections of spallation products.

2.5. Isotope Production from 10 – 90 MeV p + ^{159}Tb

This problem is to test the applicability of MCNP6 using the CEM03.03 [8], Bertini + MPM + Dresner + RAL [19, 20, 21, 22], and INCL + ABLA [23, 24] event-generators to predict cross sections for the production of isotopes of interest in medical, astrophysical, and basic science research from a thin terbium target bombarded with a proton beam of energy below 100 MeV.

The proton-induced fission cross section of Tb is very low, therefore some models like the RAL fission model used as the default option of MCNP6 for such reactions together with the Bertini INC [19], the Multistage Preequilibrium Model (MPM) [20] and the Dresner evaporation model [21], does not account for fission of Tb at all (see more details in [22]). In addition, predictions by CEM03.03 [8] and INCL + ABLA [23, 24] event generators for such processes differ significantly, therefore the ability of MCNP6 to simulate proton-induced reactions on Tb must be carefully investigated.

Experimental cross sections of nuclide production from terbium were very scarce until recently, when new measurements for this reaction at proton incident energy of 800 MeV have been completed at LANSCE, LANL. The new LANL data are published in the paper [25]. After the completion of this work, additional measurements on Tb were performed at LANSCE, by the same LANL Group, at lower proton incident energies, below 100 MeV. These new Tb data at lower energies are still under processing and analysis and are not published yet. It is interesting how MCNP6 predicts these data, especially taking into account that no experimental data on Tb in this energy region were published so far in the literature, making our MCNP6 calculations as a pure, 100% prediction for such reactions.

For this test problem, we performed MCNP6 calculations with its GENXS option, in parallel, with MPI, using 8 nodes, 64 processors, on the "Moonlight" LANL supercomputer, using the CEM03.03 [8], Bertini + MPM + Dresner + RAL [19, 20, 21, 22], and INCL + ABLA citeINCL, ABLA event-generators at 10, 20, 30, 40, 50, 60, 70, 80, and 90 MeV. Results of all our predictions will be compared with the new experimental data and published in a separate paper when the analysis of data is completed. Since MCNP6 input files at different incident energies differ only in their SDEF card, in the value of the input parameter ERG (i.e., the proton incident energy, in MeV), here, we show only one example of the MCNP6 input and output files, at 90 MeV. The main MCNP6 input files for the CEM03.03, Bertini, and INCL+ABLA event generators are p90Tb_CEM, p90Tb_Bert, and p90Tb_INCL, respectively. For the second input file required by the GENXS option we use the same file, inxc95, for all models. All these input files are presented in subdirectory */VALIDATION_CEM/Inputs/.

The main MCNP6 input file for the CEM03.03 event generator is **p90Tb_CEM**. It is provided together with the second auxiliary input file, **inxc95**, in subdirectory **/VALIDATION_CEM/Inputs/** and both are also shown below.

p90Tb_CEM:

```
MCNP6 test: p + Tb159 by CEM03.03 at 90 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   65159 1.0
  sdef erg = 90 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 ---------------------------------------------------------------
c  print 40 110 95
c  nps 10000
  nps 10000000
c  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 /
```

The main MCNP6 input files for the Bertini and INCL+ABLA models are **p90Tb_Bert** and **p90Tb_INCL**. Both of them use the same auxiliary input file, **inxc95**, shown above, and both are provided in the subdirectory **/VALIDATION_CEM/Inputs/**.

The only difference of **p90Tb_INCL** from the **p90Tb_CEM** and **p90Tb_Bert** input files is in the **LCA** and **LEA** cards. In the case of INCL+ABLA, these cards in the input file look like:

```
  LCA   2 1 0 4j -1 2    $ use INCL+ABLA                  !!!
  lea 2j 0
```

while for the Bertini option, we need to add in the MCNP6 main input file the cards:

```
  lca 2 1 5j -1 0 $ Use Bertini: LCA(9)=0
  lea 2j 0
```

otherwise MCNP6 will perform calculations using CEM03.03.

As mentioned above, the new experimental data are still under analysis and not available to us. The only preliminary experimental values we have now, are an estimation of the cross sections for the production of Tb153 and Gd153, that constitutes the most part of the total yield for products with A=153, at the incident energy of 97 MeV [26]. This preliminary experimental value for A=153 is presented in the file A153.exp.dat; we use it to compare with the MCNP6 predicted A-distributions at 90 MeV (see Fig. 7).

MCNP6 results using the CEM03.03, Bertini, and INCL+ABLA event generators are in the output files p90Tb_CEM.mpi.o, p90Tb_Bert.mpi.o, and p90Tb_INCL.mpi.o, respectively, all presented in subdirectory */VALIDATION_CEM/Experimental_data/90MeV_pTb/. Cross sections for the production of all isotopes from this reaction are printed in table entitled "Distribution of residual nuclei" of the corresponding MCNP6 output files. To help plotting these A-distributions with xmgrace, we copy them into separate files p90Tb_M6CEM.A.dat, p90Tb_M6Bert.A.dat, and p90Tb_M6INCL.A.dat, for the CEM, Bertini, and INCL+ABLA cases, respectively. The file p90Tb_A.fig is a template for plotting the mass distribution of all products from our reaction with with xmgrace. The pdf file for the figure is p90Tb_A.pdf (see Fig. 7). All these files are presented in the same subdirectory:
/VALIDATION_CEM/Experimental_data/90MeV_pTb/.

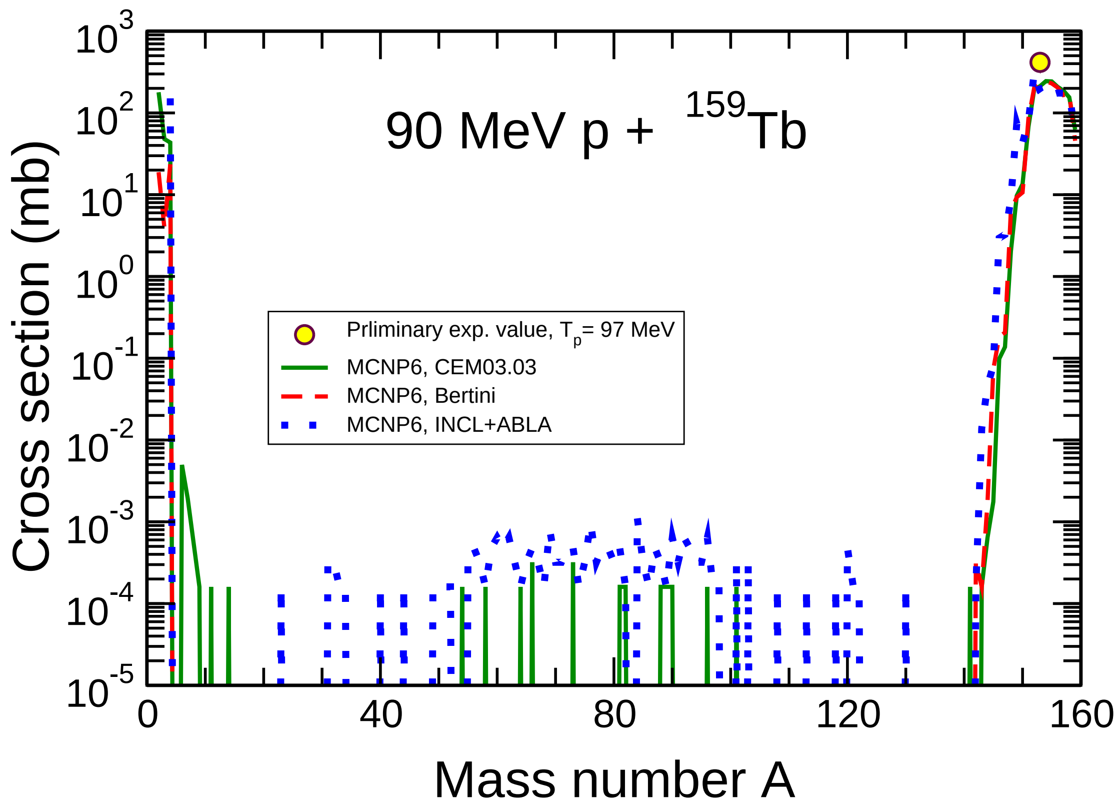


Figure 7: Comparison of mass distributions of product yields calculated with MCNP6 using CEM03.03 [8, 9], Bertini+MPM+Dresner+RAL [19, 20, 21, 22], and INCL+ABLA [23, 24] from 90 MeV p + ^{159}Tb with preliminary experimental cross section for the production of ions with A=153 at 97 MeV [26] estimated by the LANL Group that had measured and published results for this reaction at 800 MeV [25]; final experimental data at several energies below 200 MeV will be published by the same LANL Group after analysis of all measurements are completed.

3. Testing LAQGSM

All the test problems discussed in this Section are presented in the **VALIDATION_LAQGSM** subdirectory in the basic **/MCNP6/Testing/** directory.

3.1. 790 MeV/A ^{129}Xe + ^{27}Al

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to describe projectile fragmentation from nucleus-nucleus reactions at high energies. Such reactions are powerful tools to produce intensive beams of exotic nuclei even close to driplines. They are important for the planning of future experiments at Facility for Rare Isotope Beams (FRIB) and other radioactive beam facilities. Such studies should allow us to get more insight into the underlying reaction mechanisms. Also of considerable interest for the study of nuclei at the borderline of stability is whether the isotopic yields may be influenced by the use of appropriate neutron-rich or neutron-deficient projectiles.

Namely, in this test problem, we calculate with MCNP6 using LAQGSM03.03 with the GENXS option the yields of projectilelike fragments in the reaction ^{129}Xe + ^{27}Al at a laboratory energy of 790 MeV/nucleon measured at the GSI facility in Darmstadt, Germany. Numerical valued of measured data are published Tab. I of the paper [29].

The MCNP6 main input file for this problem is Xe129_Al_790, presented in subdirectory /VALIDATION_LAQGSM/Inputs/. Let us recall that the GENXS option of MCNP6 requires a second, auxiliary, input file; for this problem, we use the auxiliary MCNP6 input file xeal790, shown in the same subdirectory. Both these input files are also shown below.

Xe129_Al_790:

```
MCNP6 test: 790 MeV/A Xe129 + Al27 by LAQGSM03.03, 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 -----------------------------------------------------------------
dbcn 28j 1
  m1 13027  1.0
  sdef erg=101910 par=54129 dir=1 pos=0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:g 200
  phys:d 200
  phys:h 200
```

```
  phys:# 112100
  mode  # n a t d s h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
  tropt genxs xeal790  nreact on  nescat off
c  tropt genxs inxc69
c ---------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 10000000
  prdmp 500000 200000 1
```

xeal790:

```
MCNP6 test: 790 MeV/A Xe129 + Al27 by LASQGSM03.0, 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. 150. /
1 5 6 7 8 21 22 23 24 /
```

We calculated this test problem with MPI using 8 nodes, 64 processors, on the "Moonlight" supercomputer of LANL. The output file, Xe129_Al_790.mpi.o, is presented in subdirectory: /VALIDATION_LAQGSM/Templates/LINUX/.

The MCNP6 cross sections for the production of different isotopes are printed (in barns) in the corresponding portion of the table entitled "Distribution of residual nuclei" of the output file. To help plotting these results with xmgrace, we copy here the MCNP6 results for all measured (only) products in separate files. The cross sections for the production of isotopes with Z=40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, and 55 are presented in files 40-m6.dat, 41-m6.dat, 42-m6.dat, 43-m6.dat, 44-m6.dat, 45-m6.dat, 46-m6.dat, 47-m6.dat, 48-m6.dat, 49-m6.dat, 50-m6.dat, 51-m6.dat, 52-m6.dat, 53-m6.dat, 54-m6.dat, and 55-m6.dat, respectively.

Experimental data for all these products are presented in files with similar names, simply using in their names "exp" instead of "m6".

Template for plotting all these results compared with the measured data using xmgrace are presented in files 40.fig, 41.fig, 42.fig, 43.fig, 44.fig, 45.fig, 46.fig, 47.fig, 48.fig, 49.fig, 50.fig, 51.fig, 52.fig, 53.fig, 54.fig, and 55.fig, respectively.

Postscript files generated by xmgrace for all the plots are presented in files with similar names, simply using in their names extensions "ps" instead of "fig".

To ease an overview of all these product yields, we provide also a summary file Xe129Al27_790.pdf which shows cross sections for all products with Z from 40 to 55. This summary pdf file was produced with the LaTeX file Xe129Al27_790.tex using the listed above postscript files as input.

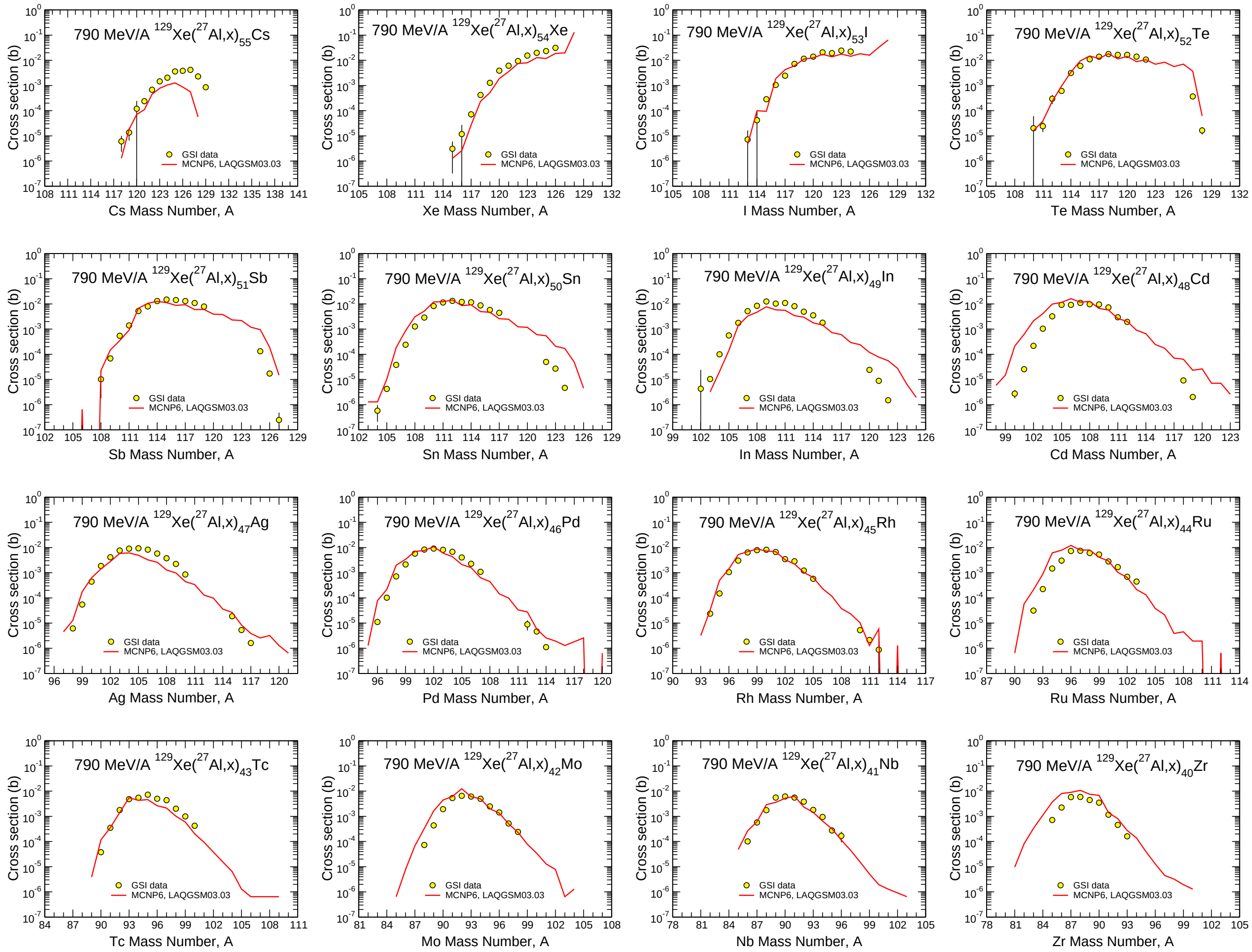


Figure 8: Experimental mass number distribution of product yields [29] (filled circles) from the 790 MeV/nucleon ^{129}Xe + ^{27}Al reaction compared with results by MCNP6 using the LAQGSM03.03 event-generator (red lines), as indicated.

3.2. 600 MeV/A ^{56}Fe + ^{12}C

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to describe the individual elemental and isotopic cross sections from carbon targets, appropriate to the interpretation of the interstellar production of secondary fragments by cosmic rays propagating through the galaxy in order to determine the source elemental and isotopic composition of cosmic rays. At the same time, such cross sections are an important input for understanding the nuclear physics involved in these collisions.

Namely, in this test problem, we calculate with MCNP6 using LAQGSM03.03 with the GENXS option the yields of projectilelike fragments in the reaction ^{56}Fe + ^{12}C at a laboratory energy of 600 MeV/nucleon measured at the Lawrence Berkeley Laboratory Bevalac and compare the MCNP6 results with experimental data and with results by LAQGSM03.03 used as a stand-alone code. Numerical valued of measured data are published Tab. II of the paper [30].

The MCNP6 main input file for this problem is Fe600C, presented in subdirectory /VALIDATION_LAQGSM/Inputs/. Let us recall that the GENXS option of MCNP6 requires a second, auxiliary, input file; for this problem, we use the auxiliary MCNP6 input file xeal790, shown in the same subdirectory, and also presented below.

Fe600C:

```
MCNP6 test: 600 MeV/A Fe56 + C12 by LAQGSM03.03, 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 -----------------------------------------------------------------
dbcn 28j 1
  m1 6012  1.0
  sdef erg=33600 par=26056 dir=1 pos=0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:g 200
  phys:d 200
  phys:h 200
  phys:# 112100
  mode  # n a t d s h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
  tropt genxs xeal790  nreact on  nescat off
c  tropt genxs inxc69
c -----------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 10000000
c  prdmp 500000 200000 1
```

xeal790:

```
MCNP6 test: 790 MeV/A Xe129 + Al27 by LASQGSM03.0, 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. 150. /
1 5 6 7 8 21 22 23 24 /
```

We calculated this test problem with MPI using 8 nodes, 64 processors, on the "Moonlight" supercomputer of LANL. The output file, Fe600C.mpi.o, is presented in subdirectory: /VALIDATION_LAQGSM/Templates/LINUX/.

The MCNP6 cross sections for the production of different isotopes are printed (in barns) in the corresponding portion of the table entitled "Distribution of residual nuclei" of the output file. To help plotting these results with xmgrace, we copy here the MCNP6 results for all measured (only) products in separate files. The cross sections for the production of isotopes with Z=3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, and 26 are presented in files 3.m6.dat, 4.m6.dat, 5.m6.dat, 6.m6.dat, 7.m6.dat, 8.m6.dat, 9.m6.dat, 10.m6.dat, 11.m6.dat, 12.m6.dat, 13.m6.dat, 14.m6.dat, 15.m6.dat, 16.m6.dat, 17.m6.dat, 18.m6.dat, 19.m6.dat, 20.m6.dat, 21.m6.dat, 22.m6.dat, 23.m6.dat, 24.m6.dat, 25.m6.dat, and 26.m6.dat, respectively. Results by LAQGSM03.03 used as a stand-alone code are presented in files with similar names, simply using in their names "laq" instead of "m6". Experimental data are presented in files with similar names, simply using in their names "exp" instead of "m6".

Template for plotting all these results compared with the measured data using xmgrace are presented in files 3.fig, 4.fig, 5.fig, 6.fig, 7.fig, 8.fig, 9.fig, 10.fig, 11.fig, 12.fig, 13.fig, 14.fig, 15.fig, 16.fig, 17.fig, 18.fig, 19.fig, 20.fig, 21.fig, 22.fig, 23.fig, 24.fig, 25.fig, and 26.fig, respectively.

Postscript files generated by xmgrace for all the plots are presented in files with similar names, simply using in their names extensions "ps" instead of "fig".

To ease an overview of all these product yields, we provide also a summary file Fe600C.pdf which shows cross sections for all products with Z from 3 to 26. This summary pdf file was produced with the LaTeX file Fe600C.tex using the listed above postscript files as input.

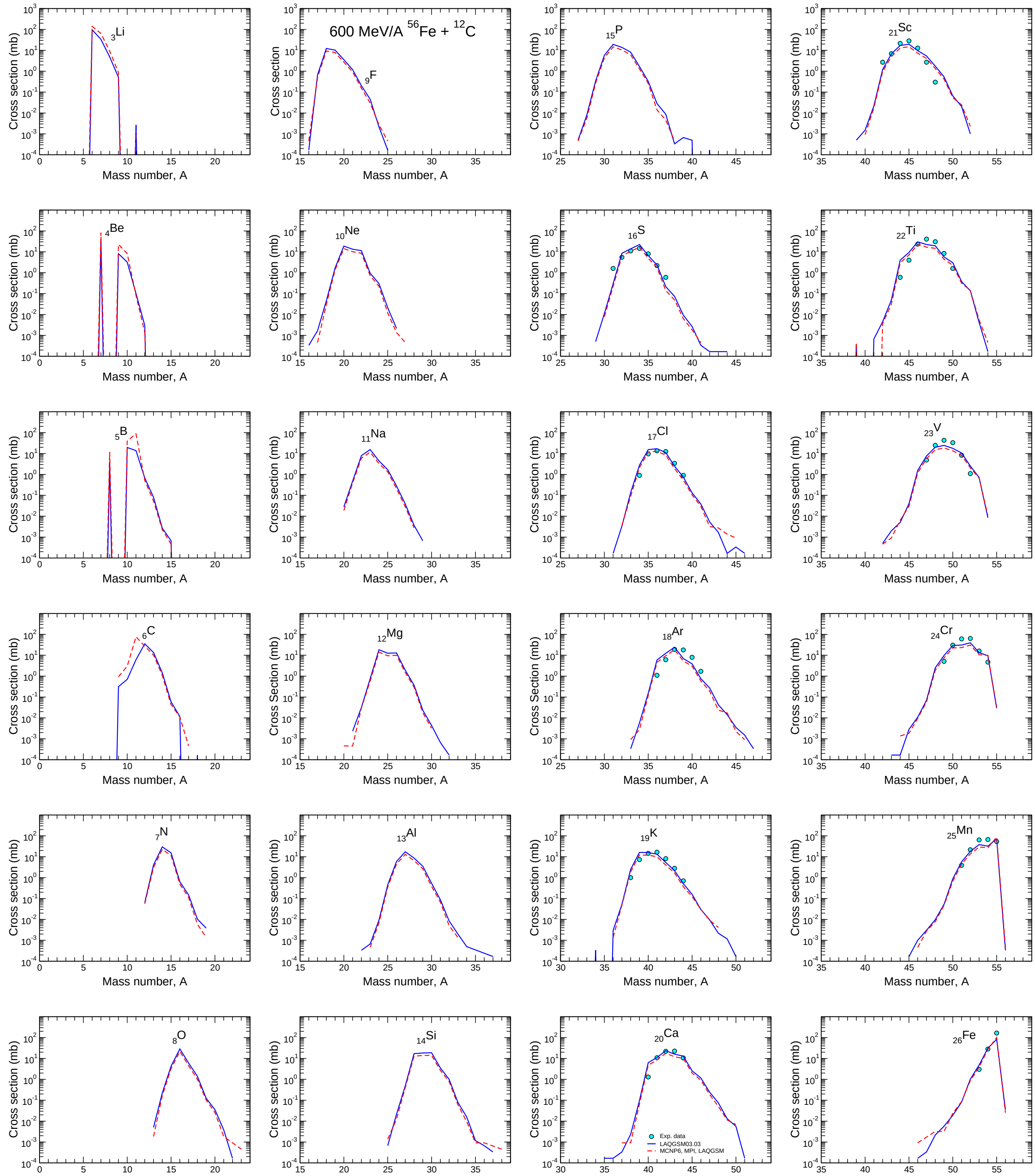


Figure 9: Experimental mass number distribution of product yields [30] (filled circles) from the 600 MeV/nucleon ^{56}Fe + ^{12}C reaction compared with results by LAQGSM03.03 [9, 27] used as a stand alone code (blue solid lines) and by MCNP6 using the LAQGSM03.03 event-generator (red dashed lines), as indicated.

3.3. 1 GeV/A ^{208}Pb + ^{9}Be

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to describe production cross sections of heavy neutron-rich nuclei approaching the nucleosynthesis r-process path around A=195. The production of heavy neutron-rich nuclei in the laboratory has been a challenging problem in the last decades. Very neutron-rich nuclei are unstable, and the more exotic they are, the shorter their half-lives. Radioactive nuclei play an important role in many cosmic phenomena, and information on these nuclei is particularly important to improve our understanding of the processes that shape our universe. In particular, one of the major challenges of nuclear astrophysics is to explain how the heavy elements are created in the universe.

Namely, in this test problem, we calculate with MCNP6 using LAQGSM03.03 with the GENXS option the yields of projectilelike fragments in the reaction ^{208}Pb + ^{9}Be at a laboratory energy of 1 GeV/nucleon and to compare our results with the experimental cross sections of heavy neutron-rich nuclei measured recently at GSI for this reaction. Numerical valued of measured data are published Tab. III of the paper [31].

The MCNP6 main input file for this problem is Pb208_Be_1000, presented in subdirectory /VALIDATION_LAQGSM/Inputs/. Let us recall that the GENXS option of MCNP6 requires a second, auxiliary, input file; for this problem, we use the auxiliary MCNP6 input file xeal790, shown in the same subdirectory. Both input files are presented below.

Pb208_Be_1000:

```
MCNP6 test: 1000 MeV/A 208Pb82 + 9Be4 by LAQGSM03.03, 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 ---------------------------------------------------------------
dbcn 28j 1
  m1 4009  1.0
  sdef erg=208000 par=82208 dir=1 pos=0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:g 200
  phys:d 200
  phys:h 200
  phys:# 208500
  mode  # n a t d s h
```

```
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
  tropt genxs xeal790  nreact on  nescat off
c  tropt genxs inxc69
c ---------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 10000000
  prdmp 500000 200000 1
```

xeal790:

```
MCNP6 test: 790 MeV/A Xe129 + Al27 by LASQGSM03.0, 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. 150. /
1 5 6 7 8 21 22 23 24 /
```

We calculated this test problem with MPI using 8 nodes, 64 processors, on the "Moonlight" supercomputer of LANL. The output file, Pb208_Be_1000.mpi.o, is presented in subdirectory: /VALIDATION_LAQGSM/Templates/LINUX/.

The MCNP6 cross sections for the production of different isotopes are printed (in barns) in the corresponding portion of the table entitled "Distribution of residual nuclei" of the output file. To help plotting these results with xmgrace, we copy here the MCNP6 results for all measured (only) products in separate files. The cross sections for the production of isotopes with Z=70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, and 83 are presented in files 70.m6.dat, 71.m6.dat, 72.m6.dat, 73m6.dat, 74.m6.dat, 75.m6.dat, 76.m6.dat, 77.m6.dat, 78.m6.dat, 79.m6.dat, 80.m6.dat, 81.m6.dat, 82.m6.dat, and 83.m6.dat, respectively. Results by LAQGSM03.03 used as a stand-alone code are presented in files with similar names, simply using in their names "noGPL" instead of "m6". Experimental data are presented in files with similar names, simply using in their names "exp" instead of "m6".

Template for plotting all these results compared with the measured data using xmgrace are presented in files PbBe1M.fig and PbBe2M.fig, respectively.

Postscript files generated by xmgrace for the two plots are presented in files with similar names, simply using in their names extensions "eps" instead of "fig". To ease an overview of all these product yields, we provide also a summary file PbBe.M6.pdf which shows cross sections for all products with Z from 70 to 83. This summary pdf file was produced with the LaTeX file PbBe.M6.tex using the listed above *.eps files as input.

As the experimental yields of products are measured (or more exactly are published) only for neutron-rich nuclei, we can not integrate (sum) the measured cross sections over the charge of the products to get a proper estimation of experimental A-distribution of all products from this reaction, or to integrate (sum) the measured yields over the mass number of products, to get experimental Z-distribution of products. However, we can do so for several values of A and Z of products near the ^{208}Pb projectile, to get a very rough estimation of experimental A- and

Z-distribution of products near the ^{208}Pb projectile: as the neutron-rich isotopes measured for these products represent the major part of the corresponding integral cross sections, and such estimations for products very near the ^{208}Pb projectile would be reliable enough and not too rough. Taking into account that A- and Z-distributions of all products from any nuclear reaction are very useful from a theoretical point of view to understand better the mechanisms of nuclear reaction, we performed such an "integration" of the measured cross sections and compare them with calculated A- and Z-distributions of all products. Experimental A-distributions of several production near the ^{208}Pb projectile are presented in the files Aexp07_1.dat (reliable estimation) and Aexp07_2.dat (not so reliable estimation); similar experimental Z-distribution of products are presented in the files Zexp07_1.dat (reliable estimation) and Zexp07_2.dat (not so reliable estimation). MCNP6 A- and Z-distributions of all products are copied from the output file in separate files A.M6.dat and Z.M6.dat, respectively. Similar results by LAQGSM03.03 used as a stand-alone code are presented in files with similar names, simply using in their names "noGPL" instead of "M". Template for plotting all these results compared with the measured data using xmgrace are presented in files A.M.fig and Z.M.fig, respectively. Postscript files generated by xmgrace for the two plots are presented in files with similar names, simply using in their names extensions "eps" instead of "fig". To ease an overview of all these product yields, we provide also a summary file PbBe_AZ.M.pdf. This summary pdf file was produced with the LaTeX file PbBe_AZ.M.tex using the listed above *.eps files as input.

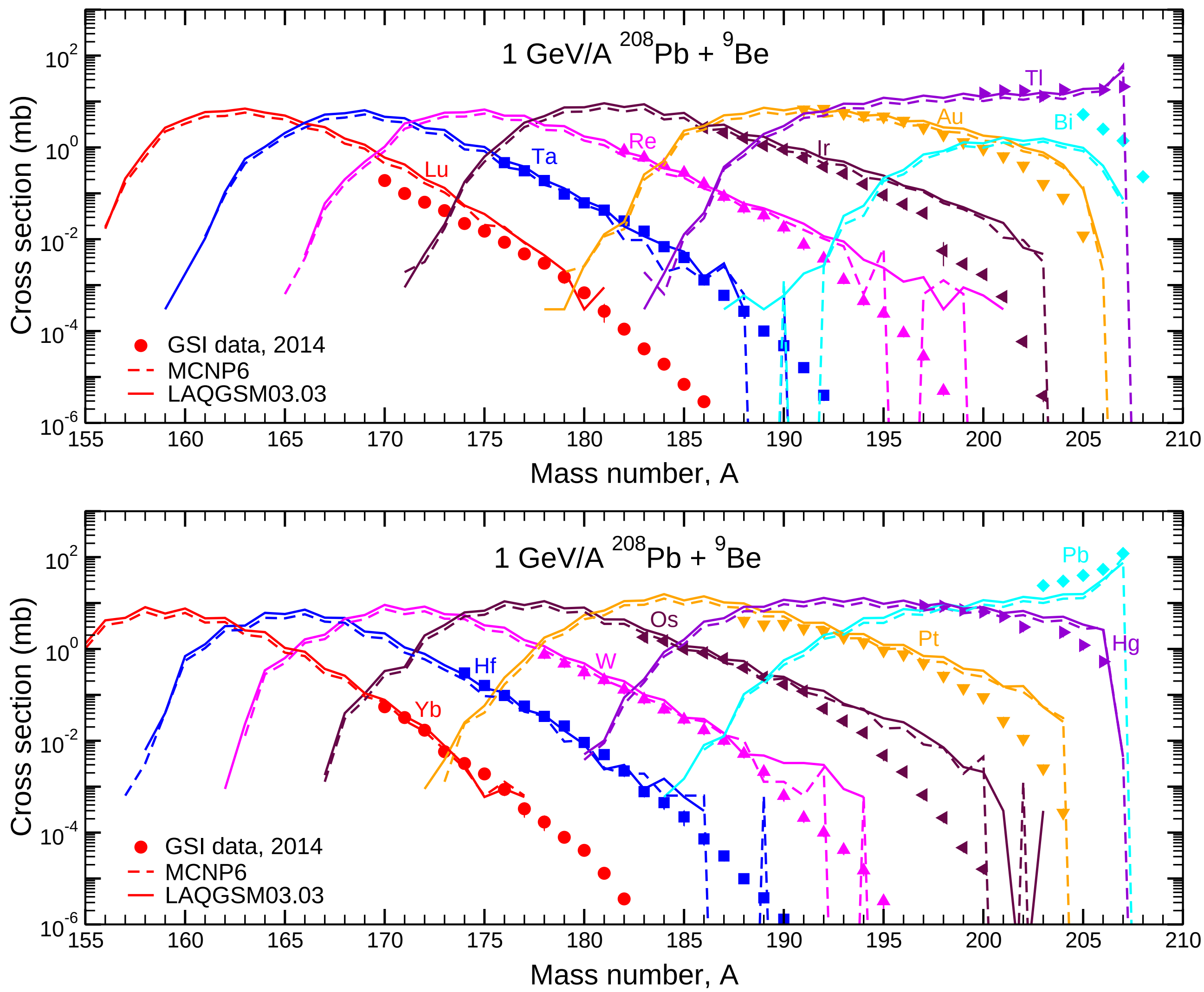


Figure 10: Experimental mass number distribution of yields of products with Z from 70 to 83 [31] (symbols) from the 1 GeV/nucleon ^{208}Pb + ^{9}Be reaction compared with results by LAQGSM03.03 [9, 27] used as a stand alone code (color solid lines) and by MCNP6 using the LAQGSM03.03 event-generator (color dashed lines), as indicated.

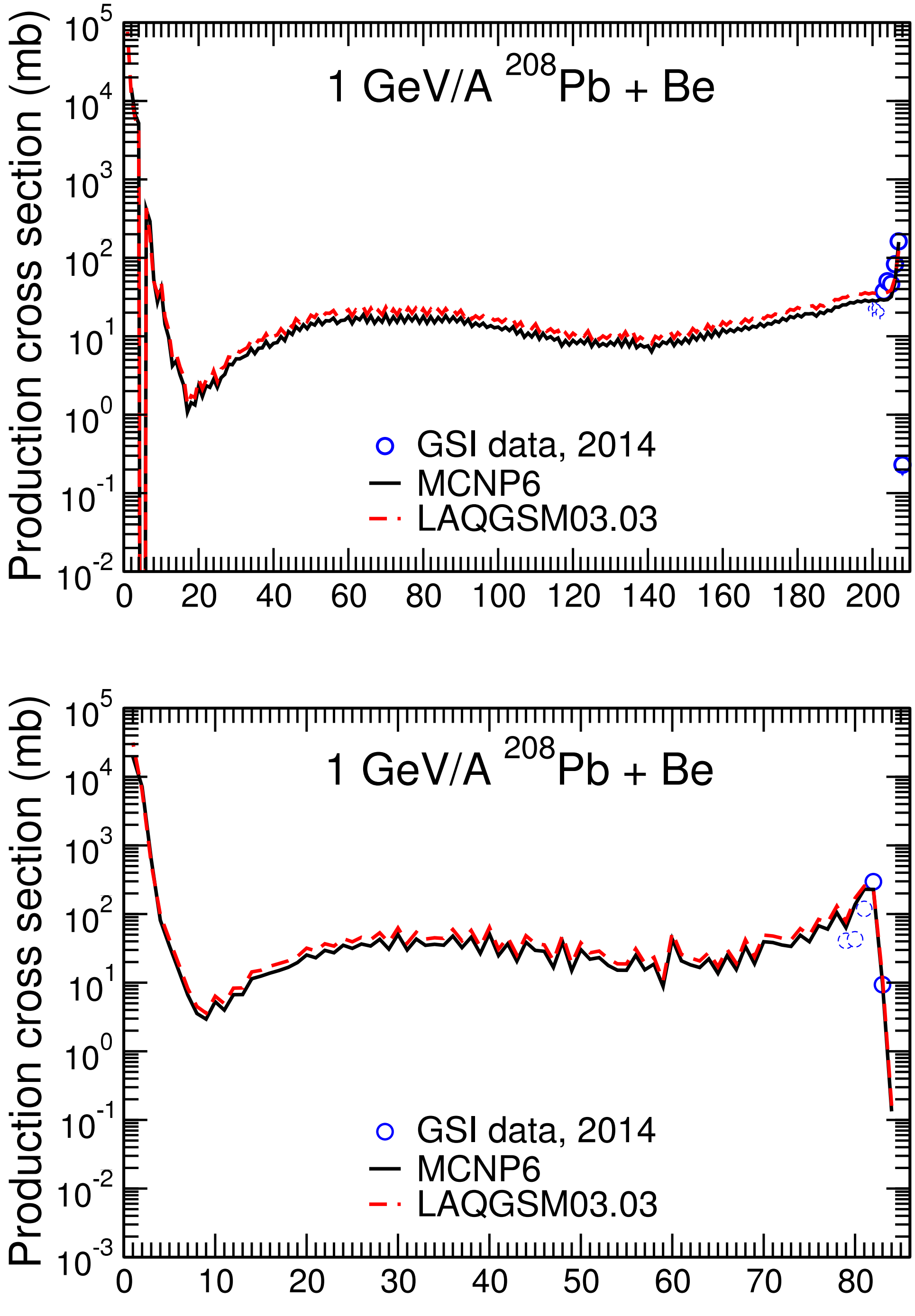


Figure 11: Comparison of calculated by MCNP6 and bf LAQGSM03.03 used as a stand alone code A- and Z-distributions of all products from the reaction 1 GeV/nucleon ^{208}Pb + ^{9}Be with a rough estimate of several experimental values for such characteristics obtained summing the measured [31] (symbols) yields of only a neutron-rich part of all products (see more details in the text) from this reaction, as indicated.

3.4. 120 GeV p and π^+ + ^{nat}Cu and ^{nat}Fe

This MCNP6 problem is to test the applicability of MCNP6 using the LAQGSM03.03 event generator to describe spallation reactions induced by protons and pions on Fe and Cu targets at ultra-relativistic energies of 120 GeV, the highest energy were experimental data are available so far for spallation reactions induced by pions. These spallation reactions are of direct relevance in activation studies, since ^{nat}Cu and ^{nat}Fe are commonly employed in high-energy particle accelerators and their surrounding structures. An accurate knowledge of the spallation product inventory within a target is important for many applications: Disposal of material, operation, maintenance, safety and decay heat analysis for neutron spallation sources, activation issues in high-energy particle accelerators, and benchmarking of Monte Carlo codes, like our MCNP6.

Namely, in this test problem, we calculate with MCNP6 using LAQGSM03.03 with the GENXS option the yields of products from reactions induced by 120 GeV/c protons and positive pions on thin natural copper and iron targets. Numerical values of measured data are published Tabs. II and III of the paper [32]. For simplicity, we assume, just as was assumed in the original paper listed above, that the particle energy is of 120 GeV, even if the actual value is slightly lower (its momentum is of 120 GeV/c).

The MCNP6 input files for proton-induced reactions on Cu and Fe are p120Cu_Laq and p120Fe_Laq, with similar input files for reaction induced by positive pions, pip120Cu_Laq and pip120Fe_Laq, presented in subdirectory /VALIDATION_LAQGSM/Inputs/. Let us recall that the GENXS option of MCNP6 requires a second, auxiliary, input file; for this test problems, we use the auxiliary MCNP6 input file inxc97 (for all four reactions), shown in the same subdirectory. All these input files are presented also below.

p120Cu_Laq:

```
MCNP6 test: p + Cu by LAQGSM at 120 GeV, nevtype=66
C To test MCNP6 at the highest energy we have data: PRC 89 (2014) 034612
  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 -------------------------------------------------------------
dbcn 28j 1
  m1   29063 0.6917 29065 0.3083
  sdef erg = 120000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:h 120100
```

```
  mode   h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                   !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc97  nreact on  nescat off
  tropt genxs inxc97
c -----------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 1000000
c  prdmp 2j -1
```

p120Fe_Laq:

```
MCNP6 test: p + Fe by LAQGSM at 120 GeV, nevtype=66
C To test MCNP6 at the highest energy we have data: PRC 89 (2014) 034612
  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 -----------------------------------------------------------------
dbcn 28j 1
  m1   26056 0.91754 26057 0.02119 26058 0.00281
  sdef erg = 120000 par = H dir = 1 pos = 0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:h 120100
  mode   h
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                   !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc97  nreact on  nescat off
  tropt genxs inxc97
c -----------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 1000000
c  prdmp 2j -1
```

pip120Cu_Laq:

```
MCNP6 test: pip + Cu by LAQGSM at 120 GeV, nevtype=66
C To test MCNP6 at the highest energy we have data: PRC 89 (2014) 034612
  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 ---------------------------------------------------------------
dbcn 28j 1
  m1   29063 0.6917 29065 0.3083
  sdef erg = 120000 par = / dir = 1 pos = 0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:/ 121000
  phys:h 121000
  mode   /
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc97  nreact on  nescat off
  tropt genxs inxc97
c ---------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 1000000
c  prdmp 2j -1
```

pip120Fe_Laq:

```
MCNP6 test: pip + Fe by LAQGSM at 120 GeV, nevtype=66
C To test MCNP6 at the highest energy we have data: PRC 89 (2014) 034612
  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 ---------------------------------------------------------------
```

```
dbcn 28j 1
  m1   26056 0.91754 26057 0.02119 26058 0.00281
  sdef erg = 120000 par = / dir = 1 pos = 0 0 0 vec 0 0 1
  imp:n 1 1 0
  imp:h 1 1 0
  phys:/ 121000
  phys:h 121000
  mode   /
LCA  2 1 5j -1 1j 1    $ use LAQGSM, nevtype = 66                  !!!
lcb  0 0 0 0 0 0
lea  2j 0
c  tropt genxs inxc97  nreact on  nescat off
  tropt genxs inxc97
c ---------------------------------------------------------------
  print 40 110 95
c  nps 1000
  nps 1000000
c  prdmp 2j -1
```

inxc97:

```
MCNP6 test: p + Te by LASQGSM03.03 at 23 GeV, 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 /
```

We calculated this test problem with MPI using 8 nodes, 64 processors, on the "Moonlight" supercomputer of LANL. The output files, p120Cu_Laq.mpi.o, p120Fe_Laq,mpi.o, pip120Cu_Laq.mpi.o, and pip120Fe_Laq,mpi.o, are presented in subdirectory: /VALIDATION_LAQGSM/Templates/LINUX/.

The MCNP6 individual cross sections for the production of different isotopes are printed (in barns) in the corresponding portion of the table entitled "Distribution of residual nuclei" of the output file. Note that some of the measured cross sections are not "individual", but are "cumulative", i.e., they contain contributions from short-lived radioactive precursors. To help plotting our MCNP6 results with xmgrace, we copy the MCNP6 values for all measured (only) products in separate files, summing the corresponding individual cross sections to get cumulative values (individual cross sections are labeled in the our plots with an "i", while cumulative ones, with a "c"). The cross sections for the production of isotopes ^{41}Ar, ^{42}K, ^{43}K, ^{43}Sc, ^{44}Sc, ^{47}Sc, ^{48}Cr, ^{48}Sc, ^{52}Mn, ^{55}Co, ^{56}Mn, ^{57}Ni, ^{58}Co, and ^{61}Cu from reactions induced by protons on ^{nat}Cu are presented in the file 120pCu.M6cum.dat, in a sequential order, with ^{41}Ar as No. 1 up to ^{61}Cu as No. 14. Similar MCNP6 results for reactions induced by pions are shown in a similar way in the file 120pipCu.M6cum.dat. Similar MCNP6 results for reactions on ^{nat}Fe are presented in the files 120pFe.M6cum.dat and 120pipFe.M6cum.dat, for protons and pions, respectively (for 16 measured products on Fe, from ^{24}Na, as No. 1, up to ^{55}Co, as No. 16).

Experimental data are presented in files with similar names, simply using in their names "e" instead of "M6cum".

Template for plotting all these results compared with the measured data using xmgrace are presented in files 120p_Cu-cum.fig, 120pip_Cu-cum.fig, 120p_Fe-cum.fig, and 120pip_Fe-cum.fig, respectively.

Postscript files generated by xmgrace for the four plots are presented in files with similar names, simply using in their names extensions "ps" instead of "fig". To ease an overview of all these product yields, we provide also summary files 120GeV-Cu.pdf and 120GeV-Fe.pdf which shows cross sections for reactions induces by both protons and pions on Cu and Fe, respectively. These summary pdf files were produced with the LaTeX files 120GeV-Cu.tex and 120GeV-Fe.tex using the listed above *.ps files as input.

As the experimental yields of products are measured only for 14 ions from Cu and 16 ions from Fe, we can not integrate (sum) the measured cross sections over the charge of the products to get a good estimation of experimental A-distribution of all products from these reactions, or to integrate (sum) the measured yields over the mass number of products, to get experimental Z-distribution of products. However, we can do so for the measured (mostly, near the target nuclei) values of A and Z of products to get a qualitative rough estimation of experimental A- and Z-distribution of products from these reactions. Taking into account that A- and Z-distributions of all products from any nuclear reactions are very useful from a theoretical point of view to understand better the mechanisms of such reactions, we performed such an "integration" of the measured cross sections from p + ^{nat}Fe (only; more products were measured from ^{nat}Fe than from ^{nat}Cu) and compare them with calculated A- and Z-distributions of all products calculated by MCNP6. Experimental A- and Z-distributions of several products from p + ^{nat}Fe are presented in the files 120pFe.exp.A.dat and 120pFe.exp.Z.dat, respectively. A- and Z-distributions of all products calculated by MCNP6 from this reaction are shown in the files 120pFe.M6.A.dat and 120pFe.M6.Z.dat, respectively. Template for plotting all these results compared with the measured data using xmgrace are presented in files 120GeVpFe.A.fig and 120GeVpFe.Z.fig, respectively. Postscript files generated by xmgrace for the two plots are presented in files with similar names, simply using in their names extensions "ps" instead of "fig". To ease an overview of all these product yields, we provide also a summary file 120GeV-Fe.AZ.pdf. It was produced with the LaTeX file 120GeV-Fe.AZ.tex using the listed above *.ps files as input.

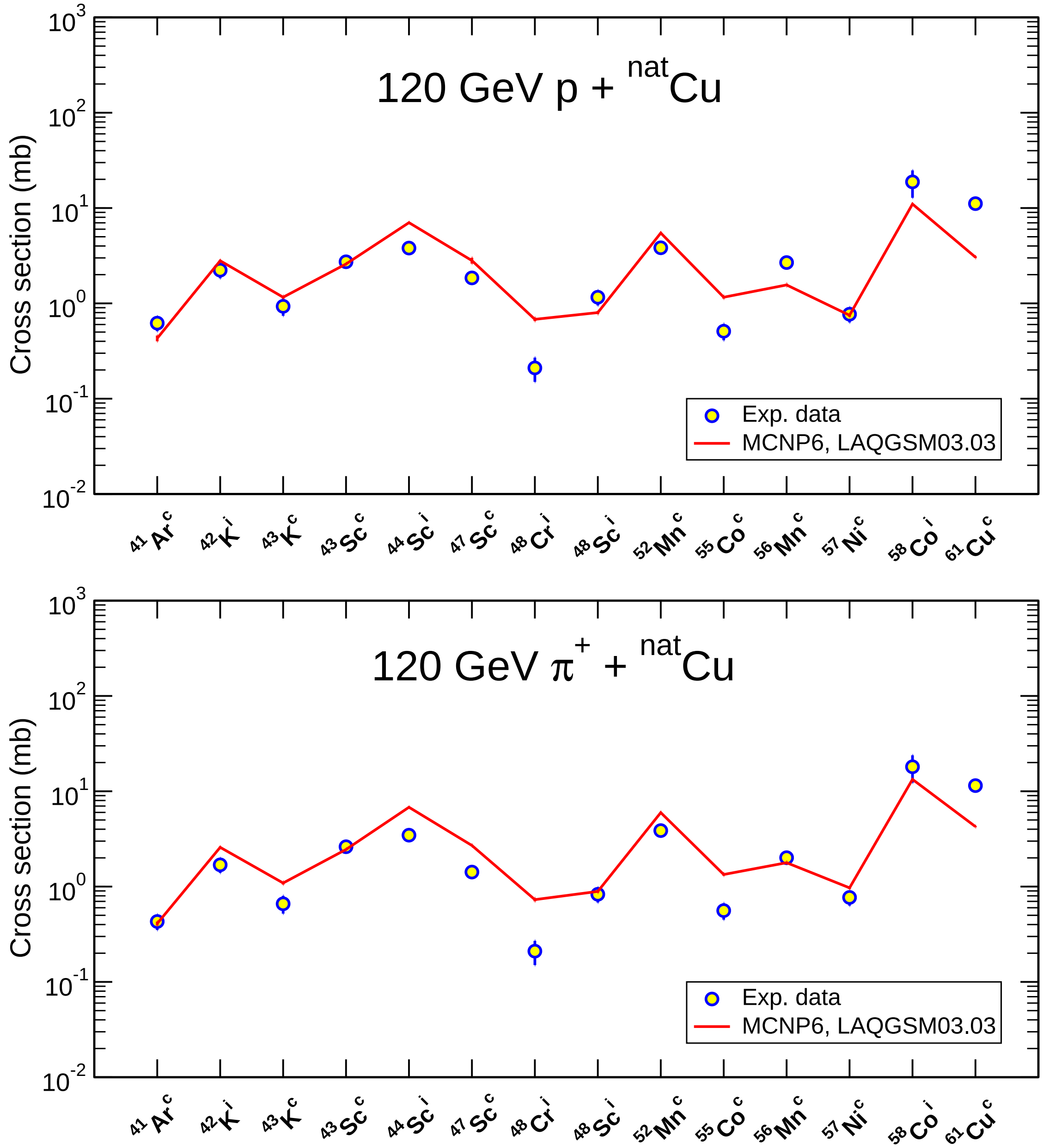


Figure 12: Detailed comparison between all cross section measured in Ref. [32] from interaction of 120 GeV protons and positive pions with ^{nat}Cu (filled circles) and those calculated by MCNP6 using the LAQGSM03.03 event-generator (red lines), as indicated.

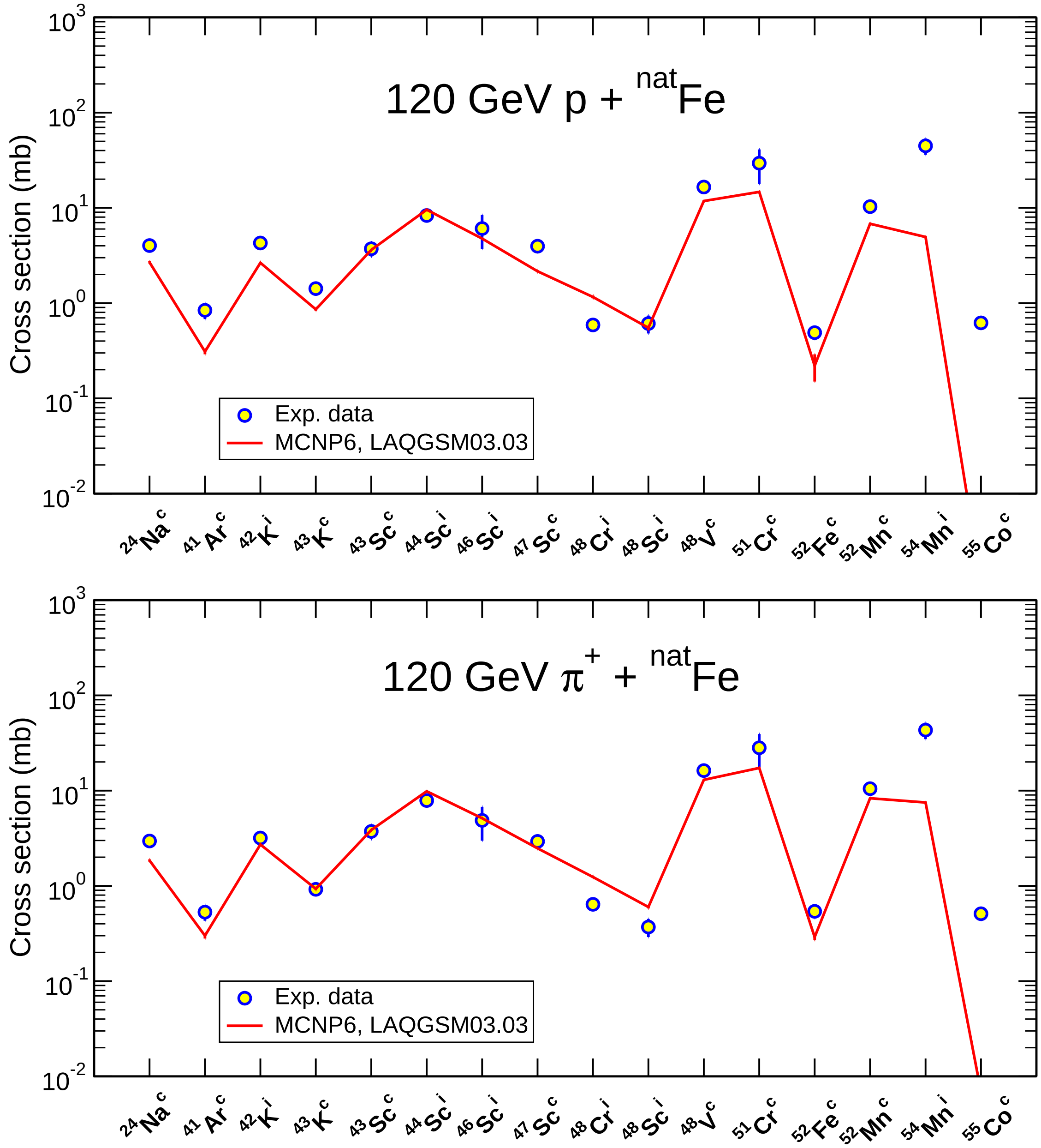
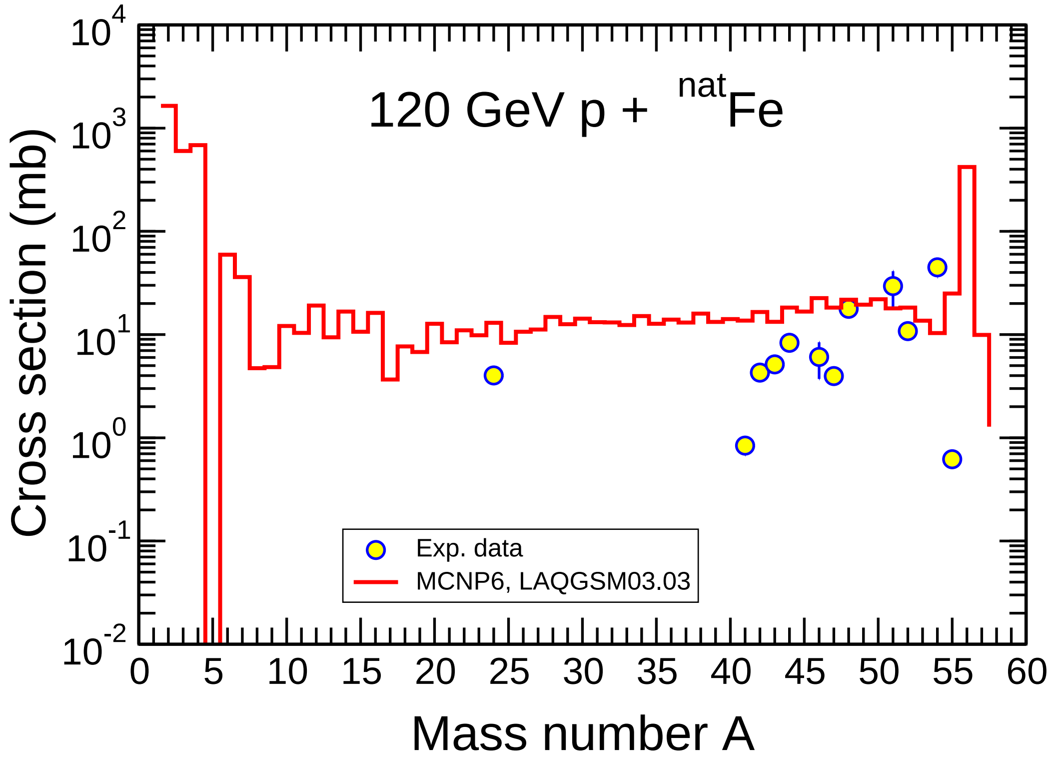


Figure 13: Detailed comparison between all cross section measured in Ref. [32] from interaction of 120 GeV protons and positive pions with ^{nat}Fe (filled circles) and those calculated by MCNP6 using the LAQGSM03.03 event-generator (red lines), as indicated.



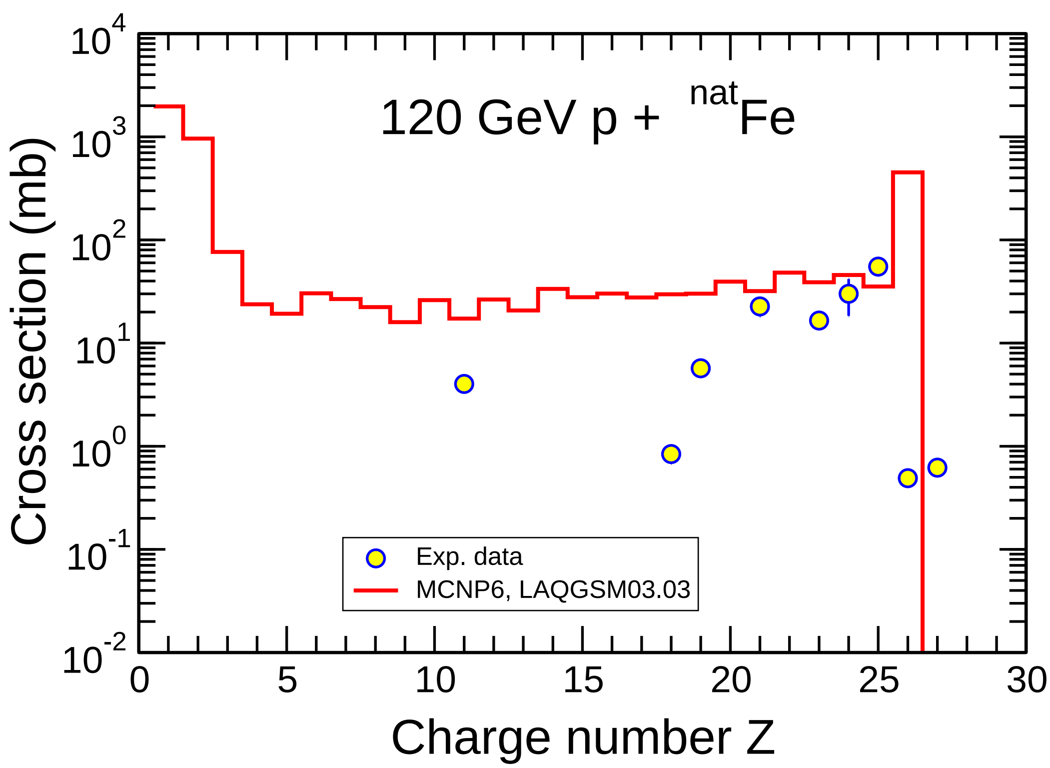


Figure 14: Experimental mass- and charge-number distributions of yields of all products measured in Ref. [32] from the 120 GeV p + ^{nat}Fe reaction (filled circles) compared with results by MCNP6 using the LAQGSM03.03 event-generator (red histograms), as indicated.

4. Conclusion

The 1.1 beta Version of MCNP6 has been validated and verified against a number of intermediate and high-energy experimental data. In the present primer, in Sections 2, we show 5 examples of test problems for MCNP6 using the Cascade-Exciton Model (CEM) event-generator, CEM03.03 and one example of results calculated using the Bertini+Dresner+RAL and INCL+ABLA event generators of MCNP6. Another 5 problems for the 1.1 beta Version of MCNP6 using the latest modifications of the Los Alamos version of the Quark-Gluon String Model (LAQGSM) event-generator LAQGSM03.03 are presented in Section 3.

We found that the 1.1 beta version MCNP6 describes reasonably well various measured reactions induced by protons, pions, and heavy-ions at incident energies from 10 MeV to about 120 GeV/nucleon and agrees very well with similar results obtained with CEM03.03 and LAQGSM03.03 used as stand alone codes. Most of several computational bugs and more serious physics problems observed during our current V&V have been fixed. We continue our work to solve all the known problems before the next distribution of MCNP6 to the public via RSICC at Oak Ridge.

From the results presented here as well as in Refs. [4, 5, 6, 7], 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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