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Title: Validation and Verification of MCNP6 Against Intermediate and High-Energy Experimental Data and Results by Other Codes

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VALIDATION AND VERIFICATION OF MCNP6 AGAINST INTERMEDIATE AND HIGH-ENERGY EXPERIMENTAL DATA AND RESULTS BY OTHER CODES

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ABSTRACT

MCNP6, the latest and most advanced LANL transport code representing a recent merger of MCNP5 and MCNPX, has been Validated and Verified (V&V) against a variety of intermediate and high-energy experimental data and against results by different versions of MCNPX and other codes. In the present work, we V&V MCNP6 using mainly the latest modifications of the Cascade-Exciton Model (CEM) and of the Los Alamos version of the Quark-Gluon String Model (LAQGSM) event generators CEM03.02 and LAQGSM03.03. We found that MCNP6 describes reasonably well various reactions induced by particles and nuclei at incident energies from 18 MeV to about 1 TeV per nucleon measured on thin and thick targets and agrees very well with similar results obtained with MCNPX and calculations by CEM03.02, LAQGSM03.01 (03.03), INCL4 + ABLA, and Bertini INC + Dresner evaporation, EPAX, ABRABLA, HIPSE, and AMD, used as stand alone 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 MCNP6 is distributed to the public.

Key Words: validation, verification, MCNP6, MCNPX, CEM03.02, LAQGSM03.03

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 Los Alamos transport code representing a merger of MCNP5 [3] and MCNPX [4]. The work on MCNP6 is not yet completed; we continue to solve the observed problems in the current version of MCNP6 and to develop and improve it further, with a plan to make it available officially to the users via RSICC at Oak Ridge, TN, USA, during 2011.

Before distributing MCNP6 to the public, we must test and validate it on as many test-problems as possible, using reliable experimental data. Extensive Validation and Verification (V&V) of our low energy transport code MCNP5 has been performed and published for many different test-problems involving interactions of neutrons, photons, and electrons with thick and thin targets, therefore V&V of MCNP6 for such problems is important but not very critical. On the other hand, our high-energy transport code, MCNPX, was not been tested against experimental data so

extensively, especially for high-energy processes induced by protons, and heavy-ions. More important, MCNP6 uses the latest modifications of the Cascade-Exciton Model (CEM) and of the Los Alamos version of the Quark-Gluon String Model (LAQGSM) event generators CEM03.02 and LAQGSM03.03 [5], and they were not tested extensively in MCNPX. This is why it is necessary to V&V MCNP6 at intermediate and high energies, to test how CEM03.02 and LAQGSM03.03 work in MCNP6 and to make sure that the latter properly transports energetic particles and nuclei through the matter.

A description of different versions of our CEM and LAQGSM event generators with many useful references may be found in our recent lecture [5]. Let's us recall here only their main assumptions. The basic version of both our CEM and LAQGSM event generators is the so-called "03.01" version, namely CEM03.01 and LAQGSM03.01. CEM describes reactions induced by nucleons, pions, and photons at energies below ~ 5 GeV. LAQGSM describes reactions induced by almost all elementary particles as well as by heavy ions at incident energies up to ~ 1 TeV/nucleon. However, our numerous tests show that CEM provides a little better agreement than LAQGSM with experimental data for reactions induced by $p, n, \pi,$ and γ at energies below several GeV, therefore we recommend using CEM in MCNP6 to describe such reaction at energies below ~ 3.5 GeV, and using LAQGSM at higher energies and for projectiles not allowed by CEM.

Both CEM and LAQGSM assume that nuclear reactions occur generally in three stages. The first stage is the IntraNuclear Cascade (INC), completely different in CEM and LAQGSM, 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 complete, CEM03.01 uses the coalescence model to "create" high-energy $d, t,$ ^{3}He, and ^{4}He via final-state interactions among emitted cascade nucleons, already outside of the target. The subsequent relaxation of the nuclear excitation is treated in terms of an improved version of the modified exciton model of preequilibrium decay followed by the equilibrium evaporation/fission stage of the reaction. But if the residual nuclei after the INC have atomic numbers with $A < 13$, CEM and LAQGSM use the Fermi breakup model to calculate their further disintegration instead of using the preequilibrium and evaporation models.
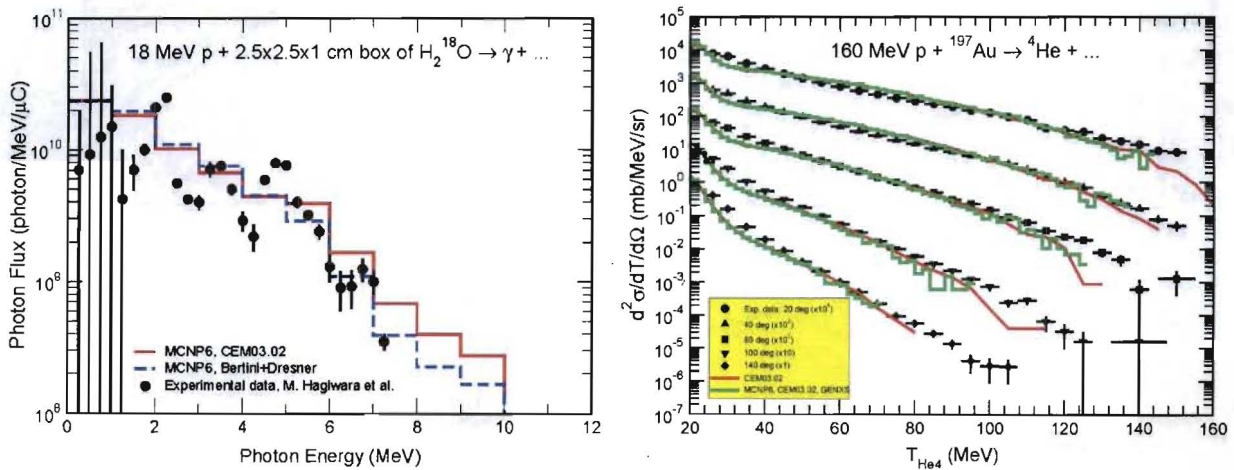
The main difference of the following, so-called "03.02" versions of CEM and LAQGSM from the basic "03.01" versions is that the latter use the Fermi breakup model to calculate the disintegration of light nuclei instead of using the preequilibrium and evaporation models only after the INC, when A < 13. It does 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 < 13. This problem was solved in the 03.02 versions of CEM and LAQGSM, where the Fermi breakup model is used also during the preequilibrium and evaporation stages of a reaction, when we get an excited nucleus with A < 13. Finally, the latest, 03.03 versions of our codes do not produce any unstable products via very asymmetric fission, allowed in very, very rare cases by the previous versions, and have several bugs fixed that were observed in the previous versions. More details and useful references on CEM and LAQGSM may be found in Ref. [5].

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2. VALIDATION AND VERIFICATION OF MCNP6

In the present work, we present only a small part of our recent extensive V&V of MCNP6 [6, 7] using as event-generators mostly CEM03.02 and LAQGSM03.03. For convenience, we start with the V&V of MCNP6 using CEM, followed by results using LAQGSM.

2.1. CEM Test Problems

Let us start our presentation of the V&V of MCNP6 using CEM with a test-problem at a very low energy of 18 MeV, namely the energy spectra of prompt γ-rays from a thick $H_2{}^{18}O$ target bombarded with 18 MeV protons. This problem is of interest for positron emission tomography (PET), as ^{18}F used in PET is usually produced via the $^{18}O(p,n)^{18}F$ reaction and energy spectrum and angular distribution of neutrons and photons produced in this reaction should be estimated for radiation safety and clearance of the production facility [8]. Generally, at energies below 150 MeV, MCNP6 uses data libraries instead of event-generators. But in cases when we do not have any data libraries for a particular isotope, MCNP6 must use an event-generator, therefore it is necessary to test how well CEM works in MCNP6 even at such low energies.
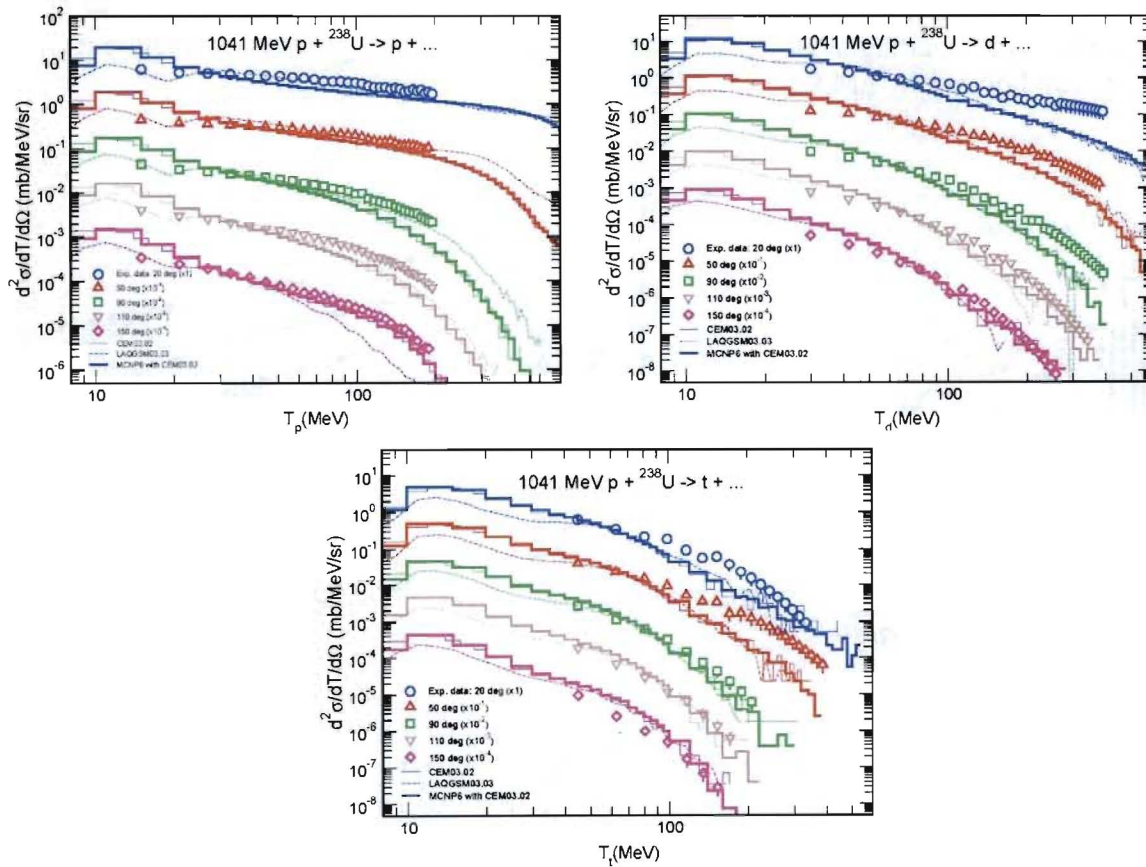

Figure 1 Comparison of the measured [8] energy spectra of prompt γ-rays from a thick $H_2{}^{18}O$ target bombarded with 18 MeV protons with our MCNP6 results using the CEM03.02 and the Bertini+MPM+Dresner [9,10,11] event-generators (left plot) and experimental [12] double-differential spectra of ^{4}He at 20, 40, 60, 100, and 140 degrees from interactions of 160 MeV protons with a thin ^{197}Au target compared with calculations by CEM03.02 as presented at the recent International Benchmark of Spallation Models [13] and with our current results by MCNP6 using CEM03.02 (right plot), as indicated.

As one can see from the left plot of Fig. 1, MCNP6 with CEM03.02 describes well the recently measured [8] spectrum of prompt γ-ray from this reaction and agrees reasonably with similar results obtained using the Bertini+MPM+Dresner [9,10,11] event-generators.
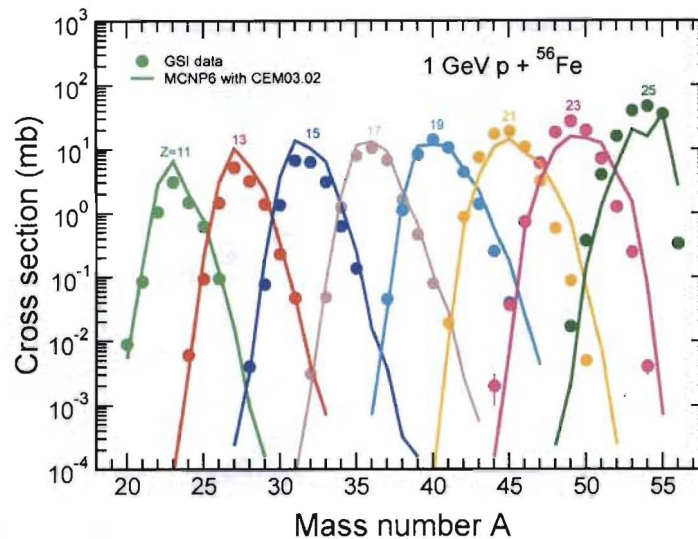
The right plot in Fig. 1 shows examples of ^{4}He spectra emitted from the 160 MeV $p + {}^{197}$Au reaction at five angles as calculated by MCNP6 using CEM03.02 compared with experimental data [12] and with results by CEM03.02 used as a stand alone code as presented at the recent International Benchmark of Spallation Models [13]. Such reactions are of interest for many applications where gas production is important and should be properly accounted; we see that MCNP6 using CEM03.02 describes them very well.

Fig. 2 shows examples of $p, d,$ and t spectra from the 1041 MeV $p + {}^{238}$U reaction calculated by MCNP6 using CEM03.02 compared with experimental data [14] and results by CEM03.02 and LAQGSM03.3 used as stand alone codes. Such reactions are of interest for several applications, especially the cases when gas production must be properly accounted; we see that MCNP6 describes them well.

Figure 2 Experimental [14] double-differential spectra of protons, deuterons, and tritons at 20°, 50°, 90°, 110°, and 150° from interactions of 1.041 GeV protons with a thin ^{238}U target compared with calculations by CEM03.02 and LAQGSM03.03 used as stand alone codes and with current results by MCNP6 using the CEM03.02 event-generator, as indicated.

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Fig. 3 shows examples of yields of eight elements produced from the reaction of 1 GeV/nucleon $^{56}Fe + p$ calculated with MCNP6 using CEM03.02 compared with recent GSI measurements [15]. Such reactions are of interest to for many technical applications using iron as a construction material, and we see that MCNP6 using CEM03.02 describes them well.

Figure 3 The measured [15] cross sections for the production of elements with the charge Z equal to 11, 13, 15, 17, 19, 21, 23, and 25 (filled color circles) from the reaction 1 GeV/A $^{56}Fe+p$ compared with results MCNP6 using the CEM03.02 event-generator, as indicated.
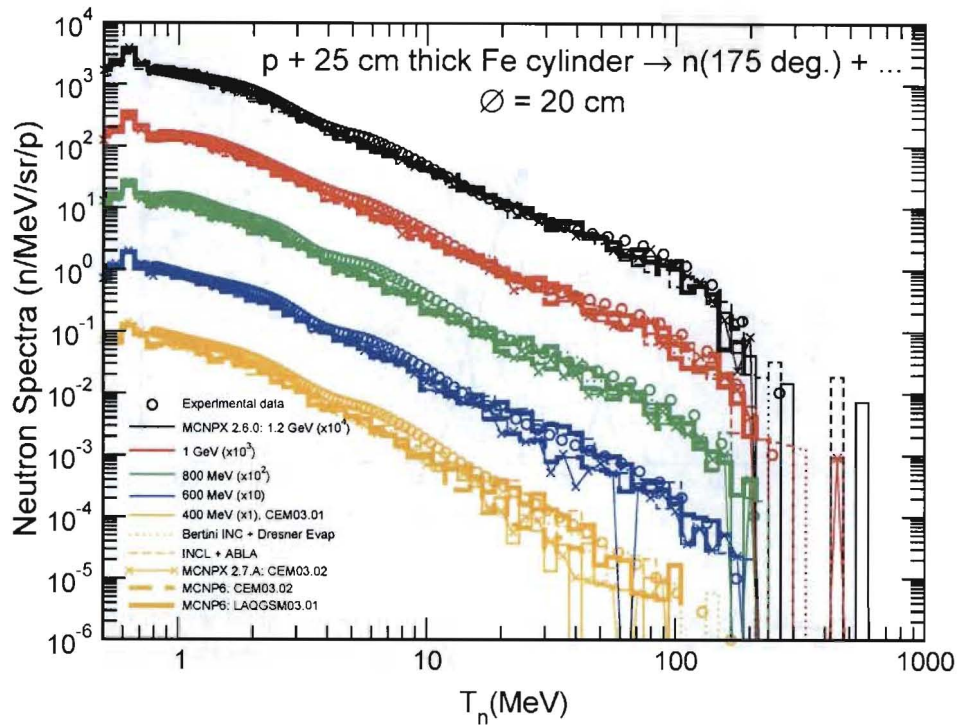
Fig. 4 shows backward angle spectra of neutrons from a thick Fe cylinder bombarded by protons of 400, 600, 800, 1000, and 1200 MeV calculated by MCNP6 using the CEM03.02 and the LAQGSM03.01 event-generators compared with experimental data [16] and results by MCNPX 2.7.A [17] using the CEM03.02, and by the 2.6.0 version of MCNPX [18] using the CEM03.01, Bertini INC [9] followed by the Multistage Preequilibrium Model (MPM) [10] and the Dresner evaporation [11], as well as using the INCL+ABLA [19, 20] event-generators. Such processes are of interest to shielding applications in predicting personnel radiation exposure from backward fluxes, to test how the event generators work in this "difficult" kinematics region, and to study the mechanisms of cumulative particle production (an academic problem under investigation for about four decades but still with many open questions). We see that MCNP6 results agree very well with the measured data and calculations by other codes. Very similar results were obtained recently also for a thick Pb target [21].

2.2. LAQGSM Test Problems

Now, let us present several results on V&V of MCNP6 using LAQGSM. Fig. 5 shows measured [14] double-differential spectra of protons at 30°, 70°, 90°, 110°, and 150° from interaction of a 1042 MeV/nucleon ^{40}Ar beam with a thin ^{40}Ca target compared with results by MCNP6 using LAQGSM03.01 and by LAQGSM03.03 used as a stand alone code. This V&V problem tests the

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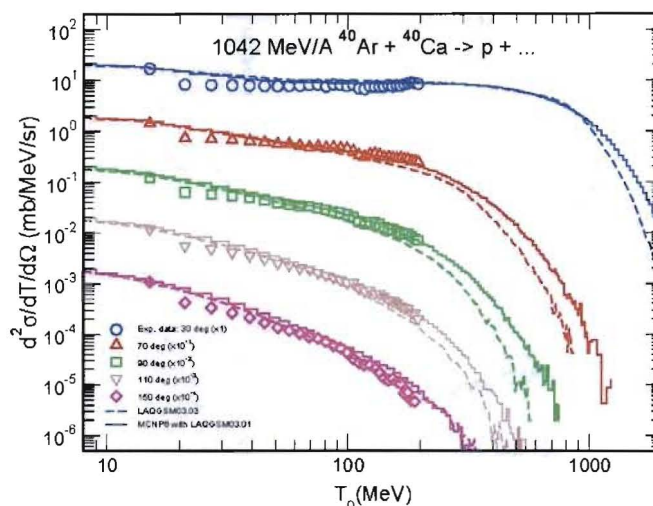Nuclear Science and Engineering (M&C 2011), Rio de Janeiro, RJ, Brazil, 2011

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applicability of MCNP6 to calculate production of protons from intermediate energy heavy-ion induced reactions for different NASA (shielding for missions in space), medical (cancer treatment with heavy-ions), FRIB (Facility for Rare Isotope Beams), and for several other U.S. DOE applications; we see that MCNP6 describes such reactions very well.

Figure 4 Experimental [16] 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 CEM03.02 and the LAQGSM03.01 event-generators, by MCNPX 2.7.A [17] using the CEM03.02 event-generator, and by the 2.6.0 version of MCNPX [18] using the CEM03.01, Bertini INC [9] followed by the Multistage Preequilibrium Model (MPM) [10] and the evaporation model described with the Dresner code EVAP [11], and by the INCL+ABLA [19, 20] event-generators, as indicated in legend.

In Fig. 6., we test the capability of MCNP6 to describe spectra of complex particles from reactions induced by heavy ions at intermediate energies. Namely, we compare the experimental [14, 22] double-differential spectra of d, t, ^{3}He, and ^{4}He from thin ^{64}Cu and ^{238}U targets bombarded with ^{20}Ne beams of several energies compared with results by MCNP6 using the LAQGSM03.01 event-generator and by LAQGSM03.03 used as a stand alone code. The interest in such types of reactions is very similar to the one listed above regarding Fig. 5. In addition, we like to note that light charged particles, i.e., p, d, t, ^{3}He, and ^{4}He from any reactions are of a major concern for material damage, as helium can cause swelling in structure materials; tritium is often an issue from a radioprotection point of view. We see that MCNP6 describes such reactions very well.

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Fig. 7. presents experimental [23] yields of the Si ions from the 140 MeV/nucleon $^{40}Ca + ^{9}Be$ reaction compared with results by MCNP6 using the LAQGSM03.03 and by LAQGSM03.03 used as a stand alone code, as well as results by EPAX [24], ABRABLA [25], HIPSE [26], and AMD [27] from [23]. Such reactions are of interest for FRIB (a modification and continuation of the former Rare Isotope Accelerator (RIA) project) and the measurements [23] were performed especially to support RIA. We see that MCNP6 describes these measurements very well and is not worse than other models. We obtained similar results for many other reactions measured for FRIB/RIA at the National Superconducting Cyclotron Laboratory (NSCL) in East Lansing, MI, USA, allowing us to conclude that MCNP6 can be a useful and reliable tool for FRIB simulations.
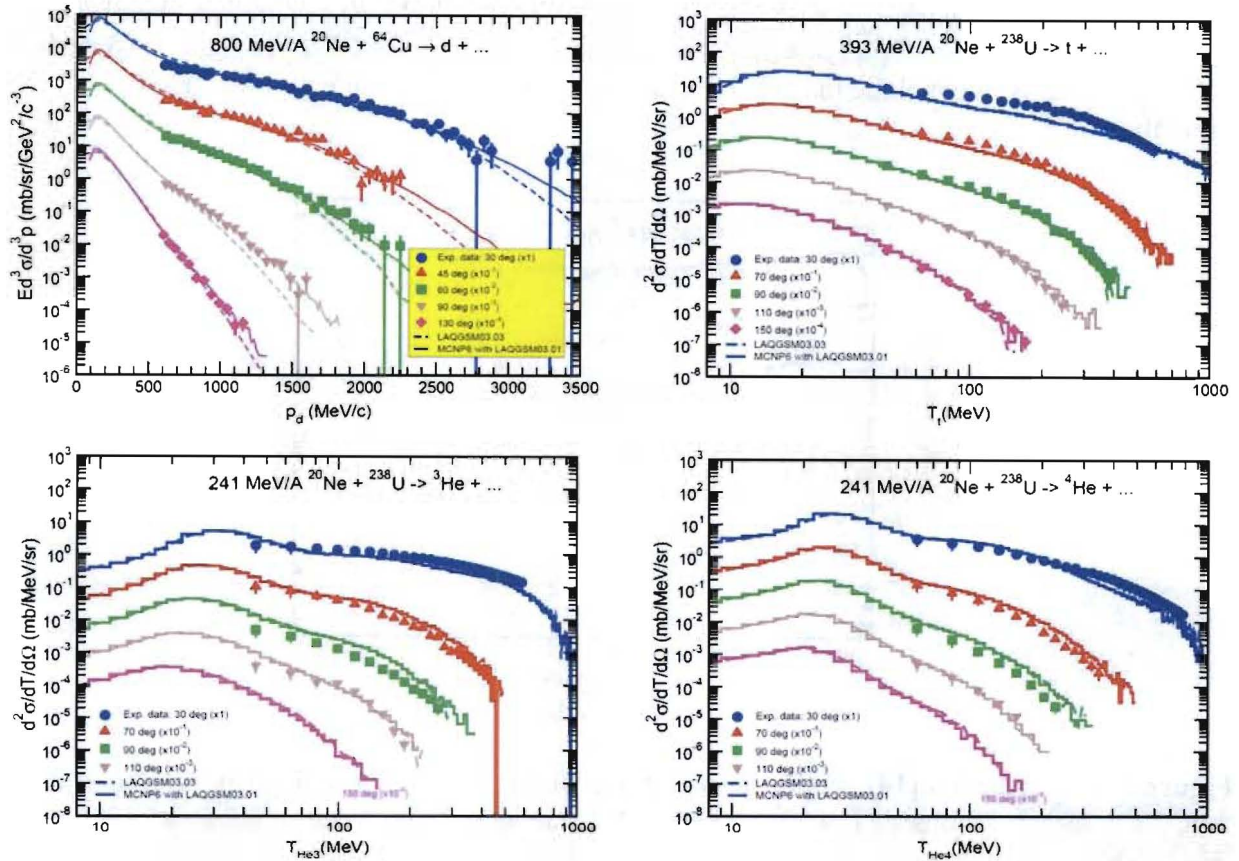

Figure 5 Experimental [14] proton spectra at 30, 70, 90, 110, and 150 degrees (symbols) from a thin ^{40}Ca target bombarded with a 1042 MeV/nucleon ^{40}Ar beam compared with results LAQGSM03.03 used as a stand alone code and by MCNP6 using the LAQGSM03.01 event-generator, as indicated.

2.3. Some Physics Problems and Bugs Fixes

Naturally, during our extensive V&V work of MCNP6, we discovered some bugs and more serious physics problems in MCNP6 or/and in MCNPX. Most of them have been fixed; we continue our work to solve all the observed problems before MCNP6 is distributed to the public. Let us present below only two examples. Fig. 8 shows the experimental [28] spectra of neutrons at 5°, 10°, 20°, 30°, 40°, 60°, and 80° from a relatively thin Cu target bombarded with a 600 MeV/nucleon ^{28}Si beam compared with results by MCNP6 using LAQGSM03.03 and by LAQGSM03.01 used as a stand alone code, as well as with calculations by MCNPX 2.7.B [28] using LAQGSM03.01. Dr. Igor Ramec of ORNL, who kindly sent us these (and many other) MCNPX 2.7.B results called our attention to a problem he observed in the MCNPX 2.7.B for neutron spectra at forward angles. For unknown reasons, MCNPX 2.7.B using LAQGSM03.01

strongly overestimates the neutron spectra at forward angles (see the magenta lines in Fig. 8), while LAQGSM03.01 used as a stand alone code describes such spectra very well (see the black lines on Fig. 8). A special investigation by Dr. Mike James of the LANL D-5 Group has identified a previously unobserved error in the implementation of LAQGSM03.01 in MCNPX, which caused that problem. This implementation error was fixed by Mike James in a
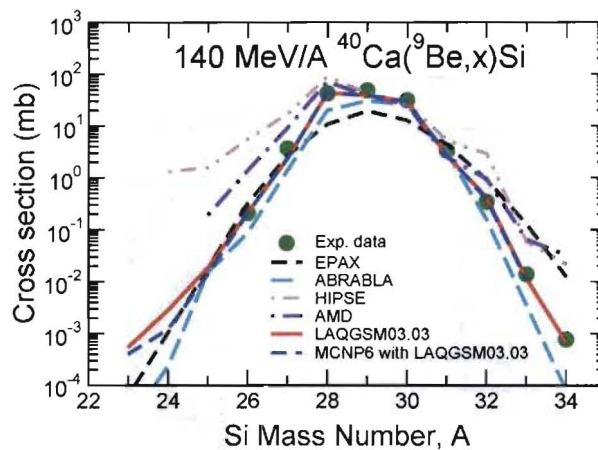

Figure 6. Experimental [14, 22] double-differential spectra of deuterons, tritons, ^{3}He, and ^{4}He at five different angles (symbols) from thin ^{64}Cu and ^{238}U targets bombarded with ^{20}Ne beams of listed energies compared with results by LAQGSM03.03 used as a stand alone code and by MCNP6 using the LAQGSM03.01 event-generator, as indicated (no ^{3}He and ^{4}He measured data are available at 150°, so we present for this angle only our predictions).

very recent version of MCNPX by replacing completely the relatively old LAQGSM03.01 with the latest version LAQGSM03.03. Such a replacement was also done in MCNP6 by Dick Prael. As we can see from Fig. 8, the current version of MCNP6 describes these measured neutron spectra very well, just as LAQGSM03.03 and LAQGSM03.01 do as stand alone codes.

Fig. 9. shows an example of another problem solved recently in MCNP6. For historical reasons,

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the initial version of MCNP6 would "tally" (i.e., would count, and provide results in the output file) particles together with antiparticles from any nuclear reactions, as would MCNPX and MCNP5. This was needed and very useful for some of our applications. But for other applications, especially at high-energies, this feature is nor convenient at all, as it does not allow users to easily get separate results for particles and antiparticles. This issue was corrected recently in MCNP6 by Dr. Grady Hughes (in the very last release of MCNPX, MCNPX 2.7.D, this problem was also addressed, but in a different way). As we see from Fig. 9, the current version of MCNP6 is able to calculate without problems separate spectra of π^+ and π^- from nuclear reactions. In this particular example, we compare the experimental [22] spectra of π^+ and π^- from a thin C target bombarded with a 800 MeV/nucleon ^{12}C with results by MCNP6 using LAQGSM03.01 and with calculations by LAQGSM03.03 used as a stand alone code; we see quite reasonable agreement.

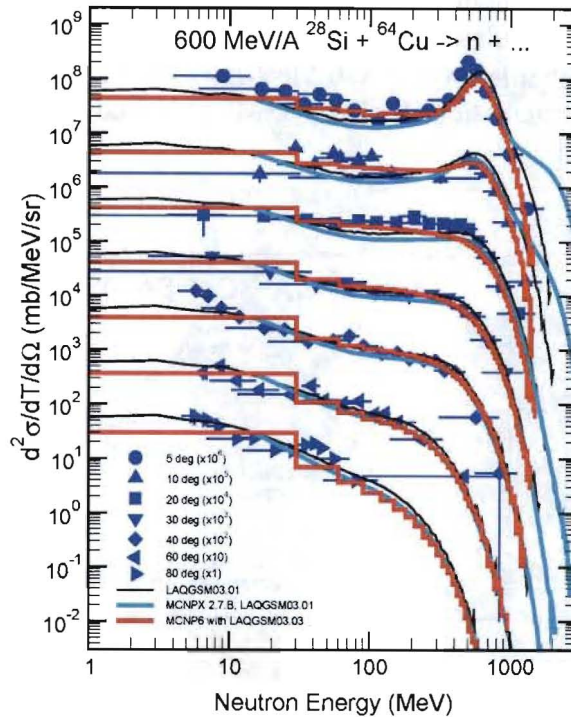**Figure 7.** Experimental [23] mass number distribution of the Si ions yield (green filled circles) from the 140 MeV/A ^{40}Ca + ^{9}Be reaction compared with results by EPAX [24], ABRABLA [25], HIPSE [26], and AMD [27] from [23], as well as with predictions by LAQGSM03.03 used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

2.4. Reactions at Ultrarelativistic Energies

Finally, let us present in Figs. 10 and 11 two examples of reactions at ultrarelativistic energies. Fig. 10 shows a test of the capability of MCNP6 to describe the same (almost) heavy-ion induced reaction in a very large range of incident energies, namely it provides a comparison of the experimental [29-32] charge distributions of product yields from 559 MeV/nucleon ^{197}Au + Cu, 10.6 GeV/nucleon ^{197}Au + Cu, and from a very similar but at an ultrarelativistic energy of 158 GeV/nucleon ^{208}Pb + Cu reaction compared with results by MCNP6 using the LAQGSM03.03 event-generator and by LAQGSM03.03 used as a stand alone code. Such capabilities of MCNP6 are needed for astrophysical applications, particularly for problems of propagation of cosmic rays through matter. Let us note that the MCNP6 results shown in Fig. 10 represent cross sections of the products from both the projectile and target nuclei, while the LAQGSM03.03
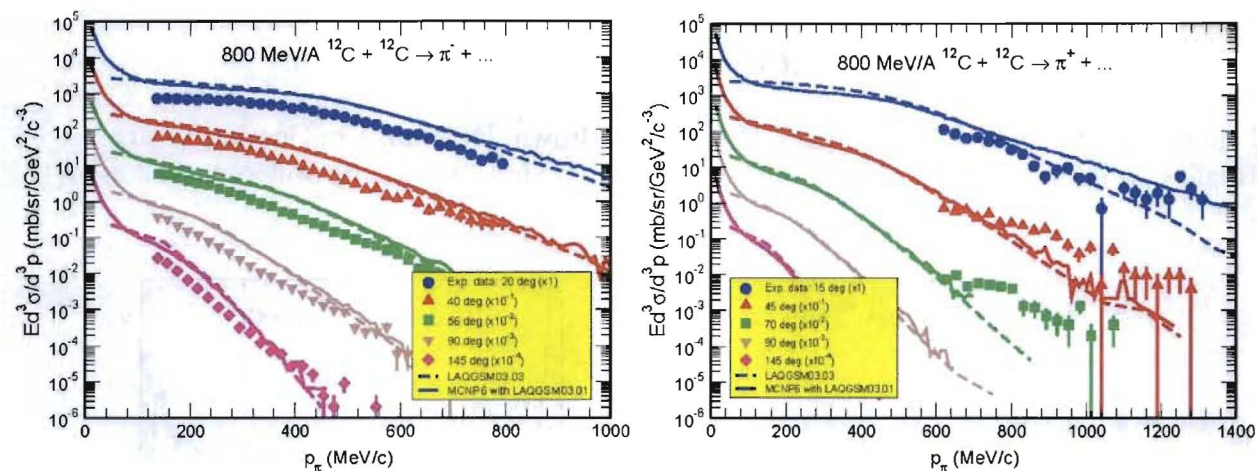
used as stand alone calculated only fragmentation products from the bombarding nuclei. This is why we see a good agreement between the MCNP6 and LAQGSM03.03 results and the measured projectile fragmentation cross sections (i.e., for products heavier than Cu), and a much higher MCNP6 yield of products lighter than Cu than the one calculated by LAQGSM03.03 from only the projectiles.

Figure 8 Experimental [28] neutron spectra at 5°, 10°, 20°, 30°, 40°, 60°, and 80° from the 600 MeV/A ^{28}Si + Cu reaction compared with results by LAQGSM03.01 used as a stand alone code, and with our MCNP6 results using LAQGSM03.03, as well as with results by MCNPX 2.7.B [29] obtained by Dr. Igor Ramec at ORNL using LAQGSM03.01, as indicated.

At the end, we like to present an example of our work still in progress. Namely, Fig. 11 shows a comparison of experimental [34, 35] invariant spectra of K^+ and t from the ultrarelativistic reaction 400 GeV p + ^{181}Ta compared with our preliminary results by MCNP6 using LAQGSM03.03 and with calculations by LAQGSM03.03 used as a stand alone code, as well as with and our 2005 results by LAQGSM03.01 from Ref. [36]. Similar preliminary results are obtained also for the measured p, d, ^{3}He, ^{4}He, K^-, and antiproton spectra from ^{181}Ta, as well as for all measured spectra from C, Al, and Cu (see [34, 35] and references therein and our LAQGSM03.01 results presented in Refs. [36, 37]). In addition to astrophysical applications, such reactions are of great academic interest in studying the production of so called "cumulative particles," i.e., energetic particles at backward angles in the kinematic region forbidden in

interactions of the projectile with free stationary nucleons of the target nucleus. It is believed that cumulative particles contain information needed for the study of the high momentum component of nuclear wave functions, or of collective phenomena in nuclei, or of quark and gluon degrees of freedom. We see that our preliminary results by MCNP6 differ a little from the results obtained with the LAQGSM03.03 used as a stand alone code, requiring more work on MCNP6. But the agreement with the experimental data is reasonably good, especially when considering that to the best of our knowledge, these "cumulative" particle spectra measured at the Fermi National Accelerator Laboratory three decades ago were described simultaneously within

Figure 9. Experimental [22] invariant π^- and π^+ spectra at five different angles (symbols) from a thin C target bombarded with an 800 MeV/nucleon ^{12}C beam compared with results LAQGSM03.03 used as a stand alone code and by MCNP6 using the LAQGSM03.01 event-generator, as indicated (no π^+ measured data are available at 90 and 145 degrees, so we present for this angle only our predictions).

a single approach and without using any "exotic" nuclear-reaction mechanisms for the first time in 2005 by our LAQGSM03.01 [36, 37] and here, with MCNP6 using LAQGSM03.03.
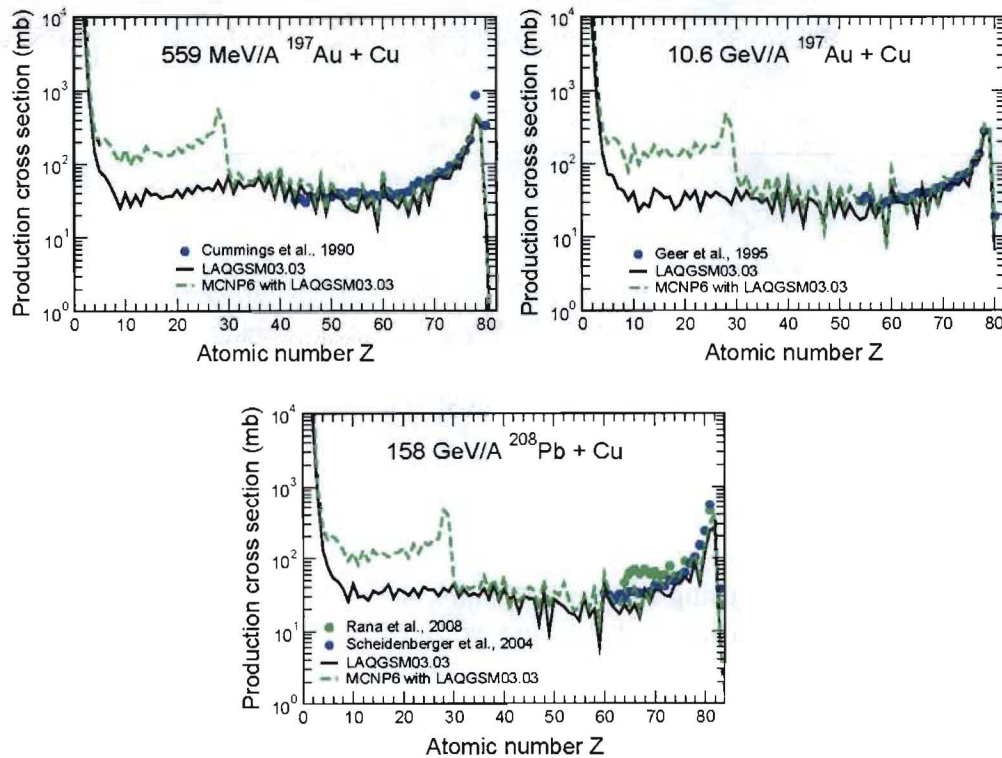
3. CONCLUSIONS

MCNP6, the latest and most advanced LANL 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 work, MCNP6 was tested using mainly the latest modifications of the Cascade-Exciton Model (CEM) and of the Los Alamos version of the Quark-Gluon String Model (LAQGSM) event generators CEM03.02 and LAQGSM03.03. We found that MCNP6 describes reasonably well various reactions induced by particles and heavy-ions at incident energies from 18 MeV to about 1 TeV/nucleon measured on both thin and thick

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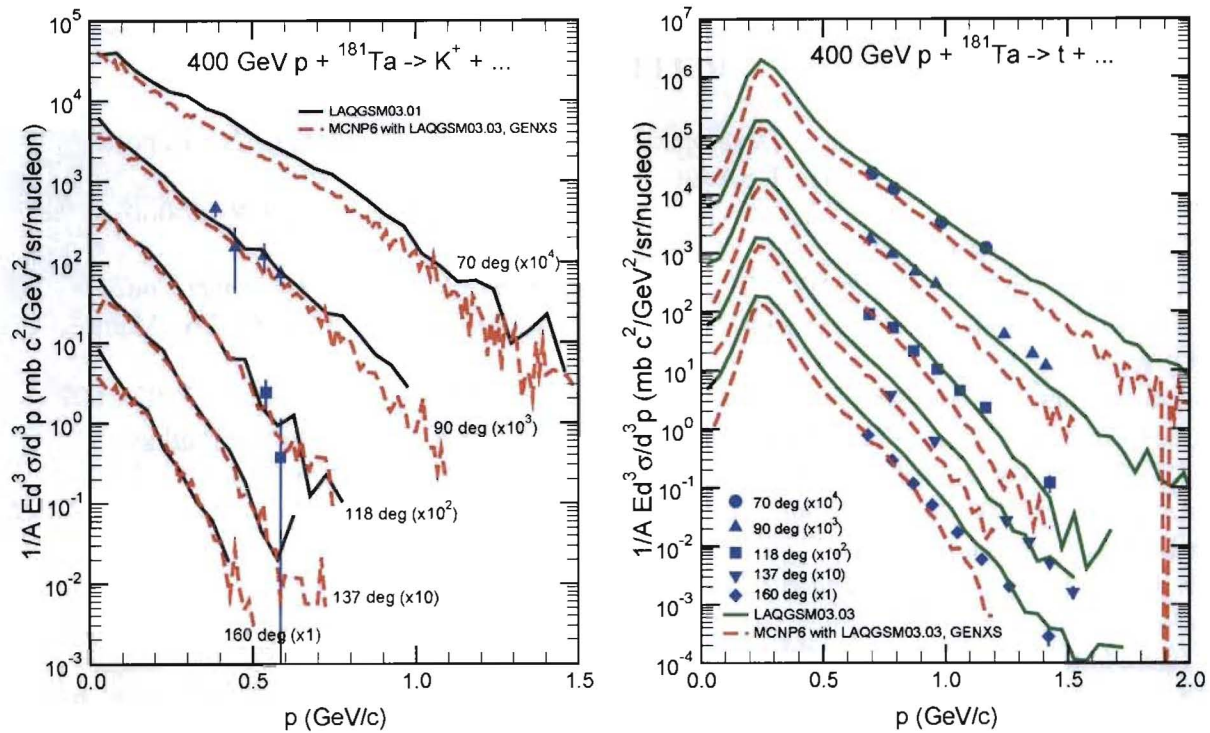Nuclear Science and Engineering (M&C 2011), Rio de Janeiro, RJ, Brazil, 2011

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targets and agrees very well with similar results 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 middle of 2011. From the current V&V, we can conclude that MCNP6 is a reliable and useful 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.

ACKNOWLEDGMENTS

Figure 10. Experimental [30-33] charge distributions of product yields (color filled circles) from 559 MeV/A ^{197}Au + Cu, 10.6 GeV/A ^{197}Au + Cu, and 158 GeV/A ^{208}Pb + Cu reactions compared with results by LAQGSM03.03 used as a stand alone code and by MCNP6 using the LAQGSM03.03 event-generator, as indicated.

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Figure 11. Experimental [34, 35] invariant spectra of K^+ and t from the reaction 400 GeV p + ^{181}Ta (symbols) compared with results by MCNP6 using LAQGSM03.03 (red dashed lines), with calculations by LAQGSM03.03 used as a stand alone code, and with our 2005 results by LAQGSM03.01 from Ref. [36], as indicated. Similar results are obtained also for the measured p, d, ^{3}He, ^{4}He, K^-, and antiproton spectra from ^{181}Ta, as well as for all measured spectra from C, Al, and Cu (see [34, 35] and references therein and our LAQGSM03.01 results in Refs. [36, 37]).

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