EVENT GENERATOR BENCHMARKING FOR PROTON RADIOGRAPHY APPLICATIONS

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Abstract

We have benchmarked the QGSM code and event generators of the MARS and LAHET3 codes as potential candidates for high-energy programs to be used in simulations for the Proton Radiography (PRad) Project. We have compiled from the literature experimental data on spectra of particles emitted from proton-induced reactions at incident energies from 30 GeV to 70 GeV on different nuclei and have performed calculations for all reactions for which we found data with these three codes without any modifications and using only default parameters and standard inputs. Our results (514 plots) show that all three codes describe reasonably most of the studied reactions, though all of them should be further improved before becoming reliable tools for PRad. We present here our conclusions concerning the relative roles of different reaction mechanisms in the production of specific secondary particles. We comment on the strengths and weaknesses of QGSM, MARS, and LAHET3 and suggest further improvements to these codes and to other models.
Introduction

The process of determining the feasibility of Proton Radiography (PRad) [1-3] as the radiographic probe for the Advanced Hydrotest Facility as well as its design and operation require information about spectra of secondary particles produced by high energy protons interacting in the target and structural materials. Reliable models and codes are needed to provide such data. We studied the literature and chose three potential candidates for high-energy codes that may be used in simulations for PRad, namely the Quark-Gluon String Model (QGSM) as developed by Amelin, Gudima, and Toneev [4], the MARS code by Mokhov et al. [5], and a version of the Los Alamos National Laboratory (LANL) transport code LAHET [6], known as LAHET3 [7].

The energy of the proton beam at PRad is supposed to be about 50 GeV. Unfortunately, there are very few measurements of particle spectra for proton-induced reactions exactly at 50 GeV or very close energies. In fact, we found only one published work at 50 GeV, namely spectra of $\pi^-$ and $\pi^+$ measured at 159° from p(50 GeV) + W published in Russian together with pion spectra for other energies and targets, in a Joint Institute for Nuclear Research (Dubna) Communication by Belyaev et al. [8].

With only a few data available at 50 GeV, we benchmarked QGSM, MARS, and LAHET3 against measured spectra of particles emitted from interaction of protons with energies 50 ± 20 GeV, i.e., from 30 to 70 GeV, with all targets for which we found experimental data. Independently of how many spectra were measured in an experiment, we performed calculations with the standard versions of QGSM, MARS, and LAHET3 without any modifications or adjustments, using only default parameters in the input of codes, and calculated double differential cross sections at 0, 4.75, 9, 13, 20, 45, 60, 90, and 159 degrees, angle-integrated energy spectra, and mean multiplicities for emission of n, p, d, t, $^3\text{He}$, $^4\text{He}$, $\pi^+$, $\pi^-$, $K^+$, $K^-$, and $\bar{p}$ for all cases listed below in Table 1. The next Section presents a brief description of the benchmarked codes, followed by results, discussion, and conclusions in the last two Sections.

Benchmarked Codes

QGSM: The core of the QGSM is built on a time-dependent version of the intranuclear cascade model developed at Dubna to describe both particle- and nuclei-induced reactions, often referred in the literature simply as the Dubna intranuclear Cascade Model (DCM) (see [2] and references therein). The DCM models interactions of fast cascade particles (“participants”) with nucleon spectators of both the target and projectile nuclei and includes interactions of two participants (cascade particles) as well. It uses experimental cross sections (or those calculated by the Quark-Gluon String Model for energies above 4.5 GeV/nucleon) for these elementary interactions to simulate angular and energy distributions of cascade particles, also considering the Pauli exclusion principle. When the cascade stage of a reaction is completed, QGSM uses the coalescence model described in [2] to “create” high-energy d, t, $^3\text{He}$, and $^4\text{He}$ by final state interactions among emitted cascade nucleons, already outside of the colliding nuclei. After calculating the coalescence
stage of a reaction, the QGSM moves to the description of the last slow stages of the interaction, namely to preequilibrium decay and evaporation, with a possible competition of fission using the standard version of the Cascade Exciton Model (CEM) \[10\]. But if the residual nuclei have atomic numbers with \( A \leq 13 \), QGSM uses the Fermi break-up model to calculate their further disintegration instead of using the preequilibrium and evaporation models.

**MARS**: The MARS Monte-Carlo code system, being developed over 29 years, allows fast and reliable inclusive and exclusive simulation of three-dimensional hadronic and electromagnetic cascades in shielding, accelerator and detector components in the energy range from a fraction of an electron-volt up to about 100 TeV \[5\]. It is under continuous development. The reliable performance of the code has been demonstrated in numerous applications at Fermilab, CERN, KEK and other centers as well as in special benchmarking studies. Description of elastic and inelastic \( hN \), \( hA \), \( \gamma A \) and \( \nu A \) cross sections is based on the newest compilations and parameterizations \[11\]. At high energies (5 GeV < \( E < 100 \) TeV), \( \sigma_{\text{tot}} \), \( \sigma_{\text{in}} \), \( \sigma_{\text{prod}} \) and \( \sigma_{\text{el}} \) are calculated in the framework of the Glauber multiple scattering theory with the \( \sigma_{hN} \) as an input. The nucleon density distribution in nuclei is represented as the symmetrized Fermi function with the parameters of \[12\] for medium and heavy nuclei (\( Z > 10 \)) and the ones of \[13\] for \( Z < 10 \). Modern evaluated nuclear data as well as fitting formulae are used to simulate hadron-nucleus elastic scattering. For protons, nuclear, Coulomb elastic scattering, and their interference is taken into account. At \( E > 5 \) GeV, a simple analytical description used in the code for both coherent and incoherent components of \( d\sigma/dt \) is quite consistent with experiment. A version of the Cascade-Exciton Model of nuclear reactions \[10\] as realized in the code CEM95 \[14\] and containing also several recent refinements \[15\] is now implemented in the 1998 version of MARS \[11\] as default for 1-10 MeV < \( E < 3-5 \) GeV. A set of phenomenological models, as described in Ref. \[5, 16, 17\], is used for inclusive production of secondary particles in \( hA \), \( dA \), \( \gamma A \) and \( \nu A \) interactions at projectile energies from 5 GeV to 100 TeV. The 2001 version \[11\] of the MARS code was employed in the present benchmark.

**LAHET3**: LAHET is a Monte-Carlo code for the transport and interaction of nucleons, pions, muons, light ions, and antinucleons in complex geometry \[6\]; it may also be used without particle transport to generate particle production cross sections. LAHET allows one to choose one of several options for the Intra-Nuclear Cascade (INC) and fission models to be employed in calculations; it is widely used and well known in the applied nuclear physics community; therefore, we do not describe it here (a comprehensive description of LAHET may be found in \[6\] and references therein). The version of LAHET realized in the code LAHET3 \[7\] uses a version of the code FLUKA, known in the literature as FLUKA96 \[19\] to describe the first, INC stage of reactions, and its own Multistage Preequilibrium Model (MPM) \[20\] to describe the following intermediate preequilibrium stage, followed by evaporation/fission slow processes (or by the Fermi break-up model after the cascade instead of preequilibrium and evaporation/fission, if the residual nuclei have atomic numbers with \( A \leq 13 \) and for \( 14 \leq A \leq 20 \) with excitation energy below 44 MeV), as described in \[6, 7\]. We mention again that only the high-energy event generator from FLUKA96 is employed here, as implemented in LAHET3; the de-
fault preequilibrium, evaporation and Fermi break-up models of LAHET3 are used for low energy nucleon and complex particle emission. More details and further references on LAHET3 with FLUKA96 can be found in [21].

Results and Discussion

Table 1 lists the cases we calculated with QGSM, MARS, and LAHET3, and provides references to experimental works where at least one spectrum of a secondary particle (from the ones listed in Introduction) was measured. A detailed report of the study containing 514 plots with spectra and multiplicities of secondary particles from reactions listed in Tab. 1 is now in preparation. Here, we present only our main conclusions and several examples of results from the study.

Our analyses have shown that all three codes tested here describe reasonably most of the secondary particle spectra. As a rule the higher the incident proton energy, the better the calculated spectra agree with experimental data. Several reaction mechanisms participate in the production of secondary nucleons and complex particles. These mechanisms are: 1) Fast INC processes; 2) preequilibrium emission from residual nuclei after the cascade stage of reactions; 3) evaporation of particles from compound nuclei after the preequilibrium stage, or from fission fragments, if the compound nucleus was heavy enough to undergo fission; 4) Fermi break-up of light excited nuclei formed after the cascade stage of reactions; 5) coalescence of complex particles by final state interactions among emitted cascade nucleons; 6) fast complex particle emission via knock out and pick up processes; 7) Multifragmentation of highly-excited residual nuclei after the INC. Their relative roles change significantly with the changing atomic mass number of the targets, and are different for different energies and angles of emission of secondary particles. Different codes describe these spectra better, worse, or do not describe them at all, depending of how these reaction mechanisms are (or are not) implemented into a specific code.

As an example, Fig. 1 shows spectra of p, d, t, and \( \pi^- \) emitted at 9.17 deg from the reaction p(70 GeV) + \(^{208}\text{Pb}\). Results for other reactions at 70 GeV are similar. One can see that all three codes describe the proton spectra well. The agreement for the pion spectra is not so good but is still reasonable, with some underestimation of the high-energy
tails of spectra by QGSM and some overestimation by MARS. Note that as the angle of pion emission changes the situation is reversed: we observe that most of the high-energy tails of pion spectra at 159 deg, and to a lesser extent at 90 deg, are over-predicted by LAHET3 and underestimated by MARS.

The situation with the deuteron and tritium spectra is quite different. We see that deuterons with momentum of up to about 15 GeV/c and tritium with momenta up to 19 GeV/c are emitted and measured in this particular reaction. Utilizing the coalescence mechanism for complex particle emission, QGSM is able to describe high-energy deuteron production, and agrees well with the measurement. LAHET3 does not consider the coalescence of complex particles and therefore describes emission of only evaporative and preequilibrium deuterons with momenta not higher than 1 GeV/c. MARS does not consider emission of complex particles at such high incident proton energies, therefore no d and t spectra by MARS are shown in Fig. 1.

For tritium, the situation is worse since LAHET3, as is the case of deuterons, describes only preequilibrium emission and evaporation of tritons with momenta not higher than 1 GeV/c and QGSM, even taking into account coalescence of tritium, describes emission of t from this reaction up to only 2.5 GeV/c while the experimental spectrum of t extends to 19 GeV/c. This deficiency can be understood by considering the coalescence mechanism: It is much more probable to emit two cascade nucleons with very similar momenta that can coalesce into a deuteron than to get three INC nucleons with very similar momenta that can coalesce into a triton. The experimental values of high-energy triton spectra are several orders of magnitude below the corresponding values of the deuteron spectra, and the statistics of our present QGSM simulation could be simply too small to get such high-energy tritium via coalescence. There is also a possibility that knock out processes of preformed clusters (or fluctuations of nuclear density, leading to “fluctons”) by bombarding protons are seen in these experimental d and t spectra, but are not taken into account by any of the tested codes, providing the observed difference in the t spectrum and less pronounced, in the d spectrum. A third possible mechanism of complex particle emission with greater than 1 GeV/c momenta would be multifragmentation of highly-excited residual nuclei after the INC. This mechanism is not taken into account by any of the tested codes and we cannot estimate its contribution.

Fig. 2 shows examples of $\pi^+$ spectra at 159 deg from 51 GeV proton collisions with $^9$Be and $^{48}$Ti. As already mentioned above for $\pi^-$, we see that LAHET3 overestimates the high-energy tails of pion spectra and MARS underestimates them a little. Similar results were obtained for other targets and incident proton energies.

Fig. 3 shows an example of how calculated proton spectra depend on the angle of emission, for the reaction p(30 GeV) + $^9$Be. We see that at 30 GeV, the agreement of calculated proton spectra with the data is not so good as we have in Fig. 1 for 70 GeV. The shapes and absolute values of proton spectra predicted by different codes depend significantly on the angle of detection, as does the agreement with the data. Similar results were obtained for other secondary particles and for other targets and incident energies.
Figure 1. Invariant cross sections $E d^3\sigma / d^3p$ for forward production of p, d, t, and $\pi^-$ at 160 mrad (9.17 deg) as functions of particle momentum $p$ from 70 GeV protons on $^{208}$Pb. Experimental data for p and $\pi^-$ are from Tab. 1 of Ref. 29 and for d and t, from Ref. 30. Calculations by QGSM, LAHET3, and MARS are shown as indicated in the legends.
Figure 2. Invariant cross sections $E d^2 \sigma / d^3 p$ for production of $\pi^+$ at 159 deg as functions of pion momentum $p$ from 51 GeV protons on $^9$Be and $^{48}$Ti. Experimental data are by Belyaev et al. Calculations by QGSM, LAHET3, and MARS are shown as indicated in legends.

Fig. 4 shows an example of mean multiplicity of secondary n, p, d, and $\pi^+$ predicted by the tested codes for interaction of protons of about 50 GeV with different nuclei as functions of the mass number of targets. We see that predicted particle multiplicities differ significantly from each other, and the differences increase with increasing mass number of the target. The observed differences point to a quite significant difference in the treatment by the codes of the cascade stage of reactions (pions are emitted only at the cascade stage of reactions) and of the subsequent preequilibrium, evaporation, and Fermi break-up stages as well (we recall that at these incident energies MARS uses its own approximations for the total particle spectra without considering separately contributions from different mechanisms of nuclear reactions). These differences indicate that further experimental data are necessary at these incident proton energies and further development and improvement of the codes is required.

Further Work

Our study shows that all three codes describe reasonably well many of the secondary particle spectra analyzed here, though all of them should be further improved before becoming reliable tools for PRad.

For instance, we find that QGSM has some problems in a correct description of several pion spectra and does not describe sufficiently the high-energy tails of measured t and $^3$He spectra. Nevertheless, QGSM is the only code tested here that accounts for coalescence of
Figure 3. Momentum spectra of secondary protons from 30 GeV protons on Be. Experimental data at 9 and 20 degrees are taken from Fig. 1 of Baker et al. [22]; at 30 degrees, from Fig. 5 of Ref. [23]; and at 90 degrees, from Fig. 2 of Ref. [24]. Calculations by QGSM, LAHET3, and MARS are shown as indicated in legends.
Figure 4. Predicted by QGSM, LAHET3, and MARS mean multiplicities of secondary n, p, d, and π⁺ emitted from 50 GeV proton-induced reactions as functions the mass number of targets. Note that actual energies of incident protons in our calculations were 47 GeV for $^{12}$C, 50 GeV for $^{184}$W, 51 GeV for $^9$Be and $^{48}$Ti, 53 GeV for $^{27}$Al, and 54 GeV for $^{96}$Mo. (MARS does not calculate production of deuterons at these incident energies.)
complex particles from cascade nucleons and provides production of high-energy complex particles.

MARS overestimates the high-energy tails of some pion, kaon, and proton spectra at small angles (4.75°, 9°, and 13°) and underestimates them a little at large angles (90° and 159°). At these incident energies, MARS does not calculate complex particle production. However, MARS has one significant advantage in comparison with the two other codes: It is several orders of magnitude faster and requires almost no computing time, providing meanwhile reliable results for many applications.

LAHET3 overestimates the high-energy tails of practically all pion spectra at 159° and some nucleon and complex particle spectra in the preequilibrium energy region. It does not consider coalescence of complex particles and does not describe production of high-energy complex particles.

We observe also big differences between predicted high-energy tails of both neutron and proton spectra at 0° and for the mean multiplicities of almost all secondary particles, though no experimental data for these quantities are available at present for the reactions studied here.

We note that many of the problems we observe in our study for particular codes have already been solved, since all benchmarked event generators are under continuous development and improvement and all of them have been further improved in comparison with the versions we use in this study.

On the basis of QGSM, we have developed the Los Alamos version of the Quark-Gluon String Model code, LAQGSM [31]. LAQGSM differs from QGSM by replacing the preequilibrium and evaporation parts of QGSM described according to the standard CEM [10] with the new physics from CEM2k [32] and has a number of improvements and refinements in the cascade and Fermi break-up models. Originally, both QGSM and LAQGSM were not able to describe fission reactions and production of light fragments heavier than 4He, as they had neither a high-energy-fission nor a fragmentation model. Recently, we addressed these problems [33] by further improving CEM2k and LAQGSM and by merging them with the Generalized Evaporation Model code GEM2 developed by Furihata [34]. The improved LAQGSM+GEM2 code describes both spectra of secondary particles and yields of produced nuclides much better than QGSM does; exemplary results by LAQGSM and further references may be found in [35].

The MARS code system is being continuously developed and improved. For instance, a new version of the code, MARS14(2002) was completed after we started the present work. It contains a large number of improvements and refinements and provides better results in comparison with the version used here. Recently, the authors of MARS started to develop new and better approximations for the double differential cross sections of inelastic $hN$ and $hA$ interactions. The new systematics allow to solve the mentioned above problems with the pion, kaon, and proton spectra at forward and large angles and describe the experimental data much better.

The FLUKA code has also been updated very significantly (see e.g., [36] and references therein) since the version FLUKA96 was incorporated into LAHET3 as used here; no updated version is yet incorporated into LAHET.
Our study points to the importance of taking into account coalescence in high-energy complex-particles production. We find it appropriate and easy to implement these processes into MARS and LAHET, as well as into other codes that do not now consider coalescence.

We think that at such high incident energies, multifragmentation of highly-excited heavy nuclei may also be of significance and should be taken into account in these event generators and in other codes.

Acknowledgment

The study was supported by the U. S. Department of Energy and by the Moldovan-U. S. Bilateral Grants Program, CRDF Project MP2-3025.

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