CEM03 and LAQGSM03—new modeling tools for nuclear applications

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Abstract. An improved version of the Cascade-Exciton Model (CEM) of nuclear reactions realized in the code CEM2k and the Los Alamos version of the Quark-Gluon String Model (LAQGSM) have been developed recently at LANL to describe reactions induced by particles and nuclei for a number of applications. Our CEM2k and LAQGSM merged with the GEM2 evaporation/fission code by Furihata have predictive powers comparable to other modern codes and describe many reactions better than other codes; therefore both our codes can be used as reliable event generators in transport codes for applications. During the last year, we have made significant improvements to the intranuclear cascade parts of CEM2k and LAQGSM, and have extended LAQGSM to describe photonuclear reactions at energies to 10 GeV and higher. We have produced in this way improved versions of our codes, CEM03.01 and LAQGSM03.01. For special studies, we have also merged our two codes with the GEMINI code by Charity and with the SMM code of Botvina. We present a brief description of our codes and show illustrative results obtained with CEM03.01 and LAQGSM03.01 for different reactions compared with predictions by other models, as well as examples of using our codes as modeling tools for nuclear applications.

1. Introduction
Following an increased interest in nuclear data for such projects as the Accelerator Transmutation of nuclear Wastes (ATW), Accelerator Production of Tritium (APT), Spallation Neutron Source (SNS), Rare Isotope Accelerator (RIA), Proton Radiography (PRAD) as a radiographic probe for the Advanced Hydro-test Facility and others, for several years the US Department of Energy has supported our work on the development of improved versions of the Cascade-Exciton Model (CEM) of nuclear reactions [1, 2, 3] and the Los Alamos version of the Quark-Gluon String Model (LAQGSM) [4] to describe reactions induced by particles and nuclei at energies up to about 1 TeV/nucleon. To describe fission and production of light fragments heavier than ⁴He, we have merged both our codes with several evaporation/fission/fragmentation models, including the Generalized Evaporation/fission Model code GEM2 by Furihata [5]. Our codes perform as well as and often better than other current models in describing a large variety of spallation, fission, and fragmentation reactions, therefore they are used as event-generators in several transport codes. The status of our codes as of the middle of 2004 together with illustrative results and comparisons with other models can be found in [6, 7, 8] and references therein. Here, we present several improvements developed during the last year leading to the new versions of our codes, CEM03.01 and LAQGSM03.01 [3, 9].
2. Basic assumptions of CEM and LAQGSM

The Cascade-Exciton Model (CEM) of nuclear reactions was proposed initially at the Laboratory of Theoretical Physics, JINR, Dubna [10] to describe intermediate-energy spallation reactions induced by nucleons and pions. It is based on the Dubna IntraNuclear Cascade (INC) [11] and the Modified Exciton Model (MEM) [12, 13]. It was extended later to consider photonic reactions and to describe fission cross sections using different options for nuclear masses, fission barriers, and level densities, and its 1995 version CEM95 was released to the public via NEA/OECD, Paris and RSICC, Oak Ridge (see corresponding references in [3]).

LAQGSM is an extension by Gudima, Mashnik and Sierk of the Quark Gluon-String Model (QGSM) by Amelin, Gudima and Toneev [14] done at Los Alamos [4] and is intended to describe both particle- and nucleus-induced reactions at energies up to about 1 TeV/nucleon. LAQGSM is based on a time-dependent version of the intranuclear-cascade model (different from the one used in CEM) developed at JINR, Dubna, often referred to in the literature simply as the Dubna intranuclear Cascade Model (DCM) (see [15] and references therein). LAQGSM [4, 9] differs from QGSM [14] by using an extended and significantly improved version of the INC model [6, 9], by replacing the preequilibrium and evaporation parts of QGSM described according to the standard CEM [10] with the new physics from CEM03.01 [3] and also has a number of improvements and refinements in the Fermi break-up and coalescence models in comparison with QGSM [14].

CEM and LAQGSM assume that the reactions occur generally in three stages. The first stage is the INC, in which primary particles can be re-scattered and produce secondary particles several times prior to absorption by, or escape from the nucleus. When the cascade stage of a reaction is completed, CEM and LAQGSM use the coalescence model as described in [15] to “create” high-energy d, t, 3He, and 4He by final-state interactions among emitted cascade nucleons. The emission of the cascade particles determines the particle-hole configuration, Z, A, and the excitation energy that is the starting point for the second, preequilibrium stage of the reaction. The subsequent relaxation of the nuclear excitation is treated in terms of an improved version of the modified exciton model of preequilibrium decay followed by the equilibrium evaporation/fission stage of the reaction. Generally, all four components may contribute to experimentally measured particle spectra and other distributions. But if the residual nuclei after the INC have atomic numbers with $A \leq 12$, CEM03.01 and LAQGSM03.01 use the Fermi break-up model [16] to calculate their further disintegration instead of using the preequilibrium and evaporation models. Fermi break-up is much faster to calculate and gives results very similar to the continuation of the more detailed models to much lighter nuclei.

3. Recent developments in CEM03.01 and LAQGSM03.01 and illustrative results

First, during 2004 we incorporated into LAQGSM the improved approximations for the total elastic and inelastic cross sections of hadron-hadron and photo-hadron elementary interactions developed previously for the code CEM97 [17] and CEM2k [1] (see details in [17]).

Second, the double differential distributions of secondary particles from elementary $NN$ and $\gamma N$ interactions were simulated by CEM2k (and all its precursors, as well as by LAQGSM and its precursors at energies below 4.5 GeV/A) still using the old Dubna INC [11] approximations that were obtained by Gudima et al. [18] 36 years ago, using the measurements available at that time. For instance, in the case of two-body reactions, the cosine of the angle of emission of secondary particles in the c.m. system is calculated by the Dubna INC as a function of a random number $\xi$, distributed uniformly in the interval [0,1] as

$$\cos \theta = 2\xi^{1/2} \left[ \sum_{n=0}^{N} a_n \xi^n + (1 - \sum_{n=0}^{N} a_n) \xi^{N+1} \right] - 1 ,$$

(1)
where $N = M = 3$,

$$a_n = \sum_{k=0}^{M} a_{nk} T_i^k .$$

The coefficients $a_{nk}$ were fitted to the then available experimental data at a number of incident kinetic energies $T_i$, then interpolated and extrapolated to other energies (see details in [11, 18] and references therein). The distribution of secondary particles over the azimuthal angle $\varphi$ is assumed isotropic. For elementary interactions with more than two particles in the final state, the Dubna INC uses the statistical model to simulate the angles and energies of products (see details in [11]).

For the improved versions of our codes referred to as CEM03 and LAQGSM03, respectively, we use currently available experimental data and recently published systematics proposed by other authors to develop new approximations for angular and energy distributions of particles produced in nucleon-nucleon and photon-proton interactions. So, for $pp$, $np$, and $nn$ interactions at energies up to 2 GeV, we did not have to develop our own approximations analogous to the ones described by Eqs. (1) and (2), since reliable systematics have been developed recently by Cugnon et al. for the Liege INC [19], then improved further by Duarte for the BRIC code [20]; we simply incorporate into CEM03 and LAQGSM03 the systematics by Duarte [20]. Similarly, for $\gamma N$ interactions, we take advantage of the event generators for $\gamma p$ and $\gamma n$ reactions from the Moscow INC [21] kindly sent us by Dr. Igor Pshenichnov. In our codes, we use part of a large data file with smooth approximations through presently available experimental data from the Moscow INC [21] and have developed a simple and fast algorithm to simulate unambiguously $d\sigma/d\Omega$ and to choose the corresponding value of $\Theta$ for any $E_\gamma$, using a single random number $\xi$ uniformly distributed in the interval $[0,1]$ [2]. For other elementary interactions, we fit new sets of parameters $a_n$ from Eq. (1) at different $T_i$ for which we found data, then we approximated the energy dependences of the parameters $a_{nk}$ in Eq. (2) using the fitted values of $a_n$.

Examples of angular distributions of secondary particles from $np$ and $\gamma p$ reactions at several energies are shown in Figs. 1 and 2 of Ref. [6]. The new approximations from CEM03 and LAQGSM03 reproduce the experimental data much better than the old Dubna INC used in our previous code versions (and in several other codes developed from the Dubna INC) and allow us to describe better particle spectra from different reactions on nuclei [see, e.g., figure 3 in [6]].

Third, we have improved the description of complex-particle spectra in CEM03 and LAQGSM03. This was done by refining the coalescence model used in our codes, by developing a better approach to estimate the probability of complex-particle emission at the preequilibrium stage of a reaction, and by incorporating into our codes the known systematics for angular distributions of complex particles developed by Kalbach (see details in [3]).

Figure 1 shows examples of proton, deuteron, and triton spectra from 542 MeV $p + Cu$ and Bi calculated by the recently improved version of CEM compared with experimental data [22]. We see that although the CEM03.01 results do not coincide exactly with these experimental data, the agreement is comparable to that provided by other modern models like FLUKA (see figure 3 in [23]) and the latest version of the Liege INC by Cugnon et al. (see figure 3 in [24]), and is significantly better than that obtained a decade ago with the initial version of CEM [10] (see Figs. 6, 7, 9 and 10 in [25]).

We note that CEM03.01 also describes reasonably well complex-particle (and nucleon) spectra from reactions at energies below 100 MeV, where more sophisticated microscopic codes like GNASH [26] or TALYS [27] are usually used to produce data libraries for applications. For example, from figure 6 of Ref. [3] one can see that CEM03.01 describes the nucleon and complex-particles spectra from 62.9 MeV $p + ^{208}Pb$ measured recently [28] in Louvain-la-Neuve for the HINDAS project quite well and agrees with the data about as well as results by TALYS [27], GNASH [26], FLUKA [23], or INCL4 [19] published in Figs. 20 and 21 of Ref. [28].
Next we extended CEM03 to calculate reactions induced by both monochromatic and bremsstrahlung photons, as described in detail in [2]. As one can see from the example shown in figure 2 and from many other results published in [2, 3], CEM03.01 now describes reasonably well photonuclear reactions at incident energies from about 30 MeV to $\sim$ 1.5 GeV. It can be used as well for estimation of photonuclear reactions for applications at higher energies, up to $\sim$ 5 GeV (see details in [2, 3]).

Finally, after making the improvements to the INC and pre-equilibrium parts CEM (and LAQGSM) as described above, the mean values of the mass and charge numbers, $A$ and $Z$ of the excited compound nuclei produced after the pre-equilibrium stage of nuclear reactions and their mean excitation energy $E^*$ have changed slightly, which affects the probability of heavy compound nuclei (especially preactinides) to fission. This means that the procedure of fitting the ratio of the level-density parameters of fissioning nuclei at the saddle point, $a_f$, and for evaporation from compound nuclei, $a_n$,
determination of the level-density ratio done in [30] for CEM2k and LAQGSM, ensuring that the latest versions of our codes describe as well as possible fission cross sections from various reactions. Figure 3 shows examples of fission cross sections for proton-induced reactions on \(^{186}\text{W},^{184}\text{W},^{183}\text{W}\) and \(^{182}\text{W}\). One can see that the improved CEM03.01 reproduces the recent Uppsala measurements [31] of proton-induced fission cross sections.

Our calculations have shown that CEM03.01 results also agree reasonably well with the recent Uppsala [32, 33, 34] and Saint-Petersburg [35] data and older measurements at LANL by Parrish Staples et al. [36] for neutron-induced fission cross sections. Results by LAQGSM03.01 for these and other fission cross sections practically coincide with ones by CEM03.01, as is expected from the fitting process [30].

The initial version of LAQGSM [4], just like its precursor QGSM [14], did not consider photonuclear reactions, while its 2003 version LAQGSM03 [6] and CEM03.01 describe such reactions only for energies up to about 1.5 GeV. This is not convenient when using our codes to solve problems for PRAD, NASA, and other high-energy applications or to analyze future high-energy measurements at the Thomas Jefferson National Accelerator Facility (CEBAF), where photons with much higher energy are created and need to be simulated by an event generator in a transport code. To address this problem, we have extended LAQGSM03 to describe photonuclear reactions at energies up to tens of GeV. For this, we took advantage of the high-energy event generators for \(\gamma p\) and \(\gamma n\) elementary interactions from the Moscow high-energy photonuclear reaction model [21] kindly sent us by one of its co-authors, Dr. Igor Pshenichnov, as mentioned previously. We have incorporated into LAQGSM03 56 channels to consider \(\gamma p\) elementary interactions during the cascade stage of reactions, and 56 channels for \(\gamma n\) interactions. These reaction channels new to LAQGSM03 are listed in Table 1 of Ref. [9] together with all corresponding details. The improved version of our code extended in this manner is referred to as LAQGSM03.01: it allows us to describe photonuclear reactions at energies both below \(\sim 1.5\) GeV where the earlier LAQGSM03 and CEM03.01 work (see, e.g. figure 11 in [9]), and at higher photon energies. Figs. 4 and 5 show two examples of results by LAQGSM03.01 for high-energy photonuclear reactions; more such results may be found in [9]. We note that to the best of our knowledge, we are able to describe with LAQGSM03.01 the data shown in Figs. 4 and 5 (and other similar reactions analyzed in [9]) for the first time; we do not know of any publication or oral presentation where these measurements were reproduced by a theoretical model, event generator, or transport code.

We have benchmarked the new versions of our codes, CEM03.01 and LAQGSM03.01, on a variety of particle-particle, particle-nucleus, and nucleus-nucleus reactions at energies from 10 MeV to 800 GeV per nucleon and find that they describe reactions generally much better than their predecessors. Two examples of this work are shown in Figs. 6 and 7. We note that the 400 GeV experimental data compared in figure 7 with our LAQGSM03.01 results and other similar measurements of \(K^+, K^-, \bar{p}, d, t, ^3\text{He}, \) and \(^4\text{He}\) spectra from \(^{181}\text{Ta}\), as well as all measured spectra from Cu, Al, and C [44]–[46] are described here simultaneously within a single approach for the first time: Though these data were measured at FNAL 25 years ago with a hope of revealing some “exotic” or unknown mechanisms of nuclear reactions leading to the production of the measured so called “cumulative” (i.e., kinematically forbidden for quasi-free inelastic collisions) particles, we do not know any publication or oral presentation where these measurements were reproduced simultaneously within a single approach by a theoretical model, event generator, or transport code. It is noteworthy that LAQGSM03.01 describes quite well all cumulative particle spectra measured in [44]–[46] in single approach, without any fitting or free parameters, and without involving any “exotic” reaction mechanisms. This is also true for the photonuclear cumulative proton yields shown in figure 4. These results do not imply, of course, that the proton- or \(\gamma\)-nucleus interaction physics is completely described by the reaction mechanisms considered by LAQGSM03.01. Our present results do not exclude some contribution
LAQGSM+GEM2 results with the older data [52] (magenta circles) on spallation product yields from this reaction agrees very well with the later measurements [53]. The agreement of LAQGSM+GEM2, a predecessor of LAQGSM03.01 for the fission-fragment mass distribution (the dates of all our calculations are shown in the legend of figure 8). The prediction by our models. The calculations were done about two years before the data [53] became available to us + d [53] (brown circles) to figure A2.3 of Ref. [8], which showed our calculations of several was made by adding the recent fission-fragment yield data from the reactions 1 GeV/A + d [53] (brown circles) to figure A2.3 of Ref. [8], which showed our calculations of several.

Finally, we wish to note that CEM03.01 and LAQGSM03.01 and their predecessors have good predictive powers and describe various nuclear reactions similarly to and often better than other current models do; therefore they can be used as reliable event generators in transport codes for applications. Figure 8 shows just one example to demonstrate this. This figure was made by adding the recent fission-fragment yield data from the reactions 1 GeV/A + d [53] (brown circles) to figure A2.3 of Ref. [8], which showed our calculations of several models. The calculations were done about two years before the data [53] became available to us (the dates of all our calculations are shown in the legend of figure 8). The prediction by our LAQGSM+GEM2, a predecessor of LAQGSM03.01 for the fission-fragment mass distribution from this reaction agrees very well with the later measurements [53]. The agreement of LAQGSM+GEM2 results with the older data [52] (magenta circles) on spallation product yields enough for an unambiguous determination of the mechanisms of particle production, just as observed heretofore at intermediate and low energies [25].

Figure 4. Proton spectra at 30, 60, 90, and 150 degrees from interaction of bremsstrahlung $\gamma$ quanta of maximum energy $E_0 = 4.5$ GeV with $^{12}$C, $^{27}$Al, $^{63}$Cu, and $^{208}$Pb. Experimental values shown by symbols are from [37, 38, 39] while histograms show results by LAQGSM03.01. Similar results [9] were obtained by LAQGSM03.01 at $E_0 = 3.0$ and 2.0 GeV, as well as for photopion spectra [40, 41]. To the best of our knowledge, using LAQGSM03.01, we are able to describe these data measured 24 years ago at Yerevan for the first time.

Figure 5. Detailed comparison between experimental yields [42] and those calculated by LAQGSM03.01 of radioactive products from the interaction of bremsstrahlung $\gamma$ quanta of maximum energy 4.5 GeV with $^{93}$Nb. The cumulative yields are labeled as “c” while the independent cross sections, as “i”. To the best of our knowledge, using LAQGSM03.01, we are able to describe these data measured 28 years ago at Yerevan for the first time.

to the production of these cumulative particles from other reaction mechanisms not considered by LAQGSM03.01. But the contribution from “exotic” mechanisms to cumulative particle production from these high-energy reactions seems to be small; inclusive particle spectra are not sensitive
(which were available to us before the calculations were performed) are also satisfactory and are comparable to that provided by LAHET3 [47] calculations using: 1) ISABEL [48] INC with the Dresner [49] evaporation and RAL [50] fission models; 2) the Liege INC code INCL by Cugnon et al. [19] merged with the Dresner [49] evaporation and RAL [50] fission models; 3) INCL [19] merged with ABLA/PROFI fission/evaporation model by Schmidt et al. [51].

4. Applications
CEM03.01 and LAQGSM03.01 and their predecessors are used as stand-alone codes to study different nuclear reactions for applications and fundamental nuclear physics (see, e.g., [3, 7, 8, 25, 54] and references therein). We outline below only two examples of applications.

The first application of CEM97 and CEM95, predecessors of CEM03.01, we like to mention here is for a medical isotope production study. Several years ago, a detailed study of the production of 22 isotopes for medical and industrial applications by high-energy protons and neutrons at the Accelerator Production of Tritium Facility project (APT) was performed (see [54, 55] and references therein). The production rate of a radioisotope can be obtained from the integral of the flux and cross section leading to the direct production of the radioisotope as a reaction product. Additional production is realized from other radionuclides that decay to the desired product. Evaluation of production rates requires knowledge of the neutron and proton fluxes at some position in the production facility and cross sections leading to production of the desired radionuclide and its progenitors. We used MCNPX version 2.1.1 to calculate neutron and proton fluxes throughout the APT model, while cross sections for reactions most likely to lead to our desired products were evaluated using all available to us experimental data and calculations by CEM95 and CEM97 at energies above 100 MeV, and the “150 MeV” activation library calculated by M. B. Chadwick with the HMS-ALICE code [57] supplemented by the European Activation File EAF-97, Rev. 1 with some recent improvements by M. Herman (see [58] and references therein), at lower energies. Our 684 page detailed report on this study [55], with 37 tables and 264 color figures is available on the Web under: http://t2.lanl.gov/publications/publications.html.

A second application of our codes is for astrophysics. A successful model for cosmic-ray propagation in the Galaxy used nowadays to study different challenging questions of astrophysics...
is realized in the code GALPROP by Strong and Moskalenko (see [59] and references therein). So, GALPROP was used recently to study propagation of different particles and nuclei in the Galaxy and to improve estimates of the Galactic halo size (see, e.g., [7], [59]-[62] and references therein). However, GALPROP relied initially on nuclear reaction cross sections calculated using the phenomenological systematics by Webber et al. [63] and Silberberg et al. [64] and on scarce available experimental data, as is usually done in astrophysics. As an example, figure 9 shows only one excitation function for the production of $^{26}$Al from the reaction $p + ^{26}$Si used by GALPROP along with hundreds of other excitation functions. We see that the phenomenological systematics [63, 64] do not reproduce correctly the available experimental cross sections for this reaction. As one can see from figure 10, using in GALPROP cross sections provided by phenomenological systematics [63, 64] leads to quite big uncertainties in the derived Galactic halo size (3–7 kpc), while using evaluated cross sections based on available experimental data and calculations by CEM2k [1] reduces uncertainties and limits the derived Galactic halo size to only 4–6 kpc. This is why we have used several versions of our CEM and LAQGSM codes to calculate cross sections of interest to astrophysics, used thereafter together with available experimental data to produce a number of reliable evaluated excitation functions for astrophysical needs (see, e.g., [60]-[62], [65] and references therein).

Finally, we mention that different versions of our CEM and LAQGSM codes are incorporated wholly as event-generators, or in part in different transport codes used in applications, among them CASCADE [66], MARS [67], MCNPX [68] GEANT4 [69], SHIELD [70], RTS&T [71], SONET [72], CALOR [73], HETC-3STEP [74], CASCADE/INPE [75], HADRON [76], CASCADO [77], CAMO [78] and others. Thus our codes are automatically employed in various nuclear applications where these transport codes are used.
5. Summary

Improved versions of the cascade-exciton model of nuclear reactions and of the Los Alamos quark-gluon string model have been developed recently at LANL and implemented in the codes CEM03.01 and LAQGSM03.01 as event-generators for transport codes MCNP6 [79], MCNPX [68], and MARS [67]. Our codes were previously incorporated into MARS and are now being incorporated into MCNPX and MCNP6. CEM03.01 was made available to the public via RSICC at Oak Ridge. We also plan to make LAQGSM03.01 available to the public via RSICC in the future.

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Figure 8. Comparison of measured mass (left panel) and charge (right panel) distributions of the nuclides produced in the reactions 1 GeV/A $^{238}$U + d with results from LAHET3 [47] using the ISABEL+Dresner/Atchison [48]-[50] (green lines), INCL+Dresner/Atchison [19, 49, 50] (blue line), and the INCL+ABLA [19, 51] (red lines) models, and by our LAQGSM+GEM2 (maroon lines), respectively. Experimental data for spallation products shown by magenta circles are from [52] and were available to us prior to the calculations being done at the dates indicated in the legend, while the fission-product data [53], shown here by brown circles, became available to us only one year after all the calculations were published in figure A2.3 of Ref. [8].

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Figure 9. Evaluated excitation function for the reaction $^{26}_{\text{Si}}$(p,x)$^{26}_{\text{Al}}$ (thick dashed line) compared with experimental data from the LANL T-16 compilation [56] (our LANL T-16 compilation is updated as new experimental data become available to us) and results from CEM2k [1] (thin solid line) and phenomenological approximations by Webber et al. [63] (dashed line) and by Silberberg et al. [64] (dot-dashed line).

Figure 10. Galactic halo size limits ($Z_h$, kpc) as derived in [60] from the calculated CR abundances of the four radioactive isotopes and ACE spacecraft data. The ranges given for each isotope were obtained using evaluated production cross-sections and reflect errors in measurements of CR isotopic ratios and CR source abundances. The dark shaded area indicates the range consistent with all ratios (4–6 kpc); for comparison the range (3–7 kpc) derived in [59] using phenomenological approximations [63, 64] for cross sections is shown by light shading.
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