CEM2K and LAQGSM codes as event generators for space-radiation-shielding and cosmic-ray-propagation applications

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Abstract

The CEM2k and LAQGSM codes have been recently developed at Los Alamos National Laboratory to simulate nuclear reactions for a number of applications. We have benchmarked our codes against most available data measured at incident particle energies from 10 MeV to 800 GeV and have compared our results with predictions of other current models used by the nuclear community. Here, we present a brief description of our codes and show some illustrative results that testify that CEM2k and LAQGSM can be used as reliable event generators for space-radiation-shielding, cosmic-ray (CR) propagation, and other astrophysical applications. Finally, we show an example of combining of our calculated cross-sections with experimental data from our LANL T-16 compilation to produce evaluated files. Such evaluated files were successfully used in the model of particle propagation in the Galaxy GALPROP to better constrain the size of the CR halo.

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1. Introduction

The radiation environment in deep space or on the moon can be very harsh (MacFarlane et al., 1991). Without the Earth’s atmosphere and magnetic field to protect them, astronauts will be directly exposed to high-energy galactic cosmic rays (GCR), to intense fluxes of protons and other particles from solar flares, and to radiation from on-board power plants or nuclear propulsion systems. Such radiation is also very dangerous to computers and electronics on spacecraft, as it may cause enough single-event upsets to lead to device failure. The economic penalties of additional mass to provide shielding may be huge. To minimize this expense, we need to be able to reliably calculate the amount of shielding required. Performing this task requires nuclear data for reactions induced by different projectiles, on different targets, for a large range of incident energies. Similarly, addressing different astrophysical problems, such as investigating the origin and propagation of cosmic rays (CR) and the nuclide abundances in the solar system and in CR, again requires a large amount of different nuclear reaction data. Experiments to obtain such data are costly, there are a limited number of facilities available to make such measurements, and some reactions of interest cannot yet be measured at accelerators. Therefore reliable models and codes are required to provide the necessary estimates.

In recent years we have worked to improve the Cascade-Exciton Model (CEM), currently implemented in the code CEM2k, which describes nuclear reactions induced by nucleons, pions, and photons with energies from a few MeV to 5 GeV (Mashnik and Sierk, 2001, 2002). Similarly, we have developed a Los Alamos version of the Quark-Gluon String Model (LAQGSM), used for particle- and nucleus-induced reactions for energies up to 1 TeV/nucleon. Both codes have been
tested against most of the available data and compared with predictions of other modern codes (Mashnik and Sierk, 2001, 2002; Mashnik et al., 2002a,b,c,d; Titarenko et al., 2002). Our comparisons show that these codes describe a large variety of spallation, fission, and fragmentation reactions quite reliably and have one of the best predictive powers compared to other available Monte-Carlo codes. In the present paper, we outline our models and show several typical results demonstrating that both CEM2k and LAQGSM are reliable event-generators which can be used in many different applications. We illustrate an astrophysical application of our evaluated cross-sections by showing an estimate of the size of the CR halo obtained using the CR propagation code GALPROP (Strong and Moskalenko, 1998; Moskalenko et al., 2002).

2. CEM2K and LAQGSM

A detailed description of the initial version of the CEM may be found in Gudima et al. (1983), therefore we outline here only its basic assumptions. The CEM assumes that reactions occur in three stages. The first stage is the IntraNuclear Cascade (INC) in which primary particles can be re-scattered and produce secondary particles several times prior to absorption by or escape from the nucleus. The excited residual nucleus remaining after the cascade determines the particle–hole configuration that is the starting point for the pre-equilibrium stage of the reaction. The subsequent relaxation of the nuclear excitation is treated in terms of an improved Modified Exciton Model (MEM) of pre-equilibrium decay followed by the equilibrium evaporative final stage of the reaction. Generally, all three stages contribute to experimentally measured outcomes.

The improved cascade-exciton model in the code CEM2k differs from the older CEM95 version by incorporating new approximations for the elementary cross-sections used in the cascade, using more precise values for nuclear masses and pairing energies, employing a corrected systematics for the level-density parameters, adjusting the cross-sections for pion absorption on quasi-deuteron pairs inside a nucleus, allowing for nuclear transparency of pions, including the Pauli principle in the pre-equilibrium calculation, and improving the calculation of the fission widths. Implementation of significant refinements and improvements in the algorithms used in many subroutines leads to a decrease of the computing time by up to a factor of 6 for heavy nuclei, which is very important when performing simulations with transport codes. Essentially, CEM2k has a longer cascade stage, less pre-equilibrium emission, and a longer evaporation stage with a higher initial excitation energy, compared to its precursors CEM97 and CEM95. Besides the changes to CEM97 and CEM95 mentioned above, we also made a number of other improvements and refinements, such as: (i) imposing momentum-energy conservation for each simulated event (the Monte-Carlo algorithm previously used in CEM provided momentum-energy conservation only statistically, but not exactly for the cascade stage of each event), (ii) using real binding energies for nucleons at the cascade stage instead of the approximation of a constant separation energy of 7 MeV used in previous versions of the CEM, (iii) using reduced masses of particles in the calculation of their emission widths instead of using the approximation of no recoil used previously, and (iv) a better approximation of the total reaction cross-sections. On the whole, this set of improvements leads to a much better description of particle spectra and yields of residual nuclei and a better agreement with available data for a variety of reactions. Details, examples, and further references may be found in Mashnik and Sierk (2001, 2002) and in Titarenko et al. (2002).

The Los Alamos version of the QGSM by Gudima et al. (2001) is a further development of the Quark-Gluon String Model (QGSM) by Amelin et al. (1990, and references therein) and is intended to describe both particle- and nucleus-induced reactions at energies up to about 1 TeV/nucleon. The core of the QGSM is built on a time-dependent version of the intranuclear-cascade model developed at Dubna, often referred in the literature simply as the Dubna intranuclear Cascade Model (DCM) (see Toneev and Gudima, 1983 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 QGSM 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 Toneev and Gudima (1983) to “create” high-energy d, t, 3He, and 4He by final state interactions among emitted cascade nucleons outside of the colliding nuclei. After calculating the coalescence stage of a reaction, QGSM moves to the description of the last slow stages of the interaction, namely to pre-equilibrium decay and evaporation, with a possible competition of fission using the standard version of the CEM by Gudima et al. (1983). 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 pre-equilibrium and evaporation models. LAQGSM differs from QGSM by replacing the pre-equilibrium and evaporation parts of QGSM described according to the standard CEM (Gudima et al., 1983) with the new physics from CEM2k (Mashnik and Sierk, 2001, 2002) and has a number of improvements.
and refinements in the cascade and Fermi break-up models (in the current version of LAQGSM, we use the Fermi break-up model only for $A \leq 12$). A detailed description of LAQGSM and further references may be found in Gudima et al. (2001).

Originally, both CEM2k and LAQGSM were not able to describe fission reactions and production of light fragments heavier than $^4\text{He}$, as they had neither a high-energy-fission nor a fragmentation model. Recently, we addressed these problems (Mashnik et al., 2002a,c) by further improving our codes and by merging them with the Generalized Evaporation Model code GEM2 developed by Furihata (2000, 2001).

We have benchmarked our codes on all reactions measured recently at GSI (Darmstadt, Germany) and on many other different reactions at lower and higher energies measured earlier at other laboratories. We found that CEM2k and LAQGSM allow us to describe quite well a large variety of spallation, fission and fragmentation reactions at energies from 10 MeV to 800 GeV, without readjusting any parameters of the models, though we still have to solve a number of problems for a better description of nuclides produced near the intersection of the spallation and fission regions. Our current versions of CEM2k and LAQGSM were incorporated recently into the MARS (Mokhov, 1995) and LAHET (Prael and Lichtenstein, 1989) transport codes and are currently being incorporated into MCNPX (Waters, 1999). This will allow others to use our codes as event-generators in these transport codes to simulate reactions with targets of practically arbitrary geometry and nuclide composition.

Fig. 1 shows examples of calculated by CEM2k and LAQGSM neutron spectra from interactions of protons with $^{208}\text{Pb}$ at 0.8 GeV, while Fig. 2 gives examples of p, d, t, $^3\text{He}$, and $^4\text{He}$ spectra from p (61 MeV) + Fe compared with experimental data by Ishibashi et al. (1997) and Bertrand and Peelle (1973).

We note that all reactions shown in Figs. 1 and 2, and in all the following figures of this paper, were calculated within a single approach, without fitting any parameters of CEM2k or LAQGSM. We see that both CEM2k and LAQGSM describe well spectra of secondary neutrons and protons. Similar results are obtained for other targets and energies of incident protons, as well as for reactions induced by neutrons, pions, and photons. Spectra of $^4\text{He}$ are also described by our codes quite well, while spectra of d, t, and $^3\text{He}$ are reproduced reasonably, but not as well as those of nucleons and $^4\text{He}$. This is partially due to the fact that we do not fit here the probability $\gamma_i$ for $p_j$ excited nucleons (excitons) to condense into a complex particle which can be emitted during the pre-equilibrium stage of a reaction to get the best agreement with the data, as is often done in the literature by other authors (see details in Gudima et al., 1983; Mashnik et al., 2002c). In the present version of our models we do not take into account direct production of complex particles like pick-up and knock-out, and this leads to some underestimation of emission of high-energy complex particles, and to under-prediction of the high-energy tails of their spectra seen in Fig. 2. We note that some of the evaporation models used often in the literature, like the GSI evaporation model ABLA by Schmidt (Gaimard and Schmidt, 1991; Junghans et al., 1998), which is used in conjunction with the Liege INC by Cugnon (Boudar et al., 2002) in the code INCL, do not consider pre-equilibrium particle emission; they only evaporate n, p, and $^4\text{He}$, and do not produce d, t, and $^3\text{He}$ at all.
Recently, Nakamura’s group measured neutron double-differential cross-sections from many reactions induced by light and medium nuclei on targets from $^{12}$C to $^{208}$Pb, at several incident energies from 95 to 600 MeV/nucleon (Iwata et al., 2001 and references therein). We have calculated all these cross-sections using LAQGSM. As an example, our results for interactions of 600 MeV/nucleon $^{20}$Ne with $^{64}$Cu are compared in Fig. 3 with experimental data and calculations with the QMD (Aichelin, 1991) and HIC (Bertini et al., 1974) models kindly provided to us by Nakamura’s group. We see that LAQGSM describes these data quite well and agrees with the measurements better than do QMD and HIC. Similar results are obtained for all the other reactions measured by this group.

We recently collected all data we could find on double-differential cross-sections for the production of particles and nuclei with $A < 4$ from reactions of 30–70 GeV protons on nuclei (Mashnik et al., 2002b). We compared these data to the predictions of the QGSM, LAQGSM, MARS, and LAHET3 (Prael, 2001) models. After analyzing more than 500 spectra of $p$, $d$, $t$, $^3$He, $^4$He, $^6$Li, $^7$Li, $^9$Be to $^{208}$Pb at angles from 0° to 159° at incident proton energies from 30 to 70 GeV, we find that LAQGSM describes well most of the measured spectra. A detailed and comprehensive report on this work is now in preparation, while Fig. 4 shows just one example, namely spectra of deuterons emitted at 9.17° from $p (70$ GeV) + $^{208}$Pb. We see that deuterons with momenta up to about 15 GeV/c are emitted and measured in this particular reaction. Utilizing the coalescence mechanism for complex particle emission, LAQGSM 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 pre-equilibrium deuterons with momenta not higher than 1 GeV/c. Even though the cross-section for emission of deuterons with momentum of $\sim 15$ GeV/c is more than six orders of magnitude lower than for evaporation of low-energy deuterons, such high-energy deuterons and other complex particles may be extremely dangerous to people and equipment in space. Therefore, we need to be able to calculate such reactions as well as possible, to accurately estimate the necessary shielding.

Recently at GSI in Darmstadt, Germany, a large number of measurements have been performed using inverse kinematics for interactions of $^{56}$Fe, $^{208}$Pb and $^{238}$U at 1 GeV/nucleon and $^{197}$Au at 800 MeV/nucleon with liquid $^1$H. These measurements provide a very rich set of cross-sections for production of practically all possible isotopes from such reactions in a “pure” form, i.e., individual cross-sections from a specific given bombarding isotope (or target isotope, when considering reactions in the usual kinematics, $p + A$). Such cross-sections are much easier to compare to models than the “camouflaged” data from $\gamma$-spectrometry.

Fig. 3. Comparison of measured (Iwata et al., 2001) double differential cross-sections of neutrons from 600 MeV/nucleon $^{20}$Ne on Cu with our LAQGSM results and calculations by QMD and HIC (Iwata et al., 2001).

Fig. 4. Invariant cross-section for the production of d by 70 GeV protons on Pb at 9.17° as a function of deuteron momentum. Experimental data (Abramov et al., 1987) and our calculations with LAQGSM and LAHET3 are shown as indicated in the legend.
measurements. These are often obtained only for a natural composition of isotopes in a target and are mainly for cumulative production, where measured cross-sections contain contributions not only from the direct production of a given isotope, but also from all its decay-chain precursors. In addition, many reactions where a beam of light, medium, or heavy ions with energy near to or below 1 GeV/nucleon interact with different nuclei, from the lightest, d, to the heaviest, 208Pb were measured recently at GSI. References on these measurements and many tabulated experimental cross-sections may be found on the Web page of Prof. Schmidt (2003). We have analyzed with CEM2k and LAQGSM all measurements done at GSI we are acquainted of, both for proton–nucleus and nucleus–nucleus interactions. Some examples of our CEM2k results compared with the GSI data and calculations by other current models for proton–nucleus reactions may be found in Mashnik (2001, 2002), Mashnik et al. (2002a,c,d), and Titarenko et al. (2002). Fig. 5 shows an example of LAQGSM results for the reaction p(1 GeV) + 208Pb compared with GSI data and calculations by a version of LAHET using the INCL + ABLA event-generator incorporated recently into LAHET. We have described INCL above; it is well known and often used in Europe. One can see that LAQGSM merged with GEM2 (LAQGSM + GEM2) describes quite well the GSI data and agrees better with the measurement than INCL + ABLA does. Similar results are obtained for all other reactions measured at GSI for which we could find data.

Fig. 6 shows an example of the highest energy we calculated so far with LAQGSM, namely results by LAQGSM + GEM2 for the reaction p(800 GeV) + Au compared with experimental data (Silberberg et al., 1998) and calculations with the phenomenological code YIELDX (Silberberg et al., 1998). For the sake of brevity, we present in this figure only every third yield measured and tabulated in Silberberg et al. (1992), though we calculated all possible products from this reaction and get similar results for nuclides not shown here. One can see that LAQGSM agrees reasonably with most of the measured yields and describes the data better than YIELDX does. More than a half of the measured products are described by LAQGSM + GEM2 with an accuracy of a factor of two or better, though we find some large discrepancies for several nuclides like 181Hf and 105Rh.

Fig. 7 shows a heavy-ion induced reaction measured at GSI (Junghans, 1997; Junghans et al., 1998), namely the yields of measured products (black circles) from the interaction of a 950 MeV/nucleon 238U beam with copper compared with our LAQGSM + GEM2 results (open circles). One can see that LAQGSM + GEM2 describes most of these data with an accuracy of a factor of two or better.

Finally, Fig. 8 shows an illustrative example of a nucleus–nucleus reaction 40Ar (1.05 GeV/nucleon) + 9Be measured recently at GSI by Ozawa et al. (2000). This interaction of a light nucleus with a medium-mass nucleus in the energy range of ~1 GeV is of interests for astrophysical and radiation shielding applications. LAQGSM + GEM2 describes most of the measured product yields quite well and reproduces correctly the change of the measured cross-sections in an interval covering about six orders of magnitude. We believe that some overestimation by LAQGSM + GEM2 of the measured very neutron-rich product yields is related to the limited statistics of our Monte-Carlo calculation (for the last
measured neutron-rich nuclides with the lowest cross-sections, we have only one or two simulated events) rather than with some serious physics problems of our code. Similar results for other $A + A$ reactions at energies of interest in space and relevant to CR shielding applications may be found in Mashnik et al. (2003a,b,c).

3. Halo size limits from the GALPROP model

This section shows an example of using cross-sections calculated by CEM2k and LAQGSM (together with available data) to put constraints on the Galactic CR halo size. For this calculation we use a state-of-the-art CR propagation code GALPROP.¹ The GALPROP models have been described in full detail elsewhere (Strong and Moskalenko, 1998; Moskalenko et al., 2002 and references therein); here we summarize their basic features.

The code solves a transport equation on a full 3D spatial grid ($x,y,z$) or 2D grid. The 2D models have cylindrical symmetry in the Galaxy, and the basic coordinates are $(R,z,p)$, where $R$ is Galactocentric radius, $z$ is the distance from the Galactic plane and $p$ is the total particle momentum. The propagation region is bounded by $R = R_h$ (taken 30 kpc), $z = \pm z_h$ (a range $z_h = 1–15$ kpc is usually considered) beyond which free escape is assumed. For a given $z_h$ the diffusion coefficient as a function of momentum and the reacceleration parameters is determined by the energy-dependence of the $B/C$ ratio. The spatial diffusion coefficient is taken as $b D_0 \left(\frac{q}{q_0}\right)^2$, assuming independence of position, where $q$ is rigidity. For the case of reacceleration the momentum-space diffusion coefficient $D_{pp}$ is related to the spatial coefficient. The reacceleration is parameterized by $v_A^2 / \omega$ where $v_A$ is the Alfvén speed and $\omega$ the ratio of wave energy density to magnetic field energy density. The source spectrum of nuclei is assumed to be a power law in momentum, $dq(p)/dp \propto p^{-\gamma}$ for the injected particle density, if necessary with a break.

¹ GALPROP model including software and data sets is available at http://www.gamma.mpe-garching.mpg.de/~aws/aws.html.
The interstellar hydrogen distribution uses HI and CO surveys and information on the ionized component; the helium fraction of the gas is taken as 0.11 by number. Energy losses of nuclei by ionization and Coulomb interactions are included. The distribution of CR sources is chosen to reproduce the CR distribution determined by analysis of EGRET gamma-ray data. The primary source abundances are adjusted to give as good agreement as possible with the observed abundances after propagation, for a given set of cross-sections. The heliospheric modulation is taken into account using the force-field approximation.

The nuclear reaction network is built using the Nuclear Data Sheets. The isotopic cross-section database now includes the LANL T-16 compilation by Mashnik et al. (1999) consisting of several tens of thousands of experimental points. This includes a critical re-evaluation of some data and cross-checks. The isotopic cross-sections are calculated in GALPROP using the authors’ fits to major beryllium and boron production cross-sections C,N,O → Be,B, and to other major reactions (Moskalenko and Mashnik, 2003); all other cross-sections are presently calculated using the Webber et al. (1990) and/or Silberberg et al. (1998) phenomenological approximations renormalized to the data where it exists. The reaction network is solved starting at the heaviest nuclei (i.e. $^{64}$Ni), solving the propagation equation, computing all the resulting secondary source functions, and proceeding to the nuclei with $A = 1$. The procedure is repeated down to $A = 1$. In this way all secondary, tertiary etc. reactions are automatically accounted for. To be completely accurate for all isotopes, e.g. for some rare cases of $\beta^+$-decay, the whole loop is repeated twice.

For some astrophysically important reactions we produced our own evaluations of excitation functions (e.g., Moskalenko et al., 2001) instead of using only scarce experimental data or calculations by standalone phenomenological systematics or nuclear reaction models. For this purpose we used all available to us experimental data from the LANL T-16 compilation (Mashnik et al., 1999) together with calculations by CEM2k, and for several reactions, by LAQGSM and the older versions of the CEM code, CEM97 and CEM95. Such evaluated data files (Mashnik et al., 1999) have proved to be useful, e.g. to study the production of radioisotopes for medical and industrial applications using high-power accelerators (Van Riper et al., 2001). One example of such an evaluated excitation function, for the reaction $^{28}$Si(p,x)$^{26}$Al, is shown in Fig. 9 together with available data, CEM2k results, and calculations using phenomenological systematics by Webber et al. (1990) and Silberberg et al. (1998). It is seen that CEM2k has some problems in a correct description of this particular cross-section near the threshold; therefore we used abundant experimental data available for this reaction to produce our evaluated excitation function at these energies. It is clear that neither the Webber et al. (1990) systematics nor the Silberberg et al. (1998) approximation describe correctly this excitation function; using their results as an input to CR propagation codes may lead to errors in results and interpretation.

The results of the calculation of Galactic propagation of radioactive isotopes $^{26}$Al, $^{36}$Cl, and $^{54}$Mn are shown in Fig. 10, where the evaluated excitation functions used were produced as described above. The radioactive isotopes of these elements are the main astrophysical “time clocks” which together with stable secondary isotopes allow us to probe global Galactic properties, such as the diffusion coefficient and the halo size. Based on the CR data from spacecraft (ACE, Ulysses, and Voyager, for details see Moskalenko et al., 2001) we...
were able to restrict the halo size as $2\theta \sim 4–6$ kpc. Using the semiempirical systematics yields less consistent results (see, e.g., Strong and Moskalenko, 2001) raising questions about the interpretation. This result supports the conclusion that large uncertainties for the halo size obtained in previous works were mostly due to cross-section inaccuracies.

In future, we plan to develop evaluated data libraries for other astrophysical reactions of interest and to use them in future studies of Galactic CR propagation.

4. Summary

From the results presented here and in the cited references, we conclude that CEM2k and LAQGSM describe well (and without any refitted parameters) a large variety of medium- and high-energy nuclear reactions and are suitable for evaluations of nuclear data for science and applications. We continue our work on further improvements and development of both CEM2k and LAQGSM, but even in their present versions they are quite reliable and may be used as event-generators for astrophysical applications. The CEM2k and LAQGSM codes have been incorporated into the transport codes MARS and LAHET, and we plan to make available our CEM2k + GEM2 code via the RSICC code distribution center at Oak Ridge and to incorporate CEM2k + GEM2 and LAQGSM + GEM2 into the MCNPX transport code in the near future.

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