Comparison Between the SMM and GEMINI++ De-Excitation Models

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Abstract. Nuclear de-excitation codes can be coupled to intranuclear-cascade models to provide coherent and comprehensive descriptions of spallation reactions above ∼150 MeV. This paper discusses the coupling of the Liège Intranuclear Cascade model with two different de-excitation codes: the Statistical Multifragmentation Model and GEMINI++. We present a selection of the results of the simulations that have been performed for the IAEA International Benchmark of Spallation Models, namely: residue yields, double-differential neutron-production cross sections and double-differential alpha-particle-production cross sections, for reactions at energies around 1 GeV. An attempt at discussing merits and demerits of the models is made.

1. Introduction

The possibility of reprocessing nuclear waste in sub-critical assemblies coupled with a proton accelerator has recently renewed the interest of the nuclear-physics community in spallation-reaction modelling. *Transmutation*, i.e. the irradiation of long-lived nuclear waste with high-energy neutrons, would significantly reduce the half-life and the required storage time of the waste and, at the same time, it would liberate enough energy to power the accelerator itself.

The design of such an Accelerator-Driven System (ADS) requires powerful and flexible tools for the optimisation of the configuration and the materials of the neutron source. First of all, one needs a quantitative understanding of the microscopic interactions between the radiation and the matter in the system. What nuclear reactions will take place? How many particles will they produce? What will their energy and angular distributions be? These are the most common problems one has to face. Secondly, it is necessary to simulate the propagation (*transport*) of the produced particles within the system and to calculate how the target composition is modified. Overall, the problem is far too complicated to be tackled by a trial-and-error method and hence one has to turn to microscopic models and transport codes.

At incident energies relevant for transmutation (from several hundreds of MeV up to a few GeV), the most appropriate theoretical tool for the description of particle-nucleus reactions is the coupling of an Intranuclear-Cascade-type model (INC) with a nuclear de-excitation model. It is assumed in the INC framework that the incoming particle starts an avalanche of binary collisions with and among the target nucleons; part of the energy of the incident particle is transferred to nucleons, which may be emitted, or is consumed in the excitation of nucleon resonances and in the production of pions. When the cascade stage terminates, a sizeable part of the target nucleus is left relatively undisturbed and forms a large, excited *remnant*. In a subsequent de-excitation stage, the remnant gets rid of the excess energy by particle emission and/or fission.

This paper discusses the coupling of the Liège Intranuclear Cascade model (INCL4.5) [1] with the GEMINI++ [2] and SMM [3] de-excitation codes and presents some simulated results.

These calculations have been performed in the framework of the International Benchmark of Spallation Models, organised by the IAEA with the goals of assessing the prediction capabilities of the spallation models, understanding the reason for the success or deficiency of the models and reaching a consensus, if possible, on some of the physics ingredients that should be used in the models.

The existence of de-excitation-insensitive observables allows one to fix the free parameters of the cascade model independently of the coupling to a de-excitation code. However, different cascade models produce slightly different remnants and can modify the de-excitation chain. Moreover, it is impossible to isolate completely the de-excitation contribution, the structure of the highly-excited remnants is only approximately known and several unverified assumptions must be made to describe their decay. Consequently, it is rather difficult to draw solid conclusions about the relative merits of different de-excitation models. Nevertheless, the results presented in this paper provide useful indications for the construction of a minimal de-excitation model of wide applicability.

2. The Models

We shall now briefly outline the most important features of the models we have considered. We direct the reader to the cited articles for more comprehensive descriptions.

2.1 INCL4.5

The INCL4.5 model [1] can be applied to collisions between nuclei and pions, nucleons, or light nuclei of energy lower than a few GeV. The particle-nucleus interaction is modelled as a sequence of binary collisions among the particles present in the system. Particles that are unstable over the time scale of the collision, notably delta resonances, are allowed to decay. The nucleus is schematised as a potential well whose radius depends on the nucleon momentum. Nucleons move on straight lines until they undergo a collision with another nucleon or until they reach the surface, where they escape if their total energy is positive and they manage to penetrate the Coulomb barrier. If the phase-space neighbourhood of the escaping nucleon is sufficiently populated, light clusters can be formed through a coalescence mechanism.

The INCL4.5 model simulates a complete collision event, its output being the velocities of all the emitted particles. The characteristics of the remnant (its mass, charge, momentum, excitation energy and intrinsic angular momentum) are derived from the application of conservation laws and are passed to the chosen de-excitation code which simulates the decay of the remnant into a nuclear-stable residue plus a number of nucleons, nuclei and/or gamma rays. The differences among different de-excitation models lie in the allowed decay modes, in the formalisms used to describe them and in the parametrisation of critical ingredients like nuclear level densities, Coulomb barriers, and collective enhancement.

2.2 GEMINI++

GEMINI++ [2] is an improved version of the GEMINI model, developed by R.J. Charity [4] with the goal of describing complex-fragment formation in heavy-ion fusion experiments. The de-excitation of the remnant proceeds through a sequence of binary decays until particle emission becomes energetically forbidden or improbable due to competition with gamma-ray emission.

Since compound nuclei created in fusion reactions are typically characterised by large intrinsic angular momenta, the GEMINI and GEMINI++ models explicitly consider the influence of spin and orbital angular momentum on particle emission. Moreover, GEMINI/GEMINI++ do not restrict binary-decay modes to nucleon and light-nucleus evaporation, which are the dominant decay channels, but allow the decaying nucleus to emit a fragment of any mass. The introduction of a generic binary-decay mode is necessary for the description of complex-fragment formation and is one of the features that set GEMINI/GEMINI++ apart from most of the other de-excitation models.

Emission of nucleons and light nuclei ($Z \leq 2$, 3 or 4, depending on the user's choice) is described by the Hauser-Feshbach evaporation formalism [5], which explicitly treats and conserves angular momentum. The production of heavier nuclei is described by Moretto [6] binary-decay formalism, which is expected to be quite accurate for intermediate-mass systems. For heavy systems, on the other hand, Moretto's formalism overpredicts the width of the fission mass and charge distributions; this shortcoming was cured in the GEMINI++ model with the introduction of the Bohr-Wheeler fission width [7] in conjunction with the systematics of mass distributions compiled by Rusanov et al. [8].

2.3 SMM

The Statistical Multifragmentation Model (SMM) [3] is a nuclear de-excitation code that combines the compound-nucleus processes at low excitation energies and multifragmentation at high energies. The model assumes that the excited, thermalised nuclear system expands, breaking up simultaneously into several fragments as the volume drops below a certain low-density freeze-out volume. Each fragment partition is assigned a thermodynamic weight, which is then used to choose a multifragmentation partition at random. In practical calculations, at low excitation energies only fragment partitions with total multiplicity smaller than four are considered, which dominate at these energies. This includes also binary and ternary decay channels, whereas at high excitation energy all available channels are taken into account. In addition, SMM takes into account competition with the compound-nucleus channel, falling back naturally to conventional evaporation and fission processes at low excitation energy.

The de-excitation of the multifragmentation products is then treated by conventional methods. Light ($A \leq 16$) fragments undergo Fermi break-up, while heavy fragments de-excite through particle evaporation or fission. Evaporation is described by the Weisskopf-Ewing formula [9] and considers ejectiles up to ^{18}O, as well as excited states of light particles. The fission width is calculated using the Bohr-Wheeler formula. Previously SMM was successfully used for analysis of multifragmentation reactions, which play an essential role at hadron beam energies higher than 2–3 GeV, and in heavy-ion collisions. However, in the present case (1-GeV proton beams) we may expect to observe only the onset of the multifragmentation process.

3. Results and Discussion

The coupling of INCL4.5 with GEMINI++ and SMM has been tested in light-target and heavy-target collisions.

Residue yields for the 1-GeV p + ^{56}Fe reaction are presented in Figure 1. Neither model is very accurate for residues close to the target ($A \simeq 50$), a deficiency which is probably due to a shortcoming of the cascade stage. The GEMINI++ model reproduces quite well the shape of the whole distribution, while SMM overestimates the production of intermediate-mass fragments

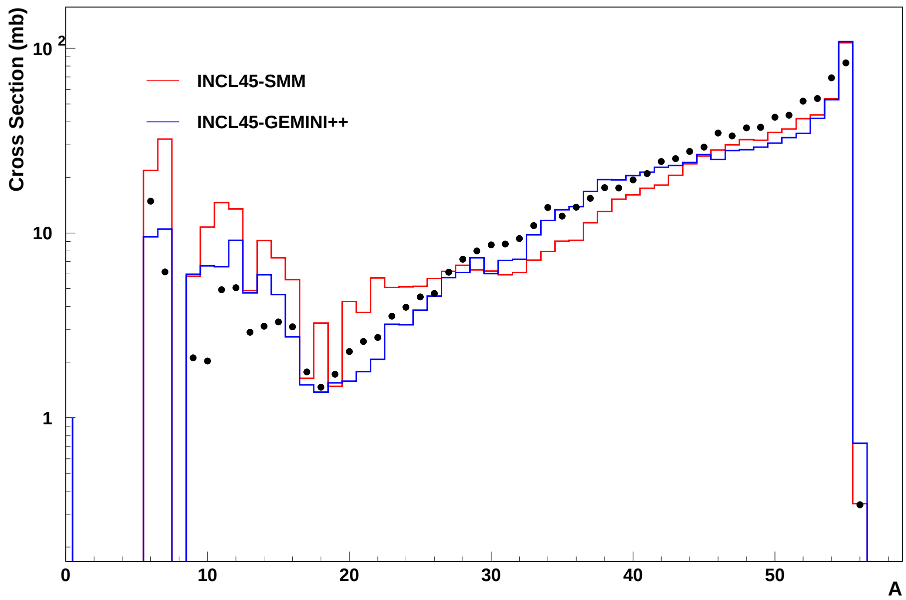

FIG. 1: Residue yields for 1-GeV p + ^{56}Fe as a function of the residue mass number, as calculated by `INCL4.5/SMM` (red) and `INCL4.5/GEMINI++` (blue). Experimental data are taken from Refs. [10] and [11].

(IMFs, $2 < A \lesssim 20$) and underestimates residues of mass between 30 and 45. However, previous studies [10] have shown that `SMM` produces better results if one introduces an intermediate pre-equilibrium stage between cascade and de-excitation. The need to include pre-equilibrium in the description of spallation reactions is the subject of a long-standing discussion and is beyond the scope of this paper. However, it has been observed that it is possible to fit heavy-ion reaction yields by assuming a parametric form of the mass/charge/energy distribution of thermalised fragments and by simulating de-excitation with `SMM` [12]. In this approach, the best-fit excitation-energy distributions are colder than those expected from cascade models, which would be consistent with the introduction of a pre-equilibrium stage after cascade. Finally, no attempt has been made to adjust the free parameters of `SMM`'s evaporation/fission module to ameliorate the agreement with the experimental data when `INCL4.5` remnants are used as input.

It is also interesting to observe that, while both models predict IMF yield in the right ballpark, the production mechanism is very different: in `SMM` IMFs can be produced in the multifragmentation stage or in evaporation, while in `GEMINI++` they are produced exclusively in asymmetric-fission events. Our result suggests that inclusive distributions (such as Figure 1) cannot help settle the question of the IMF production mechanism in spallation reactions around 1 GeV. More discriminating observables, such as correlations, are necessary.

Figure 2 shows the mass distribution of residues in 1-GeV p + ^{238}U. `GEMINI++` is again quite good in reproducing the data, except in the IMF region. It is clear that neither model is able to reproduce the abundant IMF production observed in the experiments, which might indicate that the need for refinements of the evaporation (`SMM`) or asymmetric fission (`GEMINI++`) mechanisms for highly excited heavy nuclei.

The left panel of Figure 3 reports double-differential cross sections for neutron production in a 1.2-GeV p + ^{208}Pb reaction. The cascade stage is exclusively responsible for the high-energy

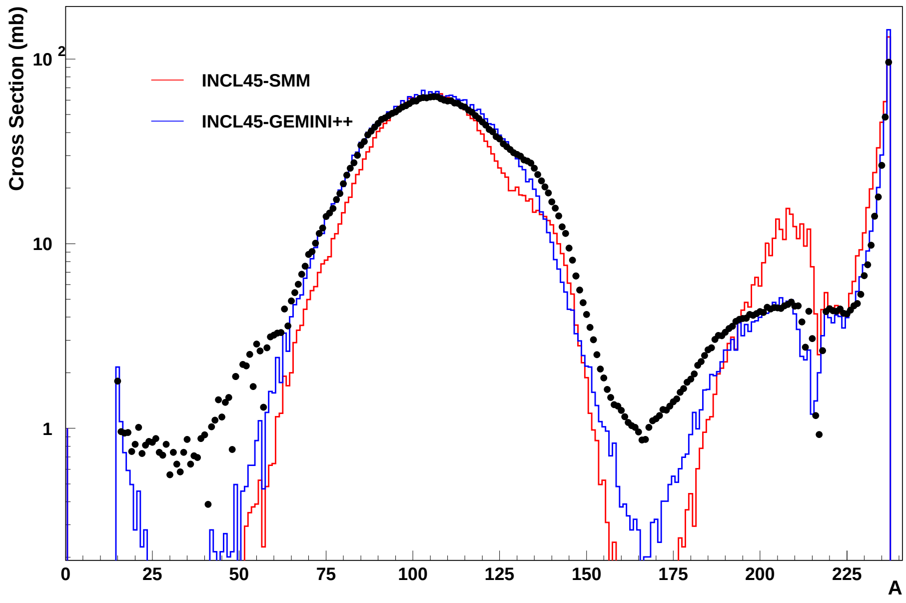

FIG. 2: Residue yields for 1-GeV p + ^{238}U as a function of the residue mass number, as calculated by `INCL4.5/SMM` (red) and `INCL4.5/GEMINI++` (blue). Experimental data are taken from Refs. [13, 14, 15, 16].

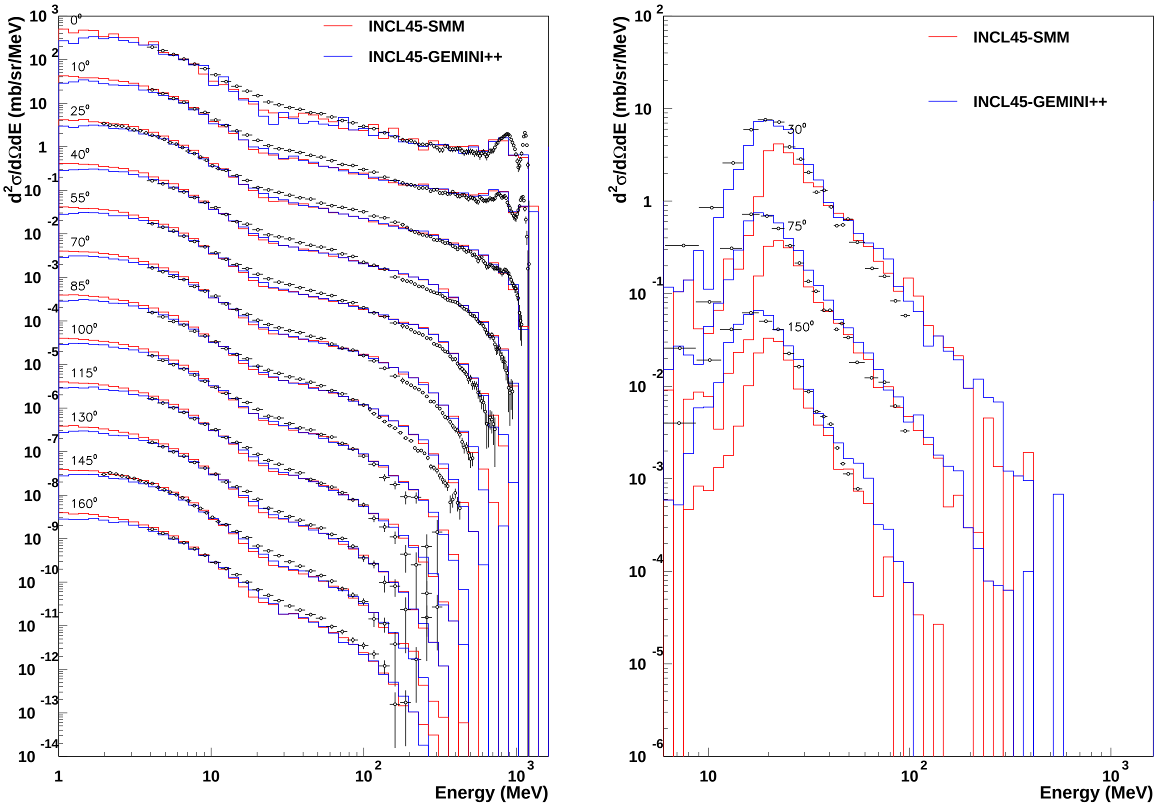

FIG. 3: Double-differential cross sections for neutron production in 1.2-GeV p + ^{208}Pb (left) and alpha production in 1.2-GeV p + ^{181}Ta (right), as calculated by `INCL4.5/SMM` (red) and `INCL4.5/GEMINI++` (blue). Experimental data are taken from Refs. [17, 18].

part of the spectra, down to about 20 MeV; this explains why the spectra are not very different above this energy (except for statistical fluctuations). Below this energy, neutron emission during de-excitation becomes gradually the dominant contribution. The choice of the de-excitation model will thus influence this part of the spectrum.

An accurate inspection of the plot leads to the following observations. Firstly, all yields seem slightly underestimated around 20 MeV; this defect has been already observed [19] and can be related to the coalescence mechanism for cluster production in `INCL4.5`. Secondly, the `SMM` spectra systematically overestimate the low-energy neutron yields and underestimate the high-energy part of the evaporation shoulder. Here, again, the introduction of a pre-equilibrium stage might help, since particles emitted during pre-equilibrium would be more energetic than the evaporated ones. Finally, the `GEMINI++` prediction is close to the data between $\sim$4–10 MeV, but it underestimates the low-energy end of the spectrum. The experimental data [17], however, refer to a 2-cm-thick target, while the calculations are performed for an infinitesimally thin target; hence, the calculation results should be slightly corrected to be compared with the experimental data. As discussed by Leray et al. [17], the effect of the correction is to soften slightly the evaporation spectrum; thus, the correction would worsen the agreement between `SMM` and the data, but it would improve `GEMINI++`'s prediction.

Finally, the right panel of Figure 3, shows double-differential cross sections for production of alpha particles in a 1.2-GeV p + ^{181}Ta reaction. The `GEMINI++` prediction shows a good production level and a realistic spectrum shape. The position of the Coulomb barrier is quite accurate, although one observes an underestimation of the production of very low-energy particles. The `SMM` result is not quite as good, mainly due to an apparent overestimation of the Coulomb barrier. On the other hand, the slopes of the high-energy tails of the spectra are consistent with the `GEMINI++` predictions and with the experimental values. A refinement of the treatment of Coulomb barriers in evaporation would sensibly improve the prediction of this observable in `SMM`.

As a concluding remark, it is important to give an indication of the calculation time necessary for the simulations; the interest lies in the possible inclusion of cascade/de-excitation models in transport codes, where computational speed represents an essential factor. The good accuracy of the `GEMINI++` code has unfortunately a high computational cost. The simulation of 10^5 events for a 1.2-GeV p + ^{208}Pb reaction on a mid-range modern PC takes about 26.7 h for `INCL4.5`/`GEMINI++` and about 1.15 h for `INCL4.5`/`SMM`. The `GEMINI++` computation time is probably too large for the model to be used regularly for transport calculations.

4. Conclusions

We have coupled the `INCL4.5` cascade code with the `SMM` and `GEMINI++` de-excitation models and we have performed simulations of proton-induced spallation reactions. The results presented in this paper represent a subset of the simulations that have been performed for the International Benchmark of Spallation Models, organised by the IAEA.

The `INCL4.5`/`GEMINI++` model seems to be able to produce accurate results on many observables, such as residue yields, and cross sections for emission of neutrons and composites (alpha particles). This good accuracy, however, comes at the price of a high computational cost.

The `INCL4.5`/`SMM` code does not suffer from the heavy computational penalty of `GEMINI++`, but its results are generally less accurate. We can identify three main reasons for these shortcomings. Firstly, the evaporation/fission module of `SMM` is quite simple; one could probably ameliorate some of `SMM`'s predictions by refining some of the ingredients, such as level densities, Coulomb barriers, or maybe by choosing other evaporation/fission formalisms. Secondly, the free parameters of SMM have not been adjusted to the INCL4.5 remnants; it is thus conceivable that the agreement could be improved with some fine tuning. Thirdly, many of the SMM results presented in this paper would be improved by the adoption of a pre-equilibrium stage between cascade and de-excitation. We did not test this possibility, which might constitute the object of future work.

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