

Heavy-ion collisions described by a new QMD code interfaced to FLUKA: model validation by comparisons with experimental data concerning neutron and charged fragment production

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Abstract

A new code, based on the Quantum Molecular Dynamics theoretical approach, has been developed and interfaced to the FLUKA evaporation/fission/Fermi break-up module. At present, this code is undergoing a series of validation tests. In this paper its predictions are compared to measured charged fragment yields and double differential neutron spectra in thin target heavy-ion reactions, at bombarding energies of about 100 MeV/A. The comparisons with the predictions of a modified version of RQMD 2.4 originally developed in Frankfurt [1], already available in the FLUKA code, are presented and potential improvements are briefly sketched.

1 Introduction

Nucleon-nucleus interactions and heavy-ion collisions at non relativistic bombarding energies can be described by macroscopic models or, at a more fundamental level, by microscopic models considering the nucleonic degrees of freedom.

The experimental information shows that *nucleon-nucleus* collisions are dominated both by mean field effects and by short-range correlations due to nucleon-nucleon forces at the shortest distances. Models based on the Intra Nuclear Cascade (INC) theory can be used to simulate these events, since they incorporate both these aspects: the projectile hadron moves along a curved trajectory in the target nucleus mean field generated by Coulomb and nuclear forces. When the projectile hits one of the target nucleons along its path, a scattering can occur, which leads to an abrupt change in the trajectory of both particles. As a first approximation, the potential originated by the incident nucleon can be neglected with respect to the one originated by the target ion, especially for heavy targets.

At the contrary, when *nucleus-nucleus* collisions are considered, each nucleus generates a potential field that affects the movement of the other. In other words, each nucleon

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of the interacting nuclei feels the field due to both the nucleons of its same nucleus, and to the nucleons of the interacting partner. Thus, the force that each nucleon globally experiences is given by a superposition of nucleon-nucleon interactions.

Quantum Molecular Dynamics (QMD) models allow to calculate this force and to study the dynamical evolution of a nucleus-nucleus collision. In these models the Hamiltonian includes an effective interaction part depending on two-nucleon forces. Many-body effects can also be incorporated. A scattering term can be included as well, as in INC codes.

Different research groups have developed models based on QMD theory, which mainly differ in the expression of the Hamiltonian. In the following of this paper the model developed by our group is briefly described (see also Ref. [2]). A few examples of the model predictions and their comparisons with those of a modified version [3] of the RQMD 2.4 code, originally developed by H. Sorge at Frankfurt [1], are presented in the following sections. The modifications were made with the aim of evaluating the yields and the double differential spectra of the fragments which may be produced in the interaction, since the original version gave only the emitted nucleon spectra. Both the new QMD code and the RQMD code have been interfaced to the evaporation/fission/Fermi break-up module available in the FLUKA Monte Carlo transport and interaction code [4], which simulates the de-excitation of the hot fragments produced at the end of the fast stage of heavy-ion collisions. Their de-excitation indeed may occur on a time scale far larger than that of the primary ion-ion collision, and is thus better described by different models, based on statistical instead of dynamical considerations.

2 Theoretical framework

In QMD models each nucleon is described in coordinate space as a gaussian wave-packet,

$$\phi_i(\vec{r}, t) = \frac{1}{(2\pi\sigma_r^2)^{3/4}} e^{-\frac{(\vec{r}-\vec{R}_i(t))^2}{4\sigma_r^2}} e^{i\frac{\vec{r}\cdot\vec{P}_i(t)}{\hbar}}. \quad (1)$$

\vec{R}_i and \vec{P}_i are the average values of the position and the momentum of the i -th nucleon, σ_r is the gaussian space width related to the nucleon momentum distribution width σ_p by the uncertainty relationship $\sigma_r\sigma_p = \hbar/2$. For a nucleus with mass number A , the nuclear wave-function is approximated by the product of A nucleon wave-functions:

$$\phi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A, t) = \prod_{i=1}^A \phi_i(\vec{r}_i, t), \quad (2)$$

neglecting the fermionic nature of the nucleons. In an approximate way, their fermionic behaviour is taken into account a) in the initialisation scheme, when nucleon spatial coordinates and momenta are sampled, according to the experimentally observed density distributions (see next section), b) by including Pauli blocking factors forbidding the collisions which lead a nucleon to a phase-space region already filled. The Hamiltonian operator is a sum of a kinetic and an interaction term:

$$\hat{H} = \hat{T} + \hat{H}_{int}. \quad (3)$$

The interaction part of the Hamiltonian is the sum of many effective terms:

$$\hat{H}_{int} = \hat{H}_{int,eff} = \hat{H}_{Skyrme-II} + \hat{H}_{Skyrme-III} + \hat{H}_{symmetry} + \hat{H}_{surface} + \hat{H}_{Coulomb}. \quad (4)$$

Here, the Skyrme-II two-body interaction term is attractive, while the Skyrme-III three-body interaction term mimics repulsive forces, that are crucial for reproducing the nuclear matter saturation properties at normal density. The symmetry term takes into account the dependence of nucleon forces on the isospin. The surface term leads to two contributions, one repulsive and the other attractive: their sum reproduces the decrease of the potential at low nuclear radii, especially for low mass nuclei. Examples of the relative importance of these contributions to the total average central potential for neutrons in ^{40}Ca (*top* panel) and ^{90}Zr (*bottom* panel) are shown in Fig. 1. These potentials are compared to those proposed by [5], which are obtained by a totally different approach. At last, a Coulomb term is added to those of eq. (4), to take into account the $p-p$ Coulomb repulsion.

Evolution of nuclear states is determined by the Hamiltonian. To evaluate nucleon-nucleon scattering we use $n-p$ and $p-p$ free cross sections which, as a first approximation, we assume to be isotropic. Inclusion of the angular distributions of scattering cross-section, as well of inelastic channels leading to pion and other particle production via resonance formation, represents an important future extension of our model, especially when approaching relativistic energies. Neutrons and protons are distinguished whenever possible in our code. In particular, the symmetry and Coulomb term of the Hamiltonian, as well as the nucleon-nucleon scattering term, take into account the different behaviour of these particles. As an example, there is a factor about three between the free $n-p$ and $p-p$ cross-sections at the energies relevant for this work, as follows from isospin and charge considerations.

3 Nuclear ground states

Nuclear states are initialized by sampling initial spatial coordinates and momenta for all nucleons in each nucleus. Nucleon-nucleon phase-space distances should be large enough to satisfy Pauli Principle, leading to smooth nuclear density and momentum profiles. Peculiar of our calculations is the fact that the total energy of each ion, calculated as a sum of the kinetic and the interaction energy, according to the Hamiltonian introduced in previous section, is exactly constrained by the experimentally observed nuclear binding energy. The difference between n and p free masses is also taken into account and attention is paid to ensure conservation of energy and momentum. The evolution of each nuclear state according to the Hamiltonian is followed for a time-scale of 250 - 300 fm/c. If, in this time interval, no spurious emission of nucleons occurs and root mean square radius oscillations maintain within a few percent, the configuration is accepted and stored off-line. It can then be used to simulate ion-ion (or nucleon-ion) collision events.

4 Ion - ion collisions

The nuclear states stored during the initialisation procedure can be used to simulate ion-ion collisions. To this purpose, for any given impact parameter value, the ions are boosted

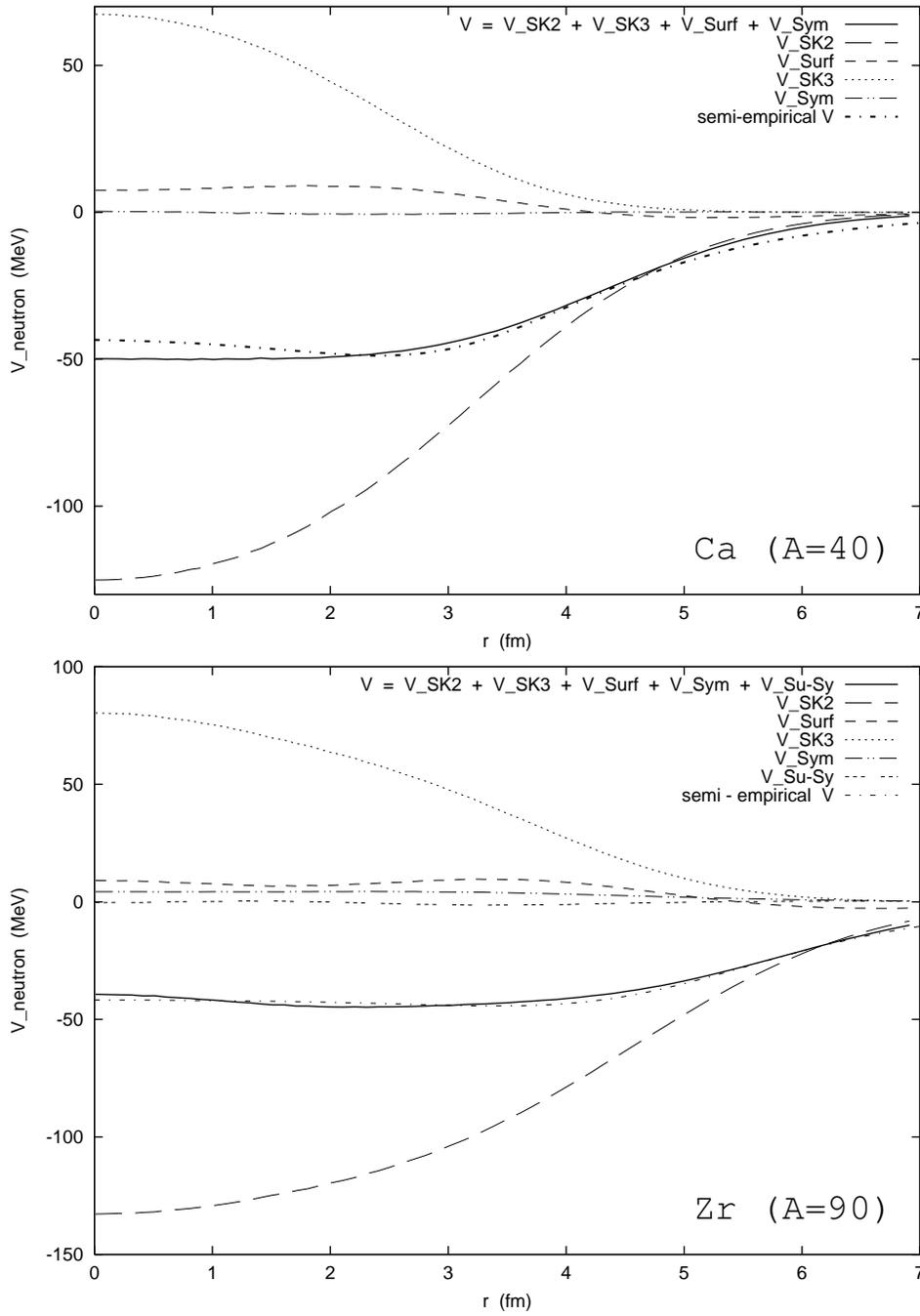


Figure 1: Radial dependence of the neutron potential for ^{40}Ca nuclei (*top*) and for ^{90}Zr nuclei (*bottom*), including the *Skyrme-II* attractive term (long-dashed line), the *Skyrme-III* repulsive term (dotted line), the *symmetry* term (dashed-double-dotted line) and the total (attractive + repulsive) *surface* term (short-dashed line). The sum of all these terms is given by the solid line and is compared to the semi-empirical central component of the neutron potential calculated according to the parameter set OB of Ref. [5] (dot-dashed line).

one towards the other to mimic the collision process. As soon as colliding nuclei come close to each other, nuclear forces due to the target (projectile) nucleons become increasingly important in affecting the projectile (target) nucleon behaviour. Additionally, Coulomb interaction, because of its infinite range, appears to be crucial since the beginning of the simulation, also when the ions are still far from each other, especially for determining the distance between the two ion centers when the ions come in contact, which slightly differs from the impact parameter. When the incoming nuclei overlap, an hot excited system, characterized by an increased density and pressure, is created. The compression phase is followed by an expansion stage, involving density fluctuations, leading to the formation of excited fragments. During this fast stage, to define a temperature can be a very difficult or even an impossible task, especially at energies of several tens MeV/A. At lower energies, repeated nucleon-nucleon collisions gradually lead to a thermalization of the biggest excited systems (pre-equilibrium phase), followed by isotropic emission. On the other hand, at higher energies, the expansion phase starts before this thermalization process could be completed.

Hot fragments are defined on the basis of nucleon final configuration, without any reference to their target or projectile initial belonging. Their de-excitation involves the competition of different processes whose probability of occurrence depends on the nuclear species and the energy. The processes considered in our calculations and simulated by the de-excitation module of the FLUKA code, account for γ emission, evaporation, Fermi break-up and fission. Fermi break-up is used for excited light nuclei and may produce up to six fragments. The FLUKA evaporation routine allows the emission of particle and light fragments, up to a mass number $A = 24$. Further details on the FLUKA de-excitation module can be found in Ref. [6].

5 Results: double - differential neutron spectra and fragment yields

We have analyzed the experimental data of Ref. [7]. These authors in an thin target experiment measured the double-differential spectra of neutrons emitted in the interaction of He, C, Ne ions, at 135 MeV/A bombarding energy, and of Ar ions, at 95 MeV/A bombarding energy, with C, Al, Cu and Pb ions. Examples of the comparison of the experimental data and our theoretical predictions are shown in Fig. 2 and Fig. 3 for the reactions induced on the aluminium and copper targets. Different sets of data on the same plot refer to different emission angles. The absolute yields have been multiplied by decreasing scaling factors (negative powers of 10) for increasing emission angle. As already mentioned at the beginning of this paper, in our analysis we used both the QMD code and the modified version of the RQMD 2.4 code [3].

The two codes differ quite substantially. The Hamiltonian included in the Sorge code is fully relativistic, but involves only Skyrme-II and Skyrme-III interactions. No distinction is made between neutrons and protons and Coulomb effects are not included. On the other hand, the Hamiltonian in our QMD code can implement relativistic or non-relativistic kinematics, according to a switch, but only instantaneous interactions are included (non-relativistic potential). As already mentioned, neutrons and protons are distinguished both considering their mass and their isospin. In the figures, the results of

the simulations performed with our QMD code coupled to FLUKA are given by triangles, while those of the simulations performed with RQMD + FLUKA are represented by histograms. No normalization factor has been included in the simulations.

In general, both models show an overall good agreement with the experimental data. At a more detailed level, the figures show that our QMD is capable of predicting better than RQMD the behaviour of neutron spectra at intermediate emission angles ($30^\circ - 80^\circ$), especially at the highest energy end of the spectra, while it underestimates the emissions in the very forward direction. Finally, both models show a comparable agreement with the experimental data at backward angles ($\geq 90^\circ$). We expect that the disagreement between data and QMD calculations in the forward and backward directions can be reduced by implementing in the code the angular dependence of n - p cross sections, which should increase the yield of particles emitted back and forth along the collision axis.

We have also calculated the yields of fragments emitted in the same reactions. Unfortunately, this information is not experimentally available, thus, we only compare the predictions of the two codes. Let us discuss the results concerning the fragment charge yield distributions. These are shown in the upper and in the lower panels of Fig. 4 for the He + Cu and Ar + Cu interactions, respectively. We find that the QMD code predicts an higher He fragment yield and the discrepancies between the two model predictions increase with increasing reaction mass asymmetry

$$\eta = \frac{|A_{proi} - A_{targ}|}{A_{proi} + A_{targ}} . \quad (5)$$

For reactions characterized by a large mass asymmetry, such as He + Cu, the yield of intermediate charge fragments predicted by QMD + FLUKA is far larger than that predicted by RQMD + FLUKA as shown in the upper part of Fig. 4. These fragments are produced as remnants of projectile and target nuclei, in central collisions, and by evaporation of projectile-like and target-like nuclei, in more peripheral collisions. The reasons of these discrepancies in predicting such a different number of IMF has still to be understood. In particular, the way the two codes treat ion-ion asymmetric systems, the role of the compressibility and that of the hot fragment definition scheme, at the end of the ion overlapping stage, are under investigation.

The description of asymmetric systems by QMD/RQMD models is more difficult than the description of the symmetric ones, because in the effective Hamiltonian the light nucleus parameters may be different from the heavy nucleus ones as suggested by many authors. Thus, while in RQMD a fixed parameter set is used for all nuclei, in QMD we try to incorporate these differences adopting parameters depending on the nuclear mass, as already done in [8]. The discrepancy may also be due to the fact that QMD Hamiltonian includes a Coulomb term while RQMD does not, and to the different way the production of fragments is evaluated in the two codes. In RQMD calculation only projectile-like and target-like hot residuals are considered, while in QMD, as previously reminded, hot fragments are defined on the basis of excited nucleon configurations, without any reference to their target or projectile initial belonging. This may lead to multifragmentation and to the production of fragments made of nucleons of both the projectile and the target. The discrepancies seem to reduce for smaller reaction mass asymmetries as shown in the lower part of Fig. 4.

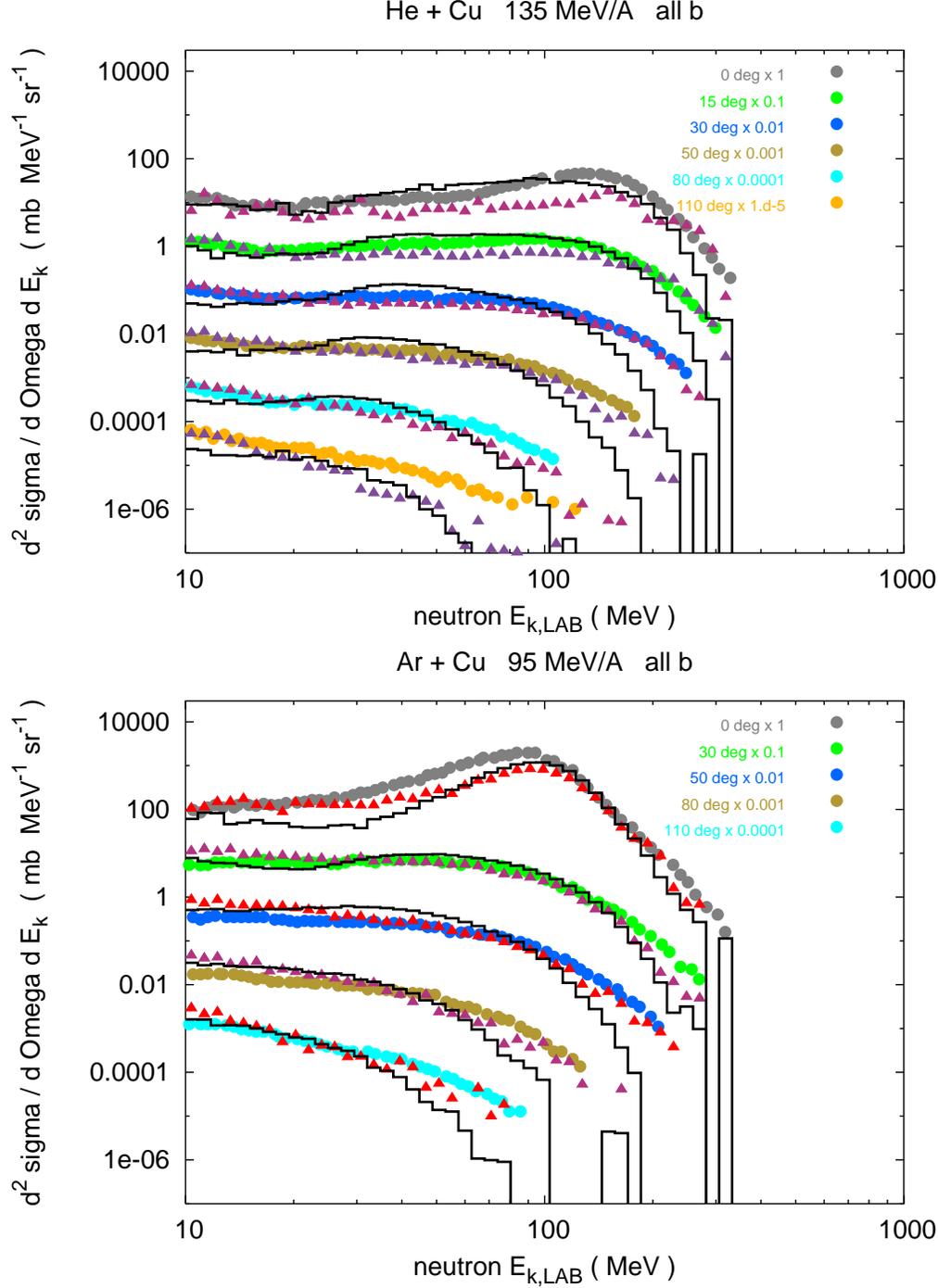


Figure 2: Double-differential neutron spectra for He + Cu at 135 MeV/A bombarding energy (upper figure) and Ar + Cu at 95 MeV/A (lower figure). In each figure the spectra are given as a function of the neutron energy, and, from top to bottom, each spectrum corresponds to emission angles $\theta = 0^\circ, 15^\circ, 30^\circ, 50^\circ, 80^\circ, 110^\circ$. The theoretical distributions predicted by QMD + FLUKA (filled triangles) and by RQMD + FLUKA (histograms) are compared to the experimental data of Ref. [7] (filled circles)

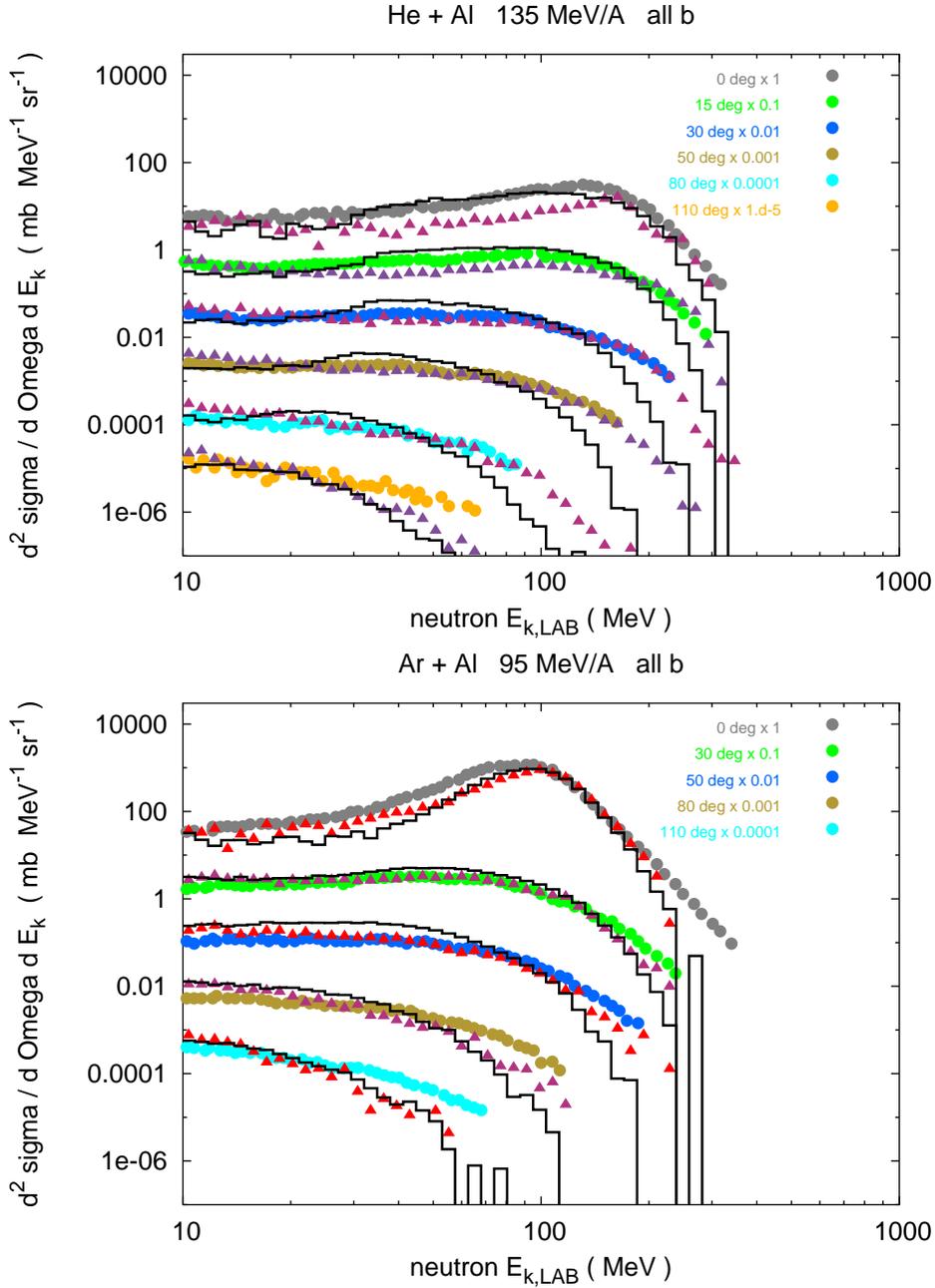


Figure 3: Double-differential neutron spectra for He + Al at 135 MeV/A bombarding energy (upper figure) and Ar + Al at 95 MeV/A (lower figure). In each figure the spectra are given as a function of the neutron energy, and, from top to bottom, each spectrum corresponds to emission angles $\theta = 0^\circ, 15^\circ, 30^\circ, 50^\circ, 80^\circ, 110^\circ$. The theoretical distributions predicted by QMD + FLUKA (filled triangles) and by RQMD + FLUKA (histograms) are compared to experimental data of Ref. [7] (filled circles).

6 Conclusions

A code, based on the Quantum Molecular Dynamics approach, has been developed for describing the fast stage of heavy-ion collisions at non-relativistic bombarding energies

and coupled to the FLUKA de-excitation module. The model is undergoing further improvements, such as the inclusion of pion and particle production via resonance formation according to the isobar model, in order to extend its predictions to higher energies. The angular dependence of nucleon-nucleon scattering cross-section needs also to be included. Comparisons with the experimental data and the predictions of other theoretical models is encouraging. In particular, the double-differential spectra of the emitted neutrons measured by [7] are quite satisfactorily reproduced.

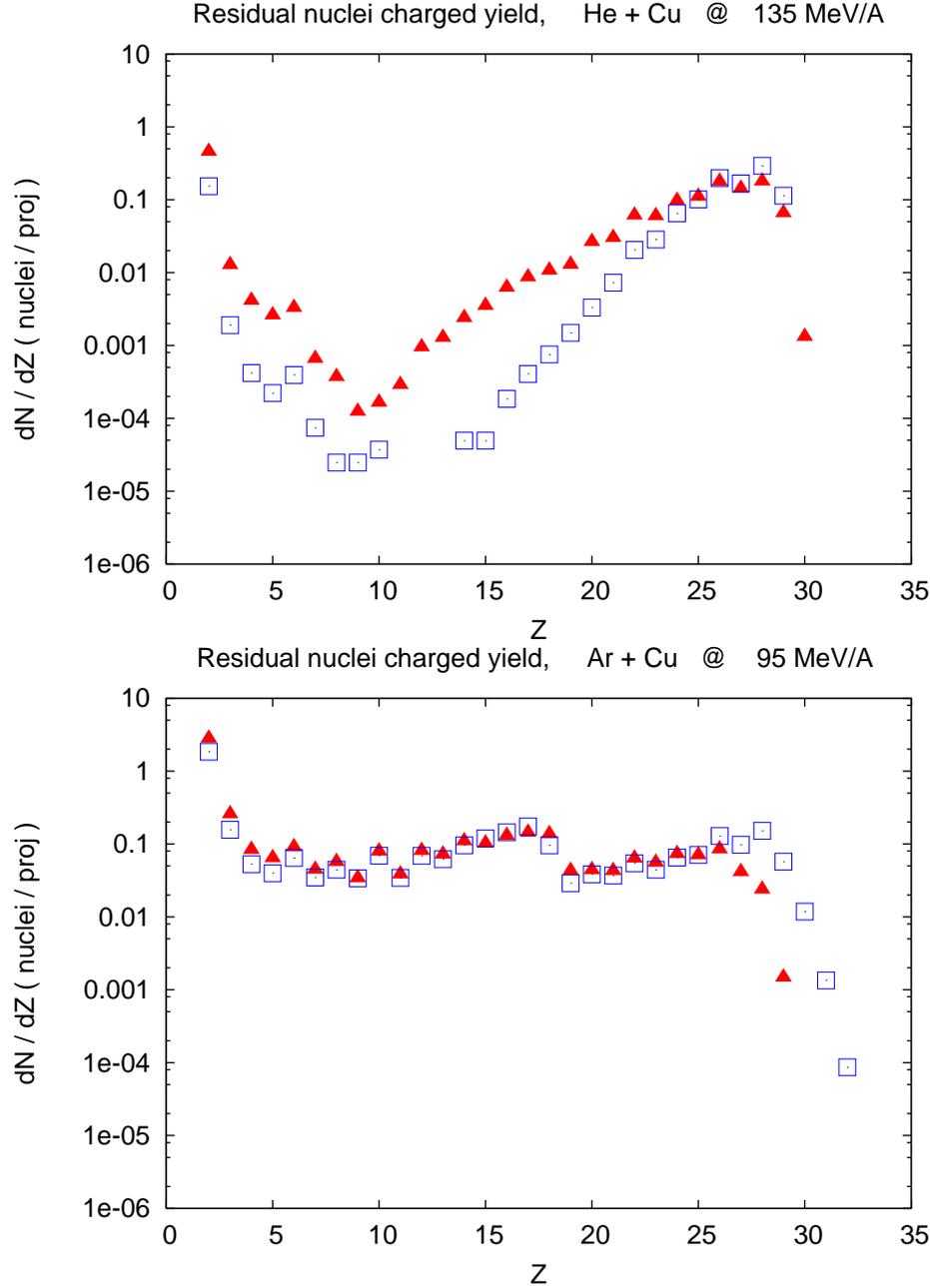


Figure 4: Residual nuclei charged yield for He + Cu at 135 MeV/A bombarding energy ($\eta = 0.88$) (*top*) and for Ar + Cu at 95 MeV/A ($\eta = 0.22$) (*bottom*), as predicted by QMD + FLUKA (filled triangles) and by RQMD + FLUKA (boxes).

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