

A Monte Carlo approach to study neutron and fragment emission in heavy-ion reactions

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Abstract

Quantum Molecular Dynamics models (QMD) are Monte Carlo approaches targeted at the description of nucleon-ion and ion-ion collisions. We have developed a QMD code, which has been used for the simulation of the fast stage of ion-ion collisions, considering a wide range of system masses and system mass asymmetries. The slow stage of the collisions has been described by statistical methods. The combination of both stages leads to final distributions of particles and fragments, which have been compared to experimental data available in literature. A few results of these comparisons, concerning neutron double-differential production cross-sections for C, Ne and Ar ions impinging on C, Cu and Pb targets at 290 - 400 MeV/A bombarding energies and fragment isotopic distributions from Xe + Al at 790 MeV/A, are shown in this paper.

Key words: heavy-ion collisions, QMD, fragmentation, evaporation

PACS: 24.10-i, 25.70.Mn, 21.60.Ka

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1 Introduction

Since several years, Quantum Molecular Dynamics models (QMD) have been introduced to simulate heavy-ion collisions (see e.g. Aichelin (1991) and references therein, Niita et al. (1995)). They are semi-classical approaches (Boal and Glosli (1988)), derived from the Classical Molecular Dynamics ones, by adding a few quantum features. The main one is that each nucleon is described by a coherent state, and is thus identified by gaussian spatial coordinate and momentum distributions, centered around mean values, and characterized by gaussian widths whose product minimizes the Heisenberg uncertainty relationship. A second quantum feature is the fact that nucleon-nucleon scattering cross-sections taken from the experiments are used to describe nucleon-nucleon collisions occurring in the fast-stage of the reactions between ions, when nuclei can overlap, depending on the impact parameter value. The impact parameters are randomly chosen, according to a Monte Carlo procedure. Thus both very peripheral reactions and more central ones can occur, on an event by event basis. Actually the measured free nucleon-nucleon cross-sections are used when a nucleon-nucleon collision occurs in these reactions, while the effects on each nucleon of all other nucleons present both in the projectile ion and in the target one are taken into account by means of effective potentials, included in the interaction part of the Hamiltonian, during the whole simulation. Another quantum feature is the fact that the collisions which lead a nucleon in an already occupied phase-space region are forbidden, according to the Pauli blocking principle. This is especially effective at non-relativistic energies, where nucleon-nucleon potentials are increasingly more important than nucleon-nucleon collisions to determine the fragmentation process, since most nucleon-nucleon collisions are blocked. Finally, a few authors have also developed fully antisymmetrized versions of QMD models (e.g. Fermionic Molecular Dynamics by Feldmeier (1990); Feldmeier and Schnack (2000), and Antisymmetrized Molecular Dynamics by Ono et al. (1992a,b)), by fully antisymmetrizing the nuclear wave-functions, which in the original QMD versions are merely given by the product of nucleon wave-functions. At present, these advanced versions are successfully used in very specific problems, such as the study of exotic nuclear structure, mainly for light nuclei due to the complexity of the underlying approaches, and their intensive CPU requirement. We limit to the original approximation for the nuclear wave-functions, instead of using a more advanced approach, since our final aim is developing a code to be used real-time to microscopically describe ion-ion collisions in general applicative problems, which can involve even the heaviest ions and composite targets. To accomplish this aim, a preliminary version of our code has been interfaced to the general purpose Monte Carlo FLUKA code, allowing the simulation of fragment formation and the study of the emission of fragmentation products, in thin and thick targets, even in complex geometries. Nevertheless, to better characterize and investigate the nuclear reaction processes, the results of simu-

lations performed in the simplest theoretical case of generating thousands of single ion-ion collision events are shown in this paper. This means that ion-ion overlapping and nuclear de-excitation effects have been accurately considered, while target thickness effects, such as ion energy loss and reinteraction in matter, were neglected in making these simulations.

2 Theoretical elements of our simulations

A QMD code has recently been developed by our Collaboration and interfaced to the FLUKA code. FLUKA (Fassò et al. (2005)) is a particle transport and interaction code, used since several years in many fields of Physics. It is currently developed according to an INFN - CERN official agreement and is made available on the web (<http://www.fluka.org>). It is based, as far as possible, on theoretical microscopic models, which are continuously updated and improved, and benchmarked with respect to newly available experimental data. Nucleon-nucleus collisions are simulated in FLUKA by means of the module called PEANUT (PreEquilibrium And Nuclear Thermalization, Ferrari and Sala (1996)), which contains also a de-excitation sub-module. This sub-module has also been used to describe the de-excitation processes which may occur at the end of the overlapping stage of ion-ion collisions, which has been simulated in this work by means of our QMD code. In particular, the QMD code has been used to follow the ion-ion system evolution for a few hundreds of fm/c, while de-excitation processes can occur on a time scale far larger (up to $\sim 10^7$ fm/c), and have been simulated by means of the statistical models contained in the FLUKA de-excitation sub-module. De-excitation is provided by different mechanisms, sometime in competition. Evaporation has been considered, both of light particles and fragments, up to a mass $A = 24$. Fission processes can occur, as well as Fermi break-up of light nuclei, with a maximum of six bodies in the final state in the present implementation. Finally, de-excitation by photon emission is also included in FLUKA. A correct description of de-excitation is crucial, since it deeply modifies the particle and fragment pattern present at the end of the fast stage of ion-ion collisions. In fact, while peripheral collisions give often rise to slightly excited projectile-like and target-like fragments, with masses very similar to the projectile and target ones, respectively, very central collisions are capable of generating intermediate mass fragments (IMF), characterized by lower masses and higher excitation energies: hot fragments in turn decay, deeply affecting the final fragment and particle emission distributions. A few features of our QMD code are presented in Subsection 2.1, while the results of our simulations are shown in Section 3.

2.1 QMD specific features

As explained in the Introduction, several QMD versions and codes have already been developed, characterized by some common features, and some specific differences, depending on the working group and the intended application. Here some features of the code we have developed are briefly sketched. The Hamiltonian is made by a kinetic and an effective interaction part. Our code can switch between non-relativistic and relativistic kinematics, according to a user initial choice, while only instantaneous interactions are included. A fully relativistic version, including relativistic potentials, is also under development thanks to the cooperation with the University of Houston and NASA, and is the object of a separate work (Zapp et al. (2006)). Neutrons and protons are distinguished both for their interaction and for their mass. The initial nuclear states, used in the ion-ion collision simulation processes, are prepared in advance, stored off-line and exactly fulfill the experimental constraints on binding energies. Binding energies are calculated by summing the kinetic energy and the potential energy of all nucleons in the nucleus. The potential energy is given by a superposition of different terms, due to the interaction of each nucleon with all other nucleons present in the ion. In particular, Skyrme-type two-body and three-body interaction terms are included, as well as two-body symmetry and surface terms. The symmetry term helps taking into account the difference among neutrons and protons, by assigning different weights to the interactions between nucleons with the same isospin and nucleons with different isospin. Furthermore, a Coulomb term is included, which acts only on protons. Further details on the effect of each term in determining the total potential energy of each ion can be found in Garzelli et al. (2006b). When two ions collide, each nucleon is subject to the effects of both the nucleons in the same nucleus and those in the other one. At ion-ion distances exceeding a few fm, only the Coulomb force is important, while nuclear interaction among nucleons of different nuclei becomes significant only at lower distances, i.e. during the ion-ion overlapping process. Also nucleon-nucleon collisions can occur in this stage, which are implemented in our code taking into account free n - p and p - p (n - n) reaction cross-sections. As an approximation, this process is assumed to be isotropic, i.e. the angular dependence of the cross-sections is neglected, as well as the pion production channel. Further extensions of the model will include these elements. Ion-ion system evolution is followed for a time of $\sim 150 - 200$ fm/c after the overlapping stage. At the end, hot excited fragments may be present, as well as emitted neutrons and protons. The de-excitation of hot fragments has been simulated thanks to the interface to the FLUKA de-excitation module, as explained at the beginning of Section 2.

3 Results of the simulations and comparisons with experimental data

As explained in Section 2, the results presented in this paper have been obtained by the interface between our QMD code and the FLUKA nuclear de-excitation routines. In Subsection 3.1 double-differential neutron production cross-sections for several projectile-target systems at energies 290 and 400 MeV/A are compared to available experimental data, while in Subsection 3.2 fragment isotopic distributions from Xe projectiles impinging on an Aluminium target at 790 MeV/A are shown. QMD + FLUKA has also been tested at energies around and below 100 MeV/A. A few results of these lower-energy tests have been presented in Garzelli et al. (2006a,b,c).

3.1 Double-differential neutron production cross-sections

Several papers presenting neutron double-differential production cross-section data have been published. Most of them consider thick targets. Nevertheless, at the aim of investigating the reliability and the prediction capabilities of theoretical ion-ion reaction models, it is better disentangling transport effects, thus data from thin target experiments are more suited. Iwata et al. (2001) present double-differential neutron production cross-sections for many systems, mostly considering thin targets. Therefore, the experimental data presented by these authors have been considered for our simulations. The targets used in their experiment are made of Carbon, Copper and Lead. The results of our simulations for a Carbon beam at a 290 MeV/A bombarding energy and Neon and Argon beams at 400 MeV/A, hitting Carbon, Copper and Lead ions, are shown in Fig. 1, and compared to the experimental data. Different histograms refer to different emission angles. In particular, from the top to the bottom of each panel one can distinguish neutrons emitted at 5° , 10° , 20° , 30° , 40° , 60° and 80° angles with respect to the incoming beam direction in the laboratory frame. The results at different angles have been multiplied by the same factors used in Iwata et al. (2001) for display purposes. The results of the theoretical simulations show an overall reasonable agreement with the experimental data, especially at emission angles $\geq 20^\circ$. On the other side, at forward emission angles ($5^\circ - 10^\circ$), the simulations give rise to neutron emission peaks lower than those experimentally observed. In the case of Carbon projectiles at 290 MeV/A these peaks are located at higher energies than the experimentally measured ones, and this can be an evidence of the fact that target thickness effects can not be neglected and have to be included in the simulations. In fact, our simulations have been made in the bare approximation of neglecting all target geometry effects, i.e. each target is merely given by a single ion. The same real targets used in the experiments

with Carbon projectiles at 290 MeV/A have also been used by Iwata et al. (2001) with Neon projectiles at 400 MeV/A. In this last case, the agreement of the results of the theoretical simulations with the experimental data is more satisfactory, both regarding the location of the peaks and their height. This point can be ascribed to the fact that projectiles at higher energies can penetrate more deeply, so that ion energy loss and reinteraction effects can be neglected more safely. To better investigate this aspect, we have planned to repeat the same simulations, taking into account geometry effects. This would be possible thanks to the FLUKA geometry package. Another source of discrepancy could be ascribed to the fact that isotropic n - p and p - p cross-sections have been used in the simulations, instead of considering the angular dependence really observed in nucleon-nucleon scattering experiments. We expect that including the last one can further improve the agreement of the theoretical simulations with the experimental data. As far as intermediate emission angles are concerned, the agreement is instead already quite satisfactory. We emphasize that the absolute results of our simulations shown in Fig. 1 have been obtained without making use of any normalization factor. The spectra at intermediate and backward angles have been attributed by Iwata et al. (2001) to the partial superposition of two components. The equilibrium component corresponds to the lower kinetic energy ($E_n < 20$ MeV) part of the spectra, where an increasing number of emitted neutrons with decreasing energy can be observed (shoulder), while the cascade/pre-equilibrium component is given by a wide peak extending up to a few hundreds MeV/A. The theoretical simulations made by QMD + FLUKA appear to agree in predicting the presence of both these distributions.

3.2 *Fragment isotopic distributions*

When two ions collide at energies of a few hundreds MeV/A, highly excited fragments can be formed, which in turn decay to lower mass and charge ones by de-excitation processes. Isotopic distributions for projectile-like fragments have been measured by Reinhold et al. (1998) at GSI in the case of ^{129}Xe ions at a 790 MeV/A bombarding energy, impinging on an Aluminium target. We have simulated about 10,000 $^{129}\text{Xe} + ^{27}\text{Al}$ reaction events at the same bombarding energy using QMD + FLUKA. The results of our simulations are presented in Fig. 2. In each panel the production cross-section is shown for the isotopes of a different element, ranging from $Z = 54$ to $Z = 40$ (projectile-like isotopes). Together with the results of our theoretical simulations, also the experimental measures taken from Reinhold et al. (1998) are plotted. We can appreciate a better agreement between the theoretical and experimental distributions for the elements whose atomic number is very close to the projectile Z value ($Z \sim 54 - 50$), than for the lighter fragments ($Z \sim 44 - 40$). While the first ones are more copiously produced, the last ones are more rarely

emitted, as follows by comparing their production cross-sections. The results of our simulations refer to fragment emitted over the whole solid angle. At the considered energy, higher mass and charge fragments are produced in more peripheral collisions, and propagate in forward direction, while the lower mass and charge ones can be emitted also at larger angles. Furthermore, at fixed Z , the simulations seem to overestimate the N richer tails, while underestimating the higher Z ones. Indeed, an asymmetry between the two tails is evident also from the experimental data, but to a lesser extent than obtained by the theoretical simulations. Reinhold et al. (1998) explain their results suggesting that neutron-deficient fragments are formed from prefragments with high excitation energies, and consequently a crucial contribution to their formation could be played by evaporation processes. Since neutrons can evaporate more easily than protons, due to Coulomb barrier effects on the last ones, the evaporation of neutrons would give rise to these fragments. According to this scenario, the theoretical excess of N richer fragments could be ascribed to the fact that the excitation energies of the fragments at the end of the fast stage of the collision process are not high enough. We observe that repeating the same simulations by using a completely different model to describe the fast stage of ion-ion collisions, i.e. the relativistic QMD code RQMD2.4 developed at Frankfurt a few years ago by Sorge et al. (1989a,b), and already coupled to FLUKA by our Collaboration (Aiginger et al. (2005)), leads to very similar results, also plotted in Fig. 2. A comparison between the results of the two models shows that at a 790 MeV/A bombarding energy the isotopic distributions are rather insensitive to the fact that fully relativistic potentials are used, or non-relativistic ones, as are the cases of RQMD and QMD, respectively. Including a pre-equilibrium phase after the fast stage of the collisions, with a smooth transition to the equilibrium stage described by statistical models, could help in gaining further insight on the reasons of the discrepancies with experimental data. Furthermore, another source of possible discrepancies could be the fact that the Aluminium target thickness has not been taken into account in our simulations. All these points are currently under investigation. The total theoretical charge fragment yield as a function of Z is presented in Fig. 3 for completeness, including also fragments with $Z < 40$, whose distributions have not been measured in the experiment by Reinhold et al. (1998).

4 Conclusions

We have performed simulations of ion-ion collision events, in the approximation of neglecting target geometry effects such as beam energy loss and reinteraction during propagation, by using the QMD we have developed in the last few years, interfaced to the statistical de-excitation module taken from the general purpose Monte Carlo FLUKA code. Results of simulations at bom-

barding energies around and below 100 MeV/A have been shown in other papers, while here results have been shown concerning different projectile-target combinations at energies of a few hundreds MeV/A. Specific observables, such as neutron double-differential production cross-sections at different angles and fragment isotopic distributions, have been calculated. Comparisons of the results with experimental data suggest an overall reasonable agreement, even if some discrepancies also appear, which need further investigation. In particular, a precise reproduction of the target geometry and the experimental setup, as well as the inclusion in the model of the angular dependence of nucleon-nucleon cross-sections, are in our opinion crucial to further improve the agreement with the experimental data.

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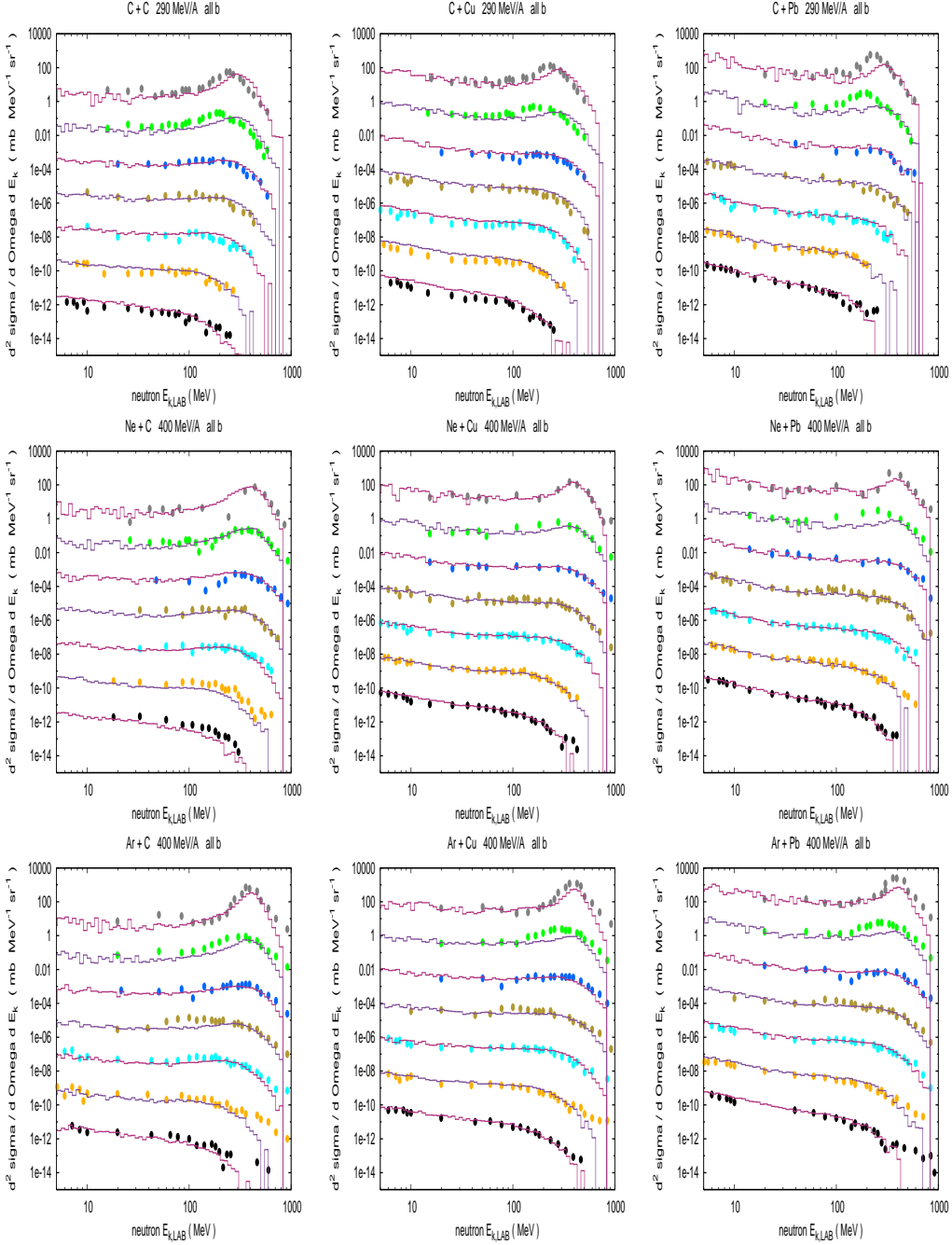


Fig. 1. Double-differential neutron production cross-section for C (top), Ne (center) and Ar (bottom) projectiles impinging on C (left), Cu (center) and Pb (right) at 290, 400, 400 MeV/A bombarding energies, respectively. The results of the theoretical simulations made by QMD + FLUKA are shown by solid histograms, while the experimental data measured by Iwata et al. (2001) are shown by filled circles. In each panel, distributions at 5° , 10° , 20° , 30° , 40° , 60° and 80° angles with respect to the incoming beam direction in the laboratory frame, have been multiplied by decreasing even powers of 10, for display purposes. The details of target geometry (thickness and shape) have not been taken into account in our theoretical simulations.

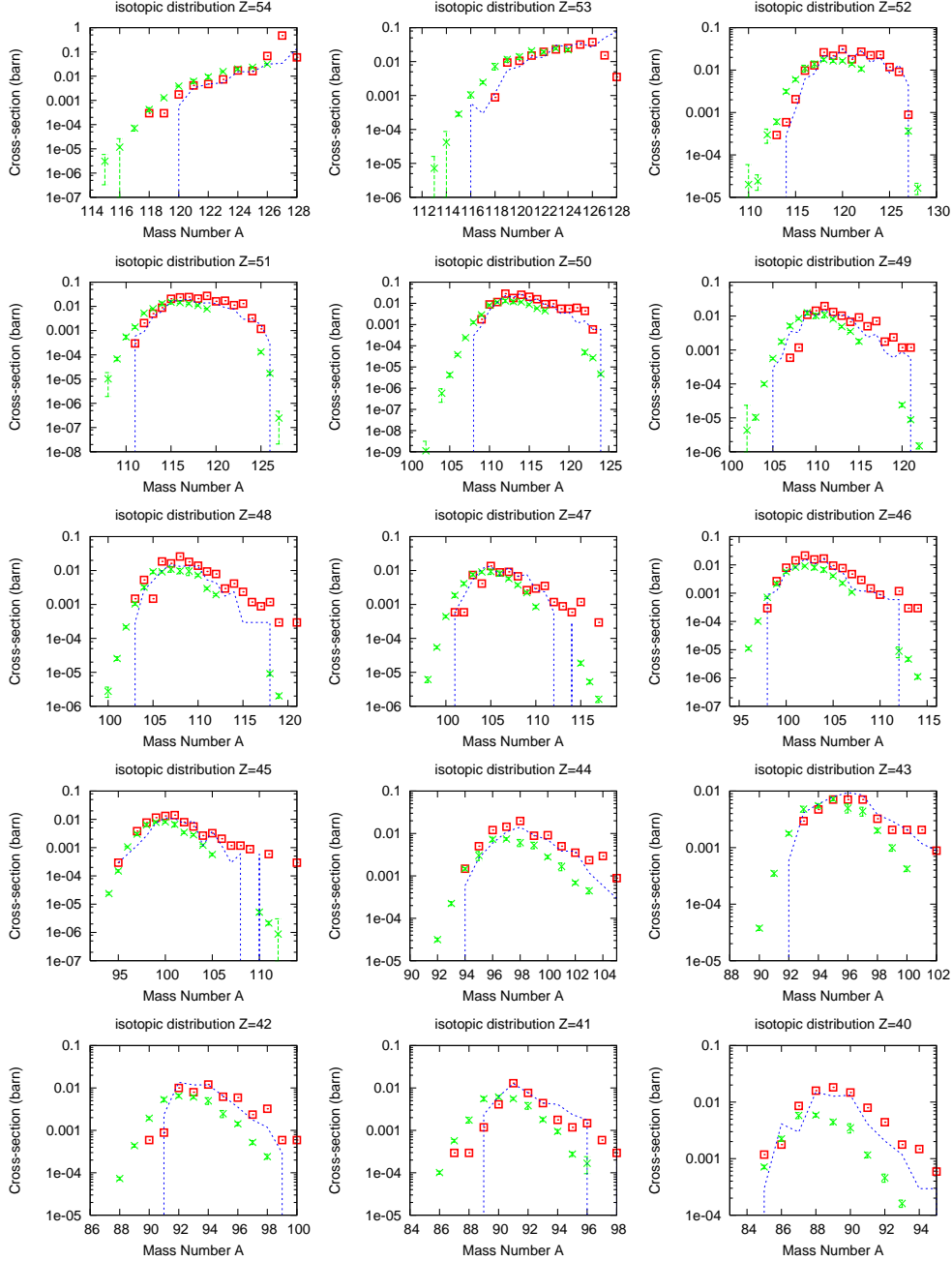


Fig. 2. Isotopic distributions of projectile-like fragment production cross-sections (barn) for a 790 MeV/A ^{129}Xe beam hitting an Al target. Each panel contains the results for the isotopes of a different element. The results of the theoretical simulations of about 10,000 $^{129}\text{Xe} + ^{27}\text{Al}$ reaction events made by QMD + FLUKA are shown by open squares, while the experimental data taken from Reinhold et al. (1998) are shown by crosses. The results obtained by a modified version of the fully relativistic code RQMD2.4 + FLUKA are also superimposed on each plot (dotted lines).

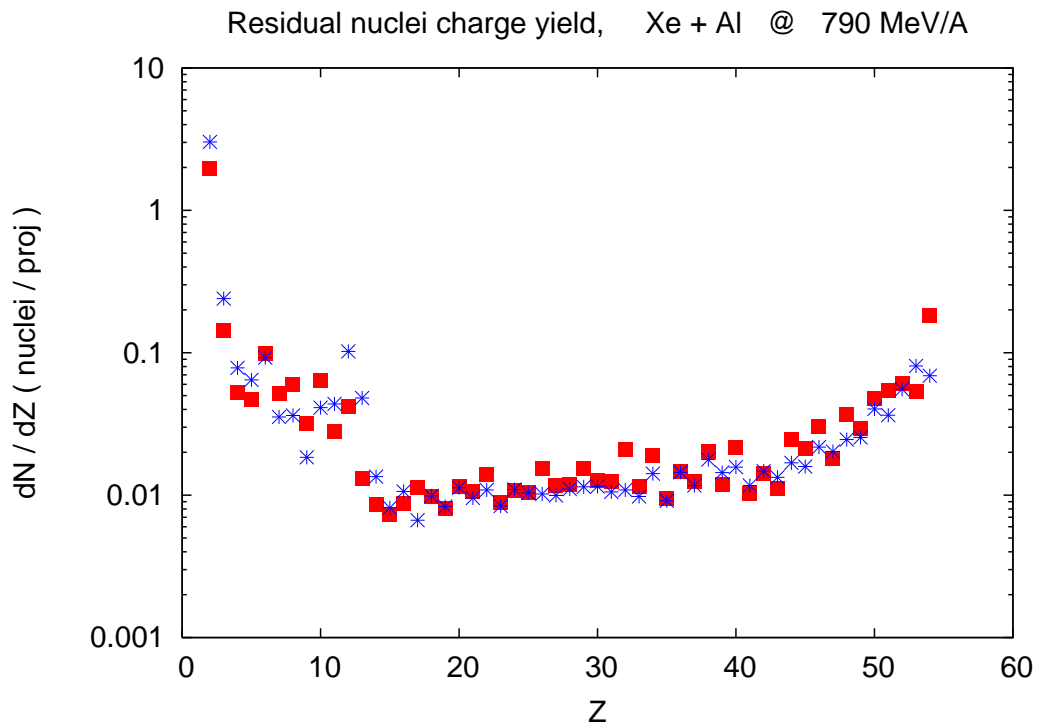


Fig. 3. Charge fragment yield for the same projectile-target combination considered in Fig. 2. The theoretical results predicted by QMD + FLUKA (filled squares) are compared to those predicted by RQMD2.4 + FLUKA (asterisks).