A QMD Description of the Interaction of Ion Beams with Matter

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Abstract. Heavy-ion collisions can be simulated by means of comprehensive approaches, to include the many different reaction mechanisms which may contribute. QMD models and their relativistic extensions are examples of these approaches based on Monte Carlo techniques. In this paper are shown some results obtained by coupling a new QMD code, which describes the fast stage of ion-ion collisions, to the evaporation/fission/Fermi break-up and γ de-excitation routines present in the FLUKA multipurpose Monte Carlo transport and interaction code. In particular, we compare the predicted neutron spectra to available experimental data from thin and thick target irradiations. We show also some predictions of particle and charged fragment fluences for the interaction of C and Fe ions with a thick PMMA target, which may be useful to assess the risk of side-effects in the hadron therapy of tumours.

1 Introduction

Heavy-ion collisions at non-relativistic bombarding energies can be simulated by Quantum Molecular Dynamics (QMD) calculations. These are comprehensive approaches which allow one, using Monte Carlo techniques, to take into account in a natural and straightforward way the whole of the different reaction mechanisms which contribute to a given two-ion interaction as a function of the impact parameter and the bombarding energy. These features make them most suitable for describing processes where yields and fluences of emitted particles and fragments have to be predicted and controlled, as it is needed in hadron therapy and radiation protection in space missions.

Since nuclear fragmentation can be interpreted as the result of nuclear density fluctuations, originated by the collisions, a proper description of nucleon correlations is crucial for understanding this process. The QMD methods allow one to take into account correlations in a natural and straightforward way. The time evolution of the projectile-target ion system in phase-space is calculated at each step of the simulation, by relating the spatial coordinates and momenta of each nucleon to the coordinates and momenta of all other particles. The nucleon wave-function evolution is evaluated by the Variational Principle, by minimizing the action corresponding to an Hamiltonian describing the nucleon-nucleon interactions.

In the original versions of QMD [1], the nuclear wave-function is merely given as a product of nucleon wave-functions. In more advanced versions, e.g. the Fermionic Molecular Dynamics (FMD) [2] and the Antisymmetrized Molecular Dynamics (AMD) [3], the fermionic nature of nucleons is properly taken into account. As far as we know, these last approaches are used for investigating nuclear structure (e.g. for light exotic nuclei), but they have never been applied in a systematic way for studying the interaction of heavy-ion beams in thick targets, due to their complexity and the required huge amount of CPU time. Since our aim is setting up an ion-ion collision event generator to be used at relatively low bombarding energies, from about one hundred up to a few hundred MeV/A, for describing the interaction and transport of heavy-ion beams in matter, considering thick composite targets of complex geometries, we choose to develop a non relativistic QMD code in which the fermionic nature of nucleons is taken into account in an approximate way. This is made using Pauli blocking factors in nucleon-nucleon scattering processes and by giving an initial nucleon state distribution which forbids that identical nucleons be in the same phase-space region [4].

2 The Hamiltonian

The QMD calculations discussed in literature mainly differ in their Hamiltonian, both considering its terms and the strenght of the nucleon interaction coefficients. In the following we briefly discuss, as reminded above, results which we have obtained using a non-relativistic Hamiltonian, i.e., assuming an istantaneous effective nucleon-nucleon interaction. Our Hamiltonian incorporates isospin and Coulomb effects, i.e. *n*-*p*, *p*-*p* and *n*-*n* interactions have different strengths and radial dependence. Its nuclear part includes an attractive Skyrme 2-body interaction term and a repulsive Skyrme 3-body interaction term. This one is crucial to reproduce the saturation properties of nuclear matter at normal density ($\rho_0 \simeq 0.17\,\mathrm{fm}^{-3}$). A symmetry term takes into account isospin effects, and a surface term, given by the sum of an attractive and a repulsive term, is also included to reproduce the decrease of the nuclear potential at low r. The nuclear terms of the Hamiltonian contain parameters fitted to reproduce the observed properties of nuclear matter and finite nuclei.

In order to compare most of the calculated observables with experimental data, an accurate description of the de-excitation of residues produced after the fast nuclear interaction stage of the reaction is also needed. In fact QMD can be used to study the fast overlapping stage of an ion-ion collision ($\Delta t_{fast} \sim 10^{-22}$ s), that leads to the formation of pre-fragments, i.e. fragments which may be excited. Other models, based on statistical considerations, are more suitable to describe the de-excitation of these fragments, which may occur on a time scale several order of magnitudes larger (Δt_{de-ex} up to $\sim 10^{-15}$ s). Thus, our QMD has been coupled to the de-excitation module available in the FLUKA Monte Carlo transport and interaction code [5, 6]. At present, the de-excitation module allows one to take into account the evaporation of light particles and intermediate mass fragments (up to $A = 24$), fission, Fermi break-up (in the case of smaller fragments), and γ emission.

3 Simulation of Thin Target Experiments

To validate the low energy limit of our calculations we have analysed neutron double differential spectra in heavy-ion collisions at bombarding energies below 150 MeV/nucleon. An example of the results obtained with our QMD + FLUKA calculations is shown in Figure 1 where our predictions are compared to the experimental spectra measured by [7] in the interaction of 95 MeV/A Ar ions with a thin Al target. In this experiment the target thickness was chosen to ensure the projectile ion energy loss be smaller than a few MeV. Our calculations (filled triangles) reproduce quite accurately the experimental data (filled circles), especially at intermediate neutron emission angles (30–80 deg).

The QMD + FLUKA calculations reproduce with fair accuracy also the other experimental results given in [7], as shown, e.g., in Figure 2 where the experimental and calculated spectra of the neutrons emitted in the interaction of Ne ions with Al ions at 135 MeV/A bombarding energy are compared.

An example of the ability of our calculations to reproduce the yield of the emitted light and intermediate mass fragment is given in Figure 3, for the reaction Ca + Ca at 35 MeV/A. To reproduce accurately the data, the calculation must simulate accurately the experimental constraints, such as those concerning the measured fragment multiplicity. The agreement of our calculations with the experimental data measured with the AMPHORA detector at SARA [8], is quite satisfactory.

4 Thick Target Applications

For applicative purposes one has often to deal with the interaction of an ion beam with a thick target of complex geometry. In this case one must describe also the interactions of secondary particles and fragments with the target. To do this our QMD code has been interfaced to the FLUKA Monte Carlo transport and interaction code which allows one to study the transport of ions and secondary particles in thick materials considering, in addition to nuclear interactions, many effects such as energy losses due to medium ionization, bremsstrahlung, multiple scattering. As reminded before, FLUKA also includes a nuclear de-excitation module, which can be used to simulate the de-excitation of the hot fragments that may be present at the end of the fast stage of the ion-ion collisions described by the QMD calculations.

An example of the ability of the QMD + FLUKA calculations to reproduce neutron spectra observed in a thick target experiment is shown in Figure 4, where our calculations are compared to the neutron spectra measured in the interaction of an Ar

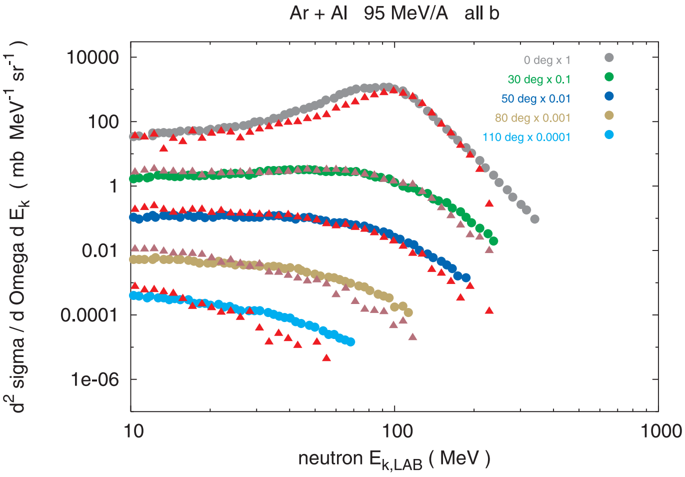

Figure **1.** Double-differential spectra of the neutrons produced in the interaction of Ar and Al ions at 95 MeV/A bombarding energy. The theoretical distributions predicted by QMD + FLUKA (filled triangles) are compared to the experimental data of [7] (filled circles).

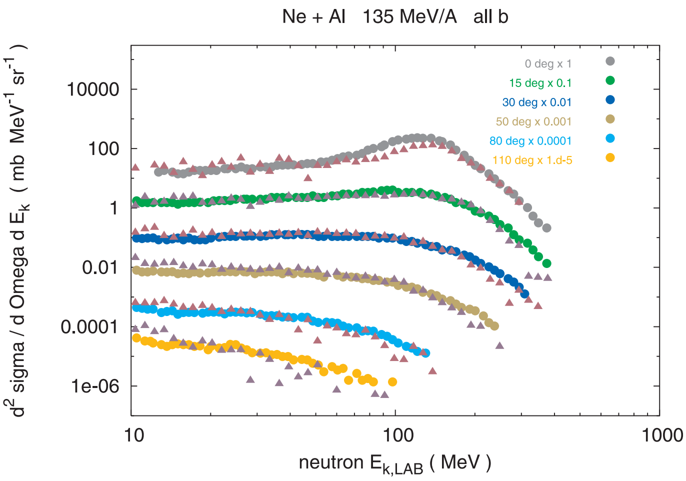

Figure **2.** Double-differential spectra of the neutrons produced in the interaction of Ne and Al ions at 135 MeV/A bombarding energy. The theoretical distributions predicted by QMD + FLUKA (filled triangles) are compared to the experimental data of [7] (filled circles).

beam with a thick Al target at 400 MeV/A bombarding energy [9]. The aluminium target used in the experiment had a thickness $d = 5.5$ cm, and was able to stop the incident beam. The agreement between the results of the calculated and the experimental spectra is very encouraging, even considering the small underestimation of

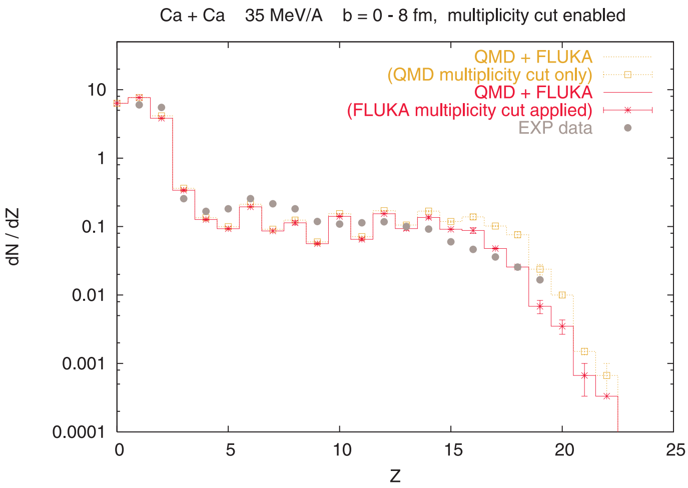

Figure **3.** The theoretical prediction of the yield of the charged fragments produced in the symmetrical Ca + Ca interaction at a 35 MeV/A bombarding energy (red filled circles and yellow squares, joined by histograms) is compared to the experimental measurement for central collisions events (grey circles) made with the AMPHORA detector at SARA [8]. The reproduction of the data requires to simulate exactly the experimental set up and contraints, as it may be appreciated by comparing the yellow histogram, obtained by imposing that the charged fragment multiplicity be more than 5 at the end of the nucleon interaction cascade described by QMD, to the red histogram, obtained by imposing that the charged fragment multiplicity be more than 10 at the end of the de-excitation stage, and fulfilling the requirement of quasicomplete events according to the detector acceptance, as in the experiment.

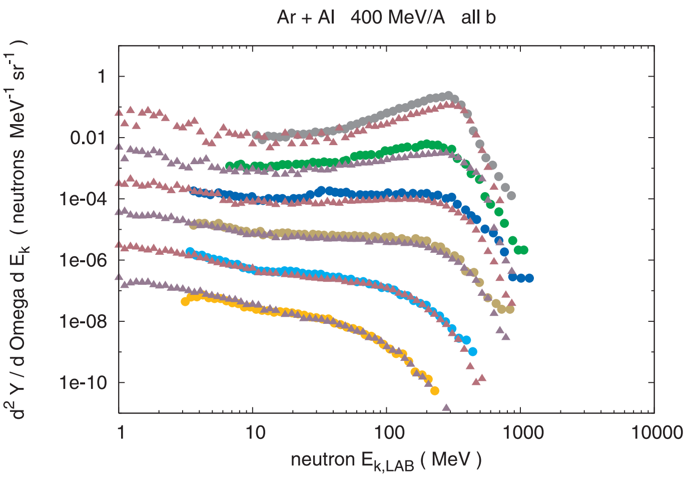

Figure **4.** Double-differential neutron spectra from the interaction of Ar and Al ions at 400 MeV/A bombarding energy. A 5.5 cm aluminium target was used to stop completely the Ar incident beam. The theoretical distributions predicted by QMD + FLUKA (filled triangles) at 0°, 7.5°, 15°, 30°, 60°, 90° emission angles are compared to the experimental data of [9] (filled circles).

the neutron yield along the beam direction. We emphasize that the reproduction of the absolute yield does not require any normalization coefficient. These calculations help to estimate the risk of side effects in patient's treatment. One of the growing applications of FLUKA concerns just this field, considering also the biological damage to the irradiated tissue [10–12].

The use of transport codes is necessary in hadron therapy studies for evaluating the spatial distribution of the physical dose given to a patient. To do this one must consider all primary and secondary particles, and their energy and angular distribution as they propagate in the biological tissue. An example of the capabilities of the calculations in describing such processes is provided by the study of the propagation of a 400 MeV/A Carbon ion beam in a 10 cm radius PMMA cylinder 10 cm deep, surrounded by air. PMMA ($C_5H_8O_2$) is a compound which allows to simulate the energy loss of a particle beam in biological tissues. The calculated spatial distribution of neutron, proton and heavy fragment fluence (expressed in particles/cm^2/primary ion) are shown in the top, central and bottom panels of Figure 5, respectively. The comparison of the emitted particle's fluences shows that neutrons are more spreaded out than protons and heavy-ions. Neutrons, originated from primary and secondary interactions of beam particles with the target, are not subject to Coulomb interaction and can thus propagate deep in matter. In Figure 6 the dose distribution predicted at different depths inside the PMMA cylinder previously considered is shown in the case of the bombardment with a 400 MeV/A iron beam. In this figure, the results of the QMD + FLUKA calculations are compared to those made with the current version of FLUKA using the Relativistic Quantum Molecular Dynamics code RQMD2.4 [13–15]. The results of the two calculations practically coincide up to the Bragg peak showing that the prediction of the dose distribution in this range region does not appear to be particularly sensitive to the differences between QMD and RQMD2.4 [4]. On the other hand, in the distal part of the peak, slight differences concerning the total released dose appear. These are due to different implementations of nuclear interaction effects in the two codes, which are more pronounced at low interaction energies.

5 Conclusions and Perspectives

Fragmentation of ion beams propagating in matter can be simulated by dinamical models, considering nucleon correlations. Quantum Molecular Dynamics models predict nucleon-nucleon phase-space correlations in a straightforward and natural way and allow one to describe the dynamical evolution of nuclear systems in the fast stage of heavy-ion collisions. In this paper results are shown concerning particle and fragment fluences and distributions, originated by the propagation and the interactions of different beams in low-Z targets. The simulations have been performed with a QMD code coupled to the FLUKA Monte Carlo general purpose transport code.

Especially gratifying is the reproduction of thick target data which are simulated by a fully microscopical calculation of the primary and secondary interac-

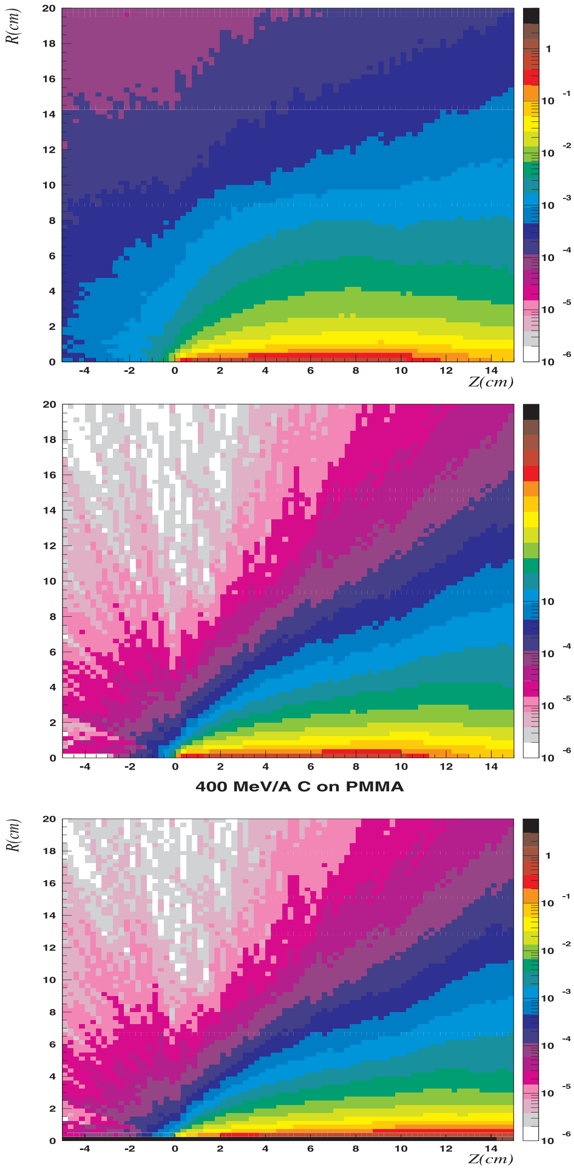

Figure **5.** Spatial distribution of the neutron (*top* panel), proton (*intermediate* panel) and ion (*bottom* panel) fluences for a 400 MeV/A C beam propagating along the axis of a 10 cm radius PMMA cylinder 10 cm deep (which is not shown in the figure) in a cylindrical symmetry geometry. The plots show the results of the simulations carried out with QMD + FLUKA. The cylinder front face is located at $Z = 0$ cm, while the beam is supposed to come from the left along the Z axis (abscissa axis in the figure). The PPMA cylinder is surrounded by air: the formation of a cascade of particles and fragments also outside the cylinder can be explained by the interactions of primary particles and secondary products with the air surrounding the cilinder.

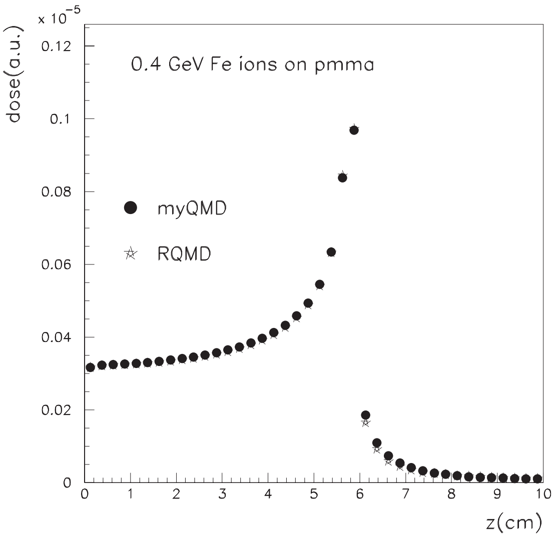

Figure **6.** Dose distribution (arbitrary unit) as a function of the propagation depth for a Fe beam propagating in the PMMA cylinder as in Figure 5, at 400 MeV/A bombarding energy. The cylinder front face is located at $Z = 0$ cm (origin of the abscissa axis). The results of the simulation made with QMD + FLUKA (full circles) are compared to those of the simulation with RQMD + FLUKA (empty stars).

tions. The obtained results are encouraging in view of their use in hadron therapy and radioprotection in space missions. For this purpose, further simulations and comparisons with experimental data to assess the ability of the code in predicting heavy fragment distributions are at present under way. As shown in the paper, charge fragment yields from symmetric central collisions are in very reasonable agreement with the experimental data.

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