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To cite this article: B Braunn *et al* 2013 *J. Phys.: Conf. Ser.* **420** 012163

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Comparisons of hadrontherapy-relevant data to nuclear interaction codes in the Geant4 toolkit.

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Abstract. Comparisons between experimental data, INCL and other nuclear models available in the Geant4 toolkit are presented. The data used for the comparisons come from a fragmentation experiment realised at GANIL facility. The main purpose of this experiment was to measure production rates and angular distributions of emitted particles from the collision of a 95.A MeV ^{12}C beam and thick PMMA (plastic) targets. The latest version of the Intra Nuclear Cascade of Liège code extended to nucleus-nucleus collisions for ion beam therapy application will be described. This code as well as JQMD and the Geant4 binary cascade has been compared with these hadrontherapy-oriented experimental data. The results from the comparisons exhibit an overall qualitative agreement between the models and the experimental data. However, at a quantitative level, it has been shown that none of this three models manage to reproduce precisely all the data. The nucleus-nucleus extension of INCL, which is not predictive enough for ion beam therapy application yet, has nevertheless proven to be competitive with other nuclear collisions codes.

1. Introduction

Hadrontherapy treatments with carbon ions consists in irradiating cancerous tumours with ^{12}C ions from 80 to 400 MeV/u. Compared to conventional radiotherapy, it presents two main advantages: a maximum of dose deposition at the end of the path of the ions (i.e. Bragg peak) and an enhanced biological efficiency in the Bragg peak region. For treatment application, a high accuracy is required for the dose value (3%) and for its location (1 mm). The largest uncertainty relies on the ion fragmentation process along its penetration path in the patient tissues [1]. This process leads to an attenuation of the beam flux which is not negligible. The table 1 gives the proportion of primary beam not consumed by nuclear fragmentation for different energies in the range of hadrontherapy. At "low" energy, nuclear interactions are already responsible for the loss of 14% of the primary beam flux.

This leads also to an increase of the number of lower Z fragments produced all along the path of the primary beam. These fragments contribute to the dose before and at the Bragg peak and must be taken into account for the evaluation of the biological effects [2]. They also contribute to spread the dose in the surrounding healthy tissues especially after the Bragg peak. The figure 1 from Gunzert-Marx *et al.*[3] illustrates the fragments contribution to the dose.

Energy (MeV/u)	100	200	300	400
N/N_0	0.86	0.66	0.45	0.27

Table 1: Proportion of primary ions reaching the Bragg peak without occurring a nuclear interaction in thick water target for four different kinetic energies. Geant4 simulations results. Courtesy of D. Cussol.

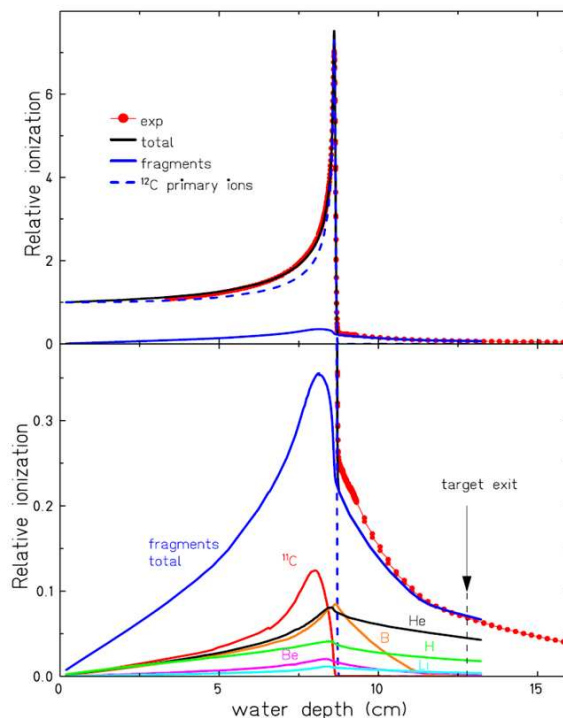


Figure 1: From [3]. The ionization function (Bragg curve) of a 200 MeV/u $^{-1}$ ^{12}C ion beam in water. The measurement was performed with parallel-plate ionization chambers and a precision water absorber [4]. Calculations with the Monte-Carlo code (particle and heavy ion transport code system (PHITS)) are in good agreement with the measurement. The lower part with magnified ordinate scale shows the contribution of fragments with different atomic numbers Z as calculated with PHITS. The thickness of the water target used in our fragmentation measurements is indicated by an arrow.

To improve the knowledge on the ^{12}C fragmentation process, experiments have been performed in Japan and in Europe for more than 15 years. Measurements of light charged fragment production in water and PMMA have been done by the Japanese treatment centers (Chiba and Hyogo). They have performed measurements of carbon ions fragmentation in PMMA phantoms in the energy range 200–400 MeV/u ([5, 6, 7]). Similar experiments have also been performed by the GSI biophysics department. Light charged ions and neutron production rates due to the fragmentation of a carbon projectile in water have been measured for beam energies ranging from 200 to 400 MeV/u ([8, 9, 3]). All these measurements allowed the determination of the integrated flux and the energy distributions of the fragments relative to the water depth. These data have been implemented in treatment planning systems (TPS) like TRiP. They can also be used to constrain nuclear reaction models ([10]). In 2008, an experiment have been

made at GANIL facility to measure the production rate of these fragments after various thick PMMA targets and at different angles with a 95 MeV/u ^{12}C beam. Results from this experiment have been published in Braunn *et al.*[11] and supplement the Japanese and German data in the hadrontherapy "low" energy region.

Here, a first comparison of these newly available data with three different nuclear models is presented.

2. Simulation

The Geant4 simulation tool-kit[12] is used as general structure to perform the comparisons. It is a Monte Carlo code developed by CERN to simulate particle interactions in matter. It can handle particle evolution "step by step" taking into account all processes that might happen. In the case of the Braunn *et al.* experiment, charged fragments produced by nuclear interactions between carbon ions and hydrogen, carbon and oxygen nuclei. The simulations were done with the Geant4 release version 9.05.

10^8 primary ^{12}C ions are generated in a Gaussian shape in position ($y, z = 0$, $\sigma = 0.4$ mm) and energy ($E = 94.6$ MeV/u, $\sigma = 0.1$ MeV) and propagated along the x axis. Targets are made of PMMA ($\text{C}_5\text{H}_8\text{O}_2$, density: $\rho = 1.19$ g/cm³) which approximate the composition of the human body. The dimensions of these targets are ($x = 5, 10, 15, 20, 25$ and 40 mm, $y = 15$ cm, $z = 3$ cm). The informations (mass, nuclear charge, total kinetic energy) on charged particles behind the target are collected with a half crown radius of 20 cm in the y-z plan and in the x positive direction. The figure 2 is a visualisation of the experimental set-up used for the simulation. The modelled detectors have been used to quantify the detection efficiency which has been found to be better than 90% [13].

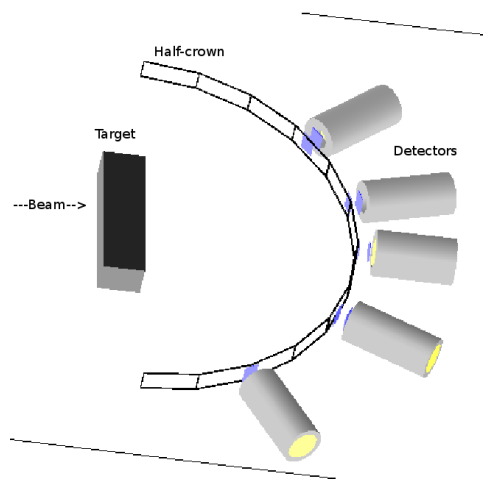


Figure 2: Experimental set-up visualisation of Braunn *et al.*[11] experiment with Geant4.

3. Nuclear models

Simulations have been done with three different nuclear models available with Geant4 while all other processes have been fixed. Table 2 summarises the models used for different processes in the Geant4 simulations.

All three nuclear models are based on a similar principle consisting on coupling a dynamical model to a statistical model. The first one treats the collision between the projectile and the target nucleus until the formation of excited compound nuclei while the second one deals with the de-excitation of these nuclei.

The first nuclear model used is the binary cascade of Geant4 developed by Folger *et al.*[14] (BIC). The model links an intra-nuclear cascade model with the de-excitation handler provided by Geant4. This handler, depending on the mass, the nuclear charge and the excitation energy of the excited nuclei provided by the cascade, chooses between three different statistical de-excitation models (a fermi break-up model, an evaporation model or a multifragmentation model) to bring back the nuclei to their fundamental state.

The second model is a Quantum Molecular Dynamic model (QMD) developed by Niita *et al.*[15], and interfaced to Geant4 by T. Koi. The dynamical part is also linked to the Geant4 de-excitation handler.

Finally, the third model tested is a preliminary version of the Intra-Nuclear Cascade of Liège (INCL) extended to nucleus-nucleus collisions. This extension is based on INCL++ v5.0[16] developed by P. Kaitaniemi and D. Mancusi. A more detailed description of the model will be done in the next section. INCL is also linked to the Geant4 de-excitation handler.

	electromagnetic	hadronic		
		elastic	inelastic	
			nucleon	ions
INCL	emstandard_opt3	HadronElasticPhysics	HadronPhysics QGSP_INCLXX	G4INCLXXInterface
BIC	”	”	”QGSP_BIC”	
QMD	”	”	HadronPhysics QGSP_BIC_HP	QMDReaction

Table 2: Models used in the Geant4 simulations.

4. Extension of INCL to Nucleus-Nucleus collisions

In this section, the general scheme (see figure 3) of INCL extended to Nucleus-Nucleus collisions is depicted. Realistic r- and p-densities are used to describe the projectile. The modification of the impact parameter due to Coulomb distortion is taken into account. The Fermi motion of the projectile is frozen and the nucleons propagate with the collective projectile velocity. However, the Fermi momentum of the nucleons is used in the computation of the elementary cross sections and in the generation of the NN scattering events. Nucleons resume normal motion as soon as they undergo a collision. At low energy, a process of complete fusion is used.

The cascade takes place in the target volume until a stopping time and the target-like pre-fragment is given by the normal INCL++ procedure. The projectile-like pre-fragment is built from projectile spectators and from non-cascading projectile participants. Its excitation energy is assigned by a semi-empirical particle-hole model, rather than by the cascade dynamics. Thus, its description is essentially semi-empirical. In contrast, the target-like pre-fragment is included in the calculation volume, which also encompasses the participant zone. The final state of the target-like pre-fragment is determined by the full collision dynamics of the cascade. Its physical description is therefore much more reliable.

Thus, the nucleus-nucleus collision is not treated symmetrically. This means that the current model cannot accurately and simultaneously describes the projectile-like and the target-like pre-fragments. Nevertheless, a method to circumvent this problem has been implemented: if the user wishes an accurate description of the target-like pre-fragment, then INCL++ is used normally (*accurate-target mode*); if the user wishes an accurate description of the projectile, the

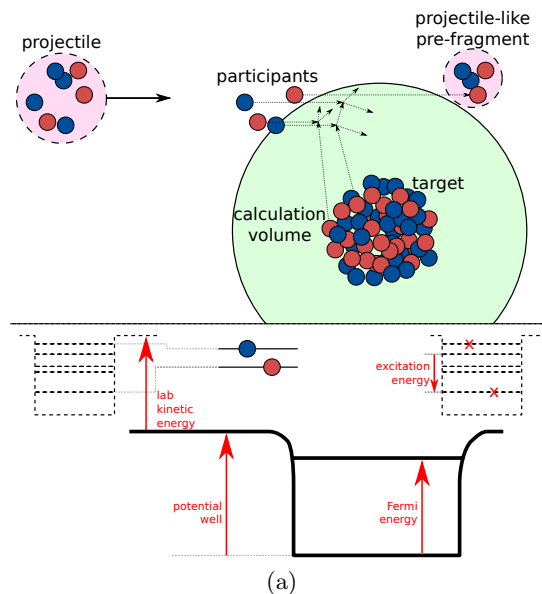


Figure 3: Scheme of a Nucleus-Nucleus collision in INCL++ v5.1.

collision event is generated in inverse kinematics (i.e. as target impinging on projectile) and then boosted back to the laboratory frame (*accurate-projectile mode*).

A comparison between these two modes has been done with experimental data from Braunn *et al.*. In this experiment, nuclear charge distributions from the fragmentation of a ^{12}C beam at 95 MeV/u as projectile have been measured with different thick PMMA targets. Figure 4, here, represents these nuclear charge distributions at five different angles after a 5 mm PMMA target. It is shown that the *accurate-projectile mode* provides globally much better results than the *accurate-target mode*, when compared with the experimental data. However, in figures 4a and 4b, results from the *accurate-projectile mode* are still underestimating the heaviest nuclear charges, albeit they definitely mark an improvement over the calculations in *accurate-target mode*. In the following, only the *accurate-projectile mode* of INCL++ will be used.

The new nucleus-nucleus capable version of INCL++ is labelled as v5.1 and has been distributed with the latest Geant4 beta release (v9.6).

5. Comparisons

In this section, comparisons between Braunn *et al.*[11] experimental data and calculation results from the Geant4 simulation detailed in the previous section are presented.

5.1. Angular distributions

Figure 5 shows the angular distributions for each nuclear charge from hydrogen to carbon from the interaction of a ^{12}C beam at 95 MeV/u with thick PMMA targets from 5 to 40 mm. The angular distributions obtained with three different models, INCL, BIC and QMD, are compared to the experimental data.

For the hydrogen production the three models are in good agreement with the experimental data. Concerning the helium production, the three models reproduce very well the data for the thinnest target (5 and 10 mm). At larger thickness, QMD continue to reproduce the entire distribution accurately. INCL tends to overestimate the production rate at low angle ($< 7^\circ$) but is quite good at larger angle (see figures 5e 5f). The opposite is observed for BIC: the model is in good agreement with the data under 7° but overestimates them largely at larger angle.

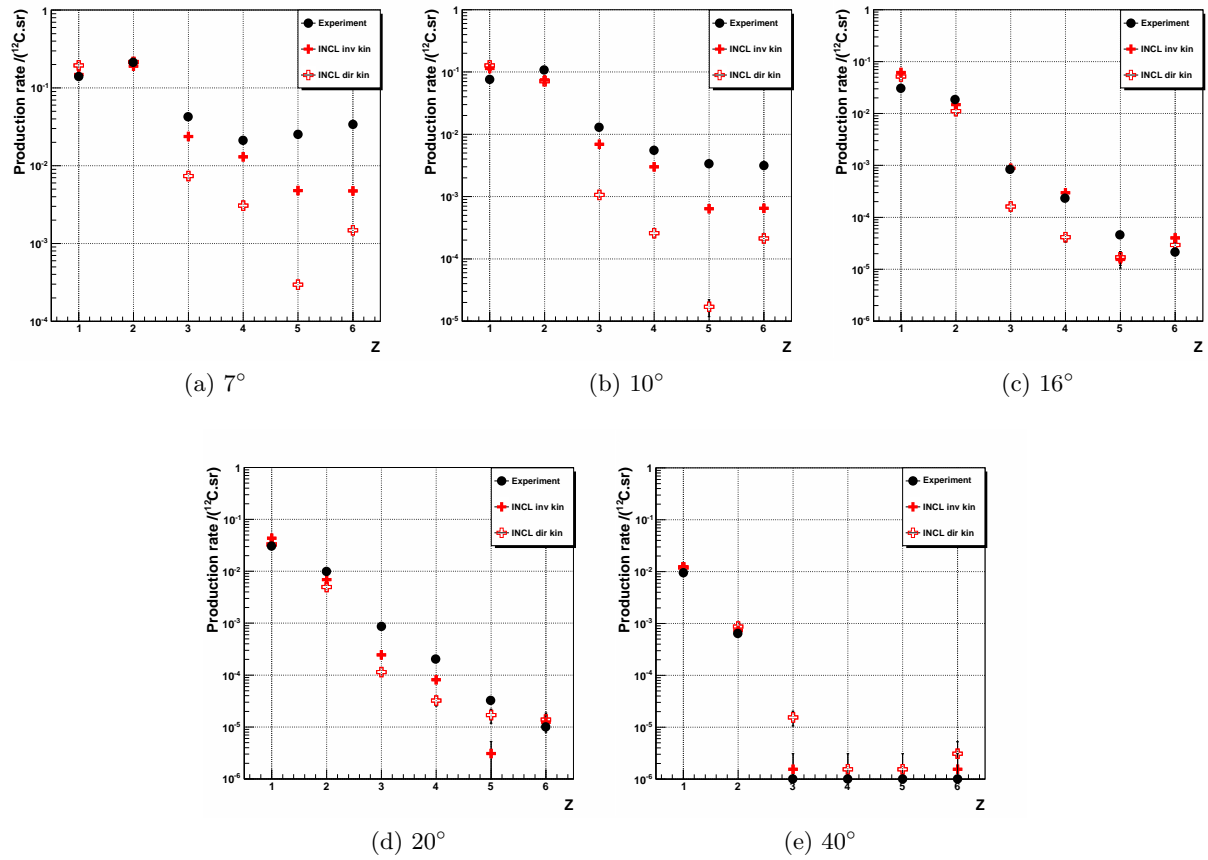


Figure 4: Nuclear charge distributions at different angles from a ^{12}C beam at 95 MeV/u interacting with a 5 mm PMMA target. The results from INCL in inverse kinematics (red cross) and in direct kinematics (open red cross) are compared to the experimental data (in black dot) from Braunn *et al.*[11].

For the fragments from $Z=3$ to 5, discrepancies between the models are more pronounced for all the targets. BIC tends to overestimate the experimental data at large angle, even a second contribution appears over 30° for the first two targets (figures 5a and 5b) which is not seen experimentally. However, at larger thickness (over 15 mm), BIC is much more accurate and the second contribution has disappeared. For the three thinnest targets, INCL tends to be the most accurate model, but for the three largest targets, the distributions are too forward peaked. The reproduction of the trend of the distributions for each thickness is only achieved by QMD.

Concerning the carbon production, one can notice the very good agreement found between the models and the data at 20 mm. Below, the models have difficulties to reproduce the shape of the distributions. Beyond, carbon ions are completely stopped inside the targets and, therefore, are not detected experimentally as well as in the simulations.

It appears that the data are rather well depicted by the models at a qualitative level. The less predictive one is BIC which fails to reproduce helium production at large angle and heavy fragments production at small thickness. INCL fails, too, to reproduce the heavy fragments, but gives encouraging results for a first version of the code attempting to take into account nucleus-nucleus reaction. The QMD model seems to be the most accurate one.

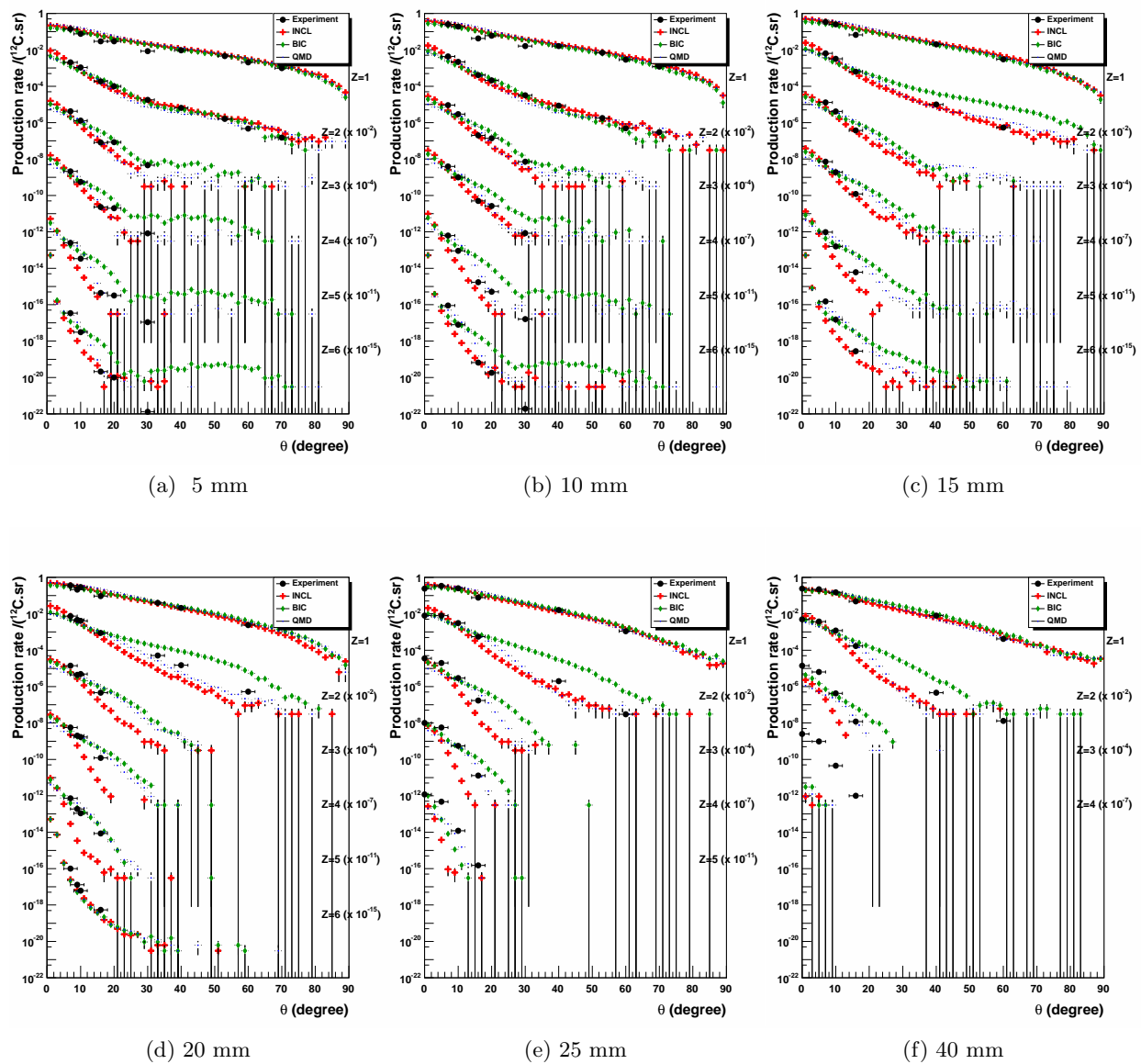


Figure 5: Angular distributions for $Z=1$ to $Z=6$ and for thick PMMA targets from 5 to 40 mm. The results from the three different models: INCL (in red cross), BIC (in green rhombus) and QMD (in blue square), are compared to the experimental data (in black dot) from Braunn *et al.*[11].

5.2. Nuclear charge distributions

In this section, focus is put on the nuclear charge distributions to see in more details the discrepancies between the models and the experimental data at low angle. The figure 6 shows the evolution of the nuclear charges for the 5 and 25 mm targets at different angles.

As mentioned in the previous section, the production of hydrogen and helium is rather well reproduced by the three models. For the other nuclear charges, discrepancies begin to appear for all the models. INCL is constantly slightly (largely) underestimating the production rate for small (big) targets, respectively. BIC has clearly problems with the angular distributions of the

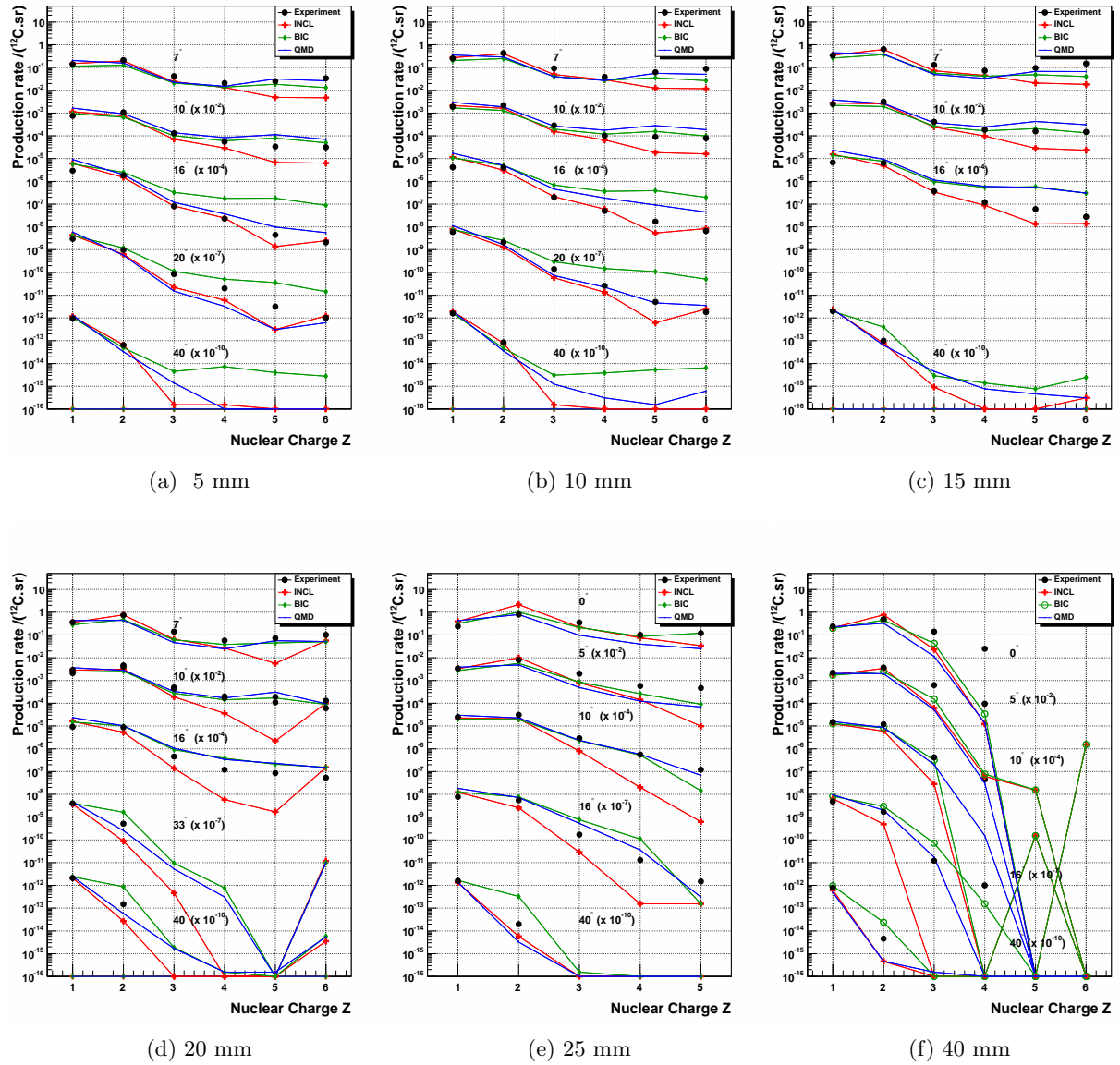


Figure 6: Nuclear charge distributions from 5 to 40 mm at different angles. The results from the three different models ; INCL (in red cross), BIC (in green rhombus) and QMD (in blue square) are compared to the experimental data (in black dot) from Braunn *et al.*[11]. The lines are here to guide the eyes.

heavy elements. At larger thickness, this effect is less visible. QMD, at low angle and at each different thickness, is the most accurate model.

5.3. Discussion

Concerning the comparisons, it has been shown that, qualitatively, the models are more (QMD) or less (BIC and INCL) in agreement with the data. It is worth noting that INCL, for a preliminary version, provides competitive results compared with the two other models. At a quantitative level, discrepancies between the data and the simulation results are often over a

factor of two even for the most reliable model, QMD. The main reason of this lack of accuracy comes from the fact that these three models are adaptation or extension of models which were not developed, at first, to treat nucleus-nucleus collision for small system and at intermediate energy (few MeV to hundreds of MeV). Improvements of these models are clearly needed if one wants to use them for hadrontherapy applications.

Concerning the experimental data, it would have been interesting to have more measurements at low angle (0°) especially for the smallest targets and in the region between 10° and 30° where the models begin to diverge.

6. Conclusion

The nuclear fragmentation process is an important effect, which can't be neglected for hadrontherapy application. An experiment have been done in 2008 at GANIL to investigate this process and, here, comparisons between these experimental data and results from three different models have been presented. The best model, QMD, only achieves an overall qualitative good agreement while the binary cascade of Geant4 has a tendency to overestimate the dispersion of the heaviest fragments and INCL has a tendency to underestimate them. In conclusion, these nuclear models used inside the Monte Carlo code Geant4 don't manage to reproduce with accuracy the experimental measurements. They are not yet predictive enough for hadrontherapy application.

To reach the accuracy required, these nuclear models have to be improved. And to do so, more comparisons may be made on other existing experimental data. More fundamental data are also needed like double differential cross section for the production of particles in the 100-400 MeV/u energy range for C-C, C-O, C-H, etc. reactions. One experiment[17] at GSI and another[18] at GANIL have been done last year to obtain this kind of data. They will soon be available and will be helpful to improve nuclear fragmentation models used in hadrontherapy applications.

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