

Investigation of the possibility to use ion beams for ADS through simulation in GEANT4

M. Paraipan

Joint Institute for Nuclear Research, Joliot Curie str.6, Dubna Moscow region, 141980 Russia
Institute of SpaceScience, Atomistilor str. 409. Bucharest-Magurele, Romania
E-mail: mihaela_paraipan@yahoo.com

A. A. Baldin

Joint institute for nuclear research, Joliot Curie str.6, Dubna Moscow region, 141980 Russia
E-mail: an.baldin@mail.ru

M. G. Kadykov

Joint institute for nuclear research, Joliot Curie str.6, Dubna Moscow region, 141980 Russia
E-mail: kadykov@jinr.ru

S. I. Tyutyunikov

Joint institute for nuclear research, Joliot Curie str.6, Dubna Moscow region, 141980 Russia
E-mail: Sergey.Tiutiunnikov@lhcp.jinr.ru

Proton and ion beams with the initial energy between 0.2 AGeV and 10 AGeV were analyzed with respect to the neutron production in different targets, the number and spatial distribution of fission acts and the energy deposited in uranium targets. In this energy range two models for the hadronic inelastic interaction are suitable: bertini cascade and binary cascade. In thin and medium thickness targets both models produce results in good agreement with the experimental data. In very thick targets the use of binary cascade gives neutron production about two times lower than the bertini cascade and the experimental data. For this reason the last model was chosen for the modeling of the hadronic inelastic interaction. In large uranium target the total number of fission acts (the energy deposited) per incident particle, reported to the energy spent to accelerate the particle and to the total number of fission acts (the energy deposited) per incident proton with the same energy per nucleon increases with the mass number of ion. Such dependence for the number of fission acts shows a quick rise for ions until Fe, followed by a slower increase. The simulations performed show that from the point of view of the energetic balance (neglecting the problem of a suitable beam intensity) it seems more useful to accelerate at the same energy per nucleon, ions with mass number between Ca and Fe, than protons.

XXI International Baldin Seminar on High Energy Physics Problems
September 10-15, 2012
JINR, Dubna, Russia

1. Introduction

An accelerator driven system (ADS) needs a powerful spallation source, neutronically coupled with the subcritical core. The target must produce the maximum number of neutrons per incident particle, and leak them into the core with minimal losses or modification in energy spectrum. In order to maximize the neutron production the target must be a heavy metal (tungsten, lead, uranium). The use as a target the material of the active core (natural uranium) allows to minimize the leakage of neutrons. In the present work the possibility to use proton and ion beam with energies between 1 and 10 AGeV for energy production in a uranium target is investigated through simulation with the code GEANT4.

2. The analyze of the models

The electromagnetic interaction was simulated with the standard electromagnetic package. For the simulation of the inelastic interaction of ions, in the energy range from 1 AGeV to 10 AGeV the binary cascade model can be used in GEANT4. The INCL model (cascade Liege) is implemented only for hadrons and light ions, and for energies below 3 AGeV. Another available model, based on quantum molecular dynamics is improper for the use in such simulations, due to its very low speed of computation. The inelastic interaction of hadrons, in the energy range of interest, can be described with two microscopic models, binary cascade and bertini cascade

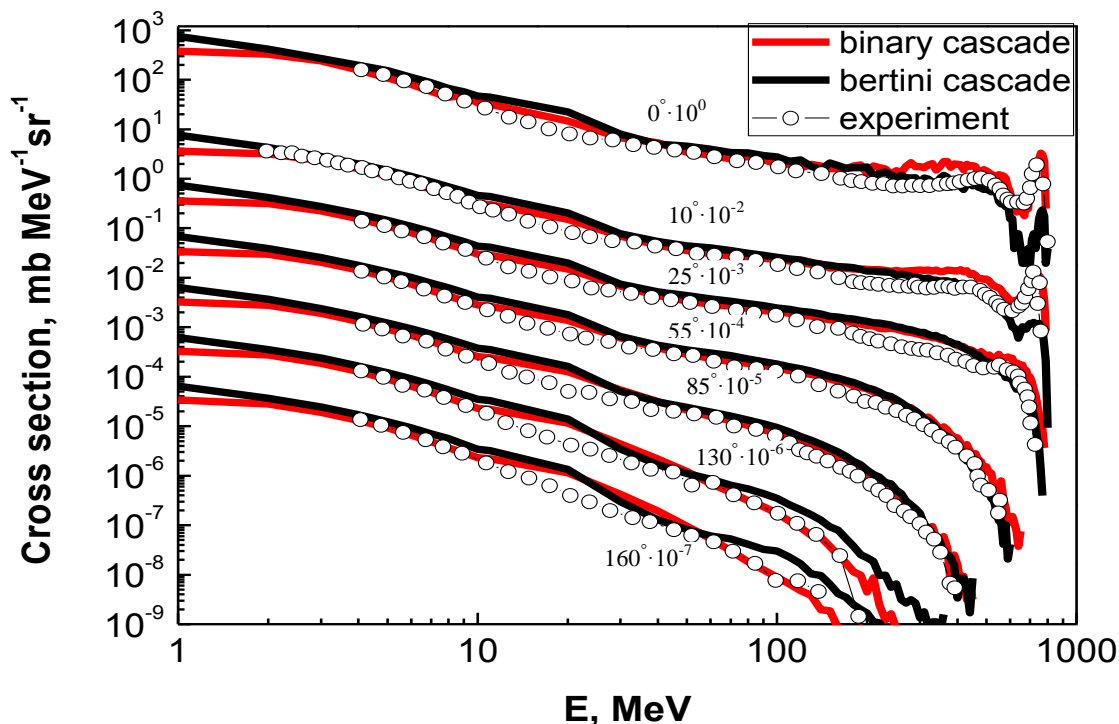


Fig. 1 Double differential cross section for neutron production, for proton beam 0.8 GeV, on lead target. Experimental data are taken from Ref [1].

. A series of simulations with proton beams, interacting in targets of different thickness, was performed, and the neutron yield was compared with the experimental data, in order to decide between these models. Targets from lead were used, a material with atomic weight close to the uranium, and for which there are published experimental data about the neutron production from thin and thick targets.

In figure 1 the simulated and experimental double differential cross section for neutron production, obtained with a 0.8 GeV proton beam, incident on thin lead target are presented. The experimental data are from Ref. [1]. The overall results are satisfactory for both models, still the binary cascade model gives a better description of the experimental results, as can be seen also from table 1, where the number of neutrons with energy higher than 5 MeV, produced on incident proton, is presented. The total is made only for the angles shown in the table. The bertini cascade underestimates the production of neutrons with energy close to the beam energy at small angles, but overestimates the neutrons with low energy, for all angles. In this way, the overall prediction for neutrons made with bertini cascade, is 40% higher than the experimental one.

Table 1 Neutrons with energy > 5 MeV produced with proton beam 0.8 GeV, in thin lead target

Angle	BC	Bert	Exp
0	$1.1 \cdot 10^{-4}$	$1 \cdot 10^{-4}$	$8.7 \cdot 10^{-5}$
10	$2.1 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	$1.6 \cdot 10^{-3}$
25	$3.6 \cdot 10^{-3}$	$4.3 \cdot 10^{-3}$	$3 \cdot 10^{-3}$
55	$4.9 \cdot 10^{-3}$	$6.2 \cdot 10^{-3}$	$4.5 \cdot 10^{-3}$
85	$4.5 \cdot 10^{-3}$	$5.8 \cdot 10^{-3}$	$3.9 \cdot 10^{-3}$
130	$2.8 \cdot 10^{-3}$	$3.6 \cdot 10^{-3}$	$2.5 \cdot 10^{-3}$
160	$1.2 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$
total	$1.9 \cdot 10^{-2}$	$2.36 \cdot 10^{-2}$	$1.68 \cdot 10^{-2}$

For a target with intermediate thickness the situation is similar. The target used in the simulation was a cylinder with diameter 20 cm, 20 cm length, at which arrived a beam of protons with energy 2.55 GeV. The neutron yield registered at three angles (30° , 90° , 150°) is shown in figure 2, in comparison with the experimental data, taken from Ref. [2]. In table 2 the neutron yield on incident proton is given for the analyzed angles. Binary cascade gives better predictions than the bertini model, in this case, also.

Table 2 Neutron yield for proton beam, 2.55 GeV, in lead target

Angle	BC	Bert	Exp
30	$6.57 \cdot 10^{-2}$	$5.36 \cdot 10^{-2}$	$5.76 \cdot 10^{-2}$
90	$9.99 \cdot 10^{-2}$	$6.23 \cdot 10^{-2}$	$9.37 \cdot 10^{-2}$
150	$5.04 \cdot 10^{-2}$	$3.64 \cdot 10^{-2}$	$4.23 \cdot 10^{-2}$
Total	0.216	0.152	0.193

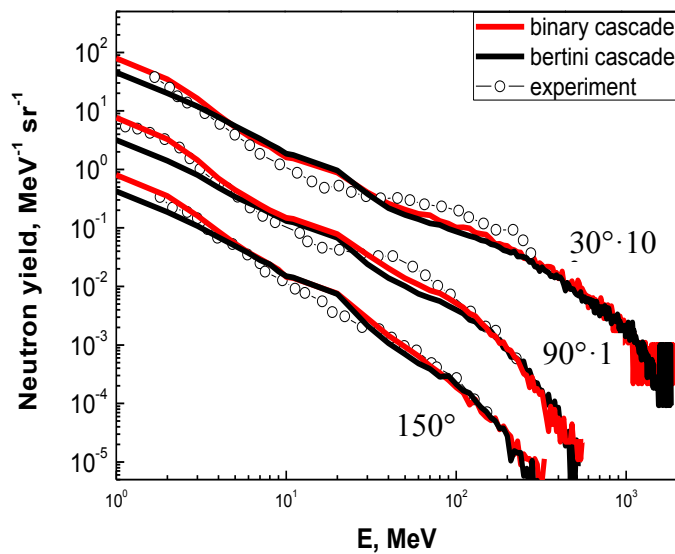


Fig. 2 Neutron yield for proton beam 2.55 GeV, in lead target. Experimental data from Ref. [2].

When we analyze the neutron production in very thick target the results are different. In table 3 are presented the results of the simulation, in comparison with the experimental data (taken from Ref. [2]) for proton beam with energies 1 GeV, 2.55 GeV and 3.65 GeV, interacting in a cylinder of lead with 20 cm diameter and 60 cm length. The neutrons were registered in 4π geometry. In the table the total yield of neutrons and the yield of neutrons with energy higher than 20 MeV are shown. In very thick targets binary cascade model underestimates both the total neutron yield and the high energy component, and the underestimation is accentuated with the increase in energy, reaching 45% for proton energy 3.65 GeV. Bertini cascade model maintains its behavior with the underestimation of the high energy part of neutron spectrum (within about 30%), but with predictions for the total neutron yield close to the experimental values. For this reason it is preferable to use bertini model for the simulation of hadron inelastic interaction.

Table 3 Neutron yield from proton beam in lead target (ϕ 20cm, length 60 cm)

E_p , MeV	N_{total}			$E_n > 20$ MeV		
	exp	bc	bert	exp	bc	bert
1	24.1±2.9	21.2	26.7	2.1±0.4	1.3	1.4
2.55	63.5±7.6	44.6	64.5	5.8±1.0	3.38	4.2
3.65	80.6±9.7	57.6	87.1	8.5±1.5	4.5	6.1

The capability to simulate the neutron production obtained with ion beams in thick targets was also checked. Such experimental data for ion beams in the energy range 1 AGeV- 10 AGeV are not available. Systematic measurements were performed with ion beams with lower energy, from 100 AMeV until 1 AGeV. In consequence the binary cascade model was checked against the experiment for ion beams with the same energy per nucleon (400 AGeV) interacting

in thick lead target. The results for the double differential neutron yield, obtained with beams of ^{40}Ar , ^{56}Fe and ^{129}Xe , for angles between 0° and 90° are shown in figure 3.

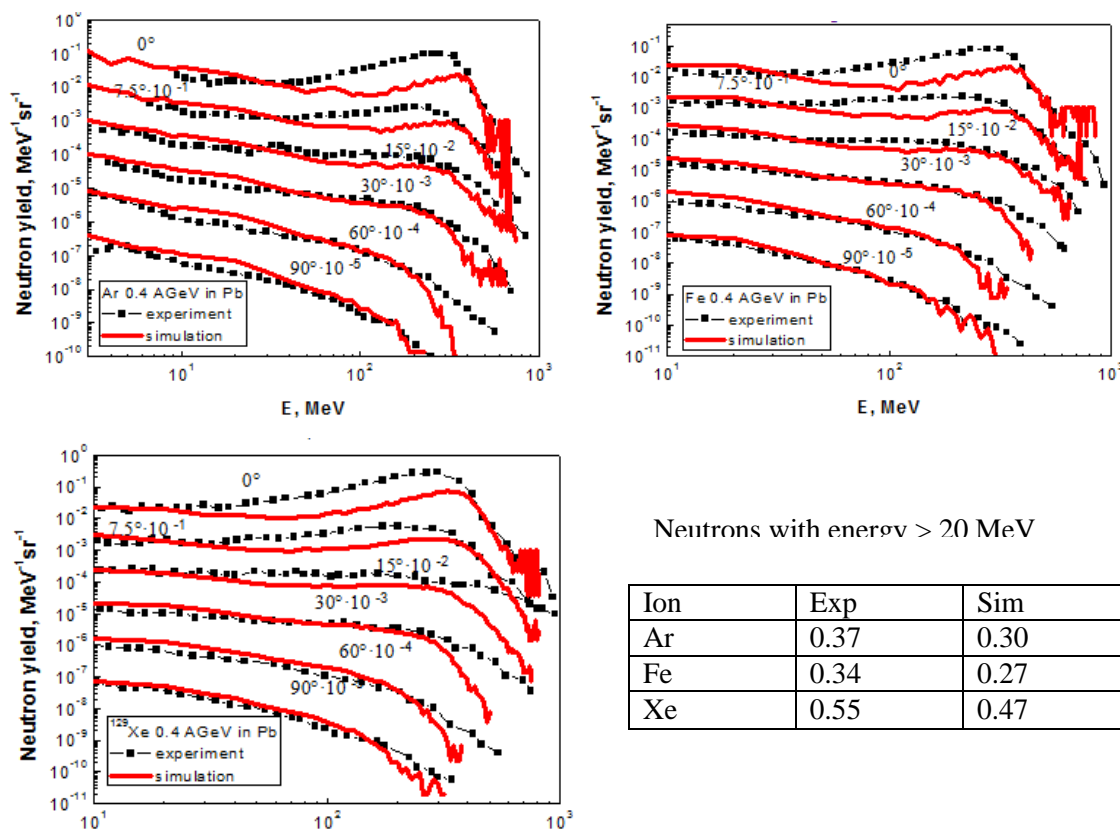


Fig. 3 Neutron yield for Ar, Fe and Xe beams with energy 400 AMeV, in thick lead target. Experimental data are taken from Ref. [3] and [4].

In the table is presented the neutron yield on incident ion for neutrons with energy higher than 20 MeV (the values presented are only for the angles shown in the figure). The model behaves in a similar way for all the ions. It systematically underestimates the yield for neutrons with energy above 100 MeV, and gives total results with 15 -20 % lower than the experimental values.

For an accurate description of the neutron interaction in target it is preferably to use the high precision models for neutron energy lower than 20 MeV. These models are based on the detailed implementation of the cross sections in ENDL format. In this case it was necessary to change the high precision model for neutron fission. In the original implementation from GEANT4 this model does not produce fission fragments. The model was rewritten, the mass distribution of fragments before the prompt neutron emission and the kinetic energy of fragments were adapted from the model G4CompetitiveFission. The excited fragments are de-excited through neutron and gamma emission. In order to reproduce correctly the dependence of the mean number of prompt neutrons on the fragment mass, it is necessary to assume

different nuclear temperatures for the fission fragments, as in [5]. Some results for the fission of ^{238}U with 14.5 MeV neutrons, obtained with this model, are shown in figure 4. The model reproduces well the tooth structure for the dependence of the mean prompt neutron number on the fragment mass. The dependence of the total kinetic energy of the fragments on the fragment mass is well reproduced, too, but the simulated mass distribution of the fragments is shifted towards higher mass numbers, comparing with the experimental distribution.

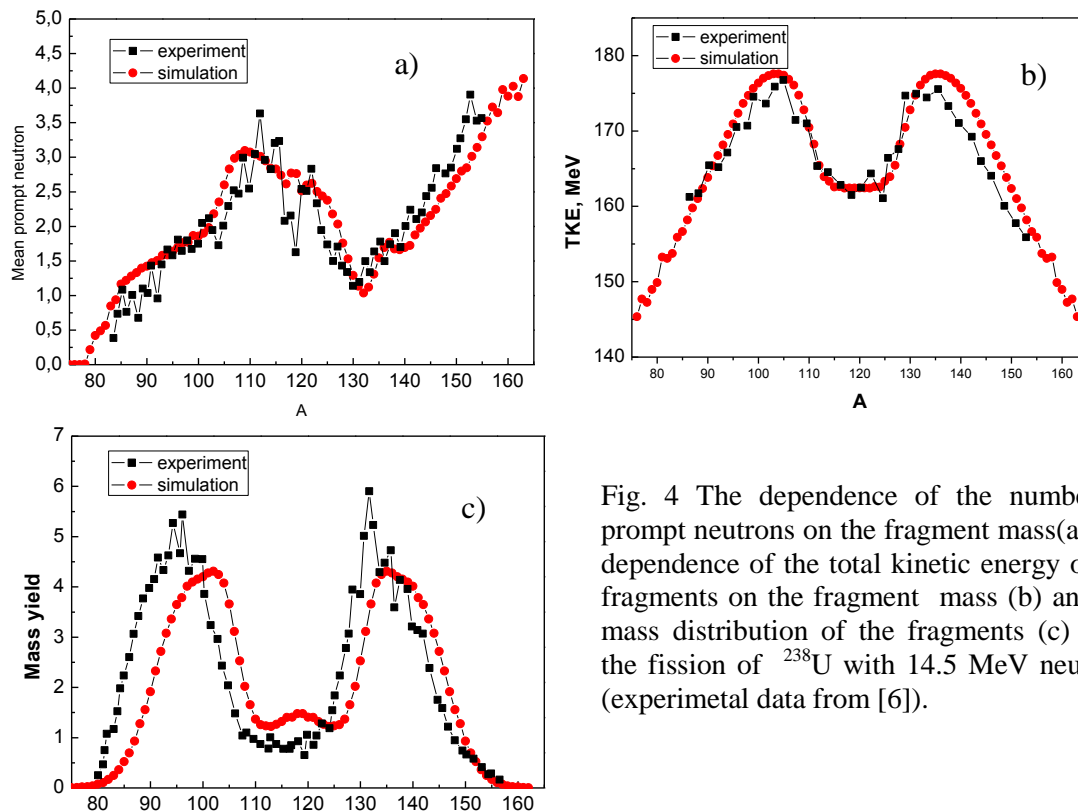


Fig. 4 The dependence of the number of prompt neutrons on the fragment mass(a), the dependence of the total kinetic energy of the fragments on the fragment mass (b) and the mass distribution of the fragments (c) from the fission of ^{238}U with 14.5 MeV neutrons (experimental data from [6]).

3. Results in uranium target

The purpose of these simulations was to analyze the efficiency of rising the beam energy and of using ions with higher mass.

In the first set of simulations a cylindrical target from natural uranium, with radius 10 cm and length 52 cm was irradiated with proton and ion beams, with energies between 1 AGeV and 10 AGeV, and the neutron yield was registered. The neutron yield reported to the beam kinetic energy on nucleon, as a function of the beam kinetic energy on nucleon is shown in figure 5. For proton (fig. 5a) and deuteron (fig 5b) beams the results obtained with bertini and binary cascade are given, in the energy range from 0.2 AGeV to 10 AGeV. The predictions realized with the INCL cascade, for beam energies between 0.2 AGeV and 4 AGeV are presented, too. All the curves have the same form, with a maximum at beam energy around 1 AGeV. Bertini model predicts neutron yields 1.7-2 times higher. Binary and INCL cascade models give results close to each other, but the falling down with the increase in energy is

stepper for the binary cascade model. These results are similar with the results obtained with MCNP code (Ref.[7]) , but in contradiction with the experimental measurements from Ref. [2]. The simulation shows that the rise in energy is inefficient for beams of proton or deuteron.

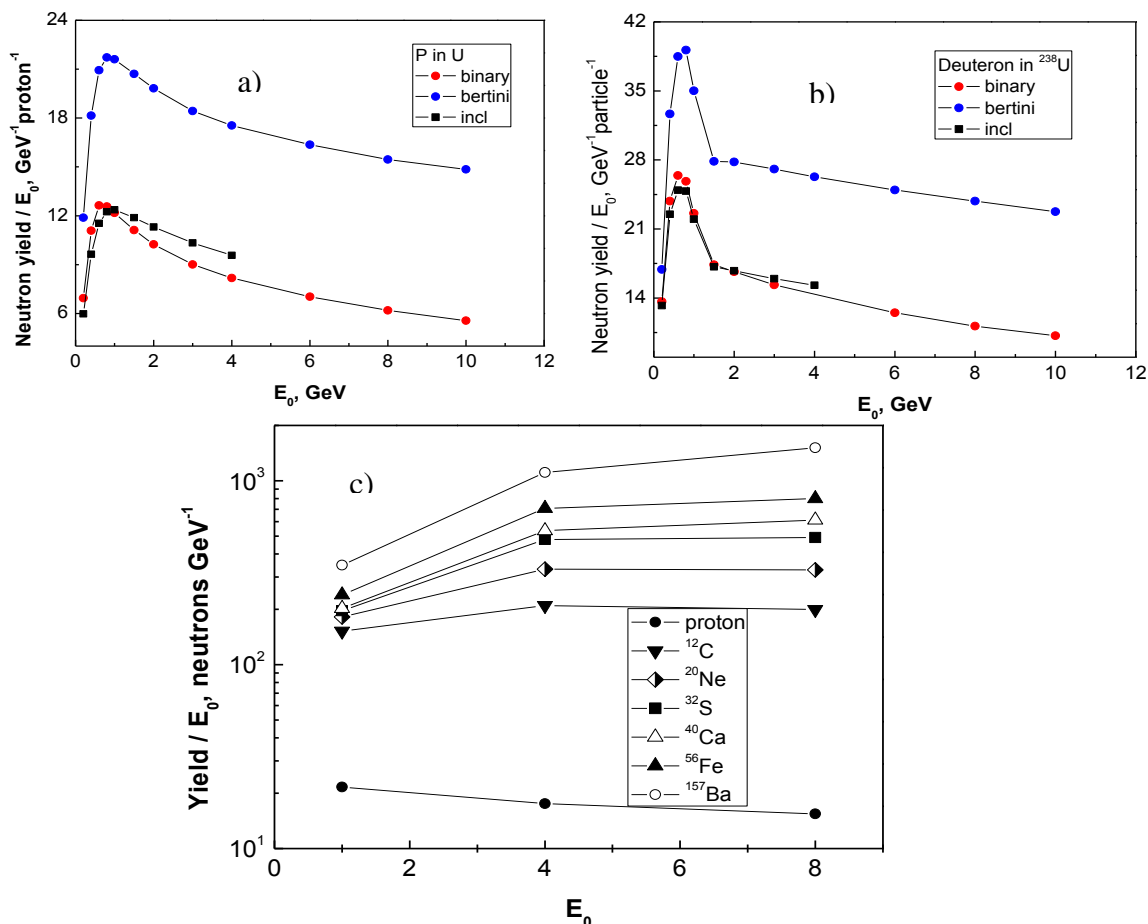


Fig. 5 The neutron yield reported to the initial energy per nucleon for proton beams (a), deuteron beams (b), and ion beams (c).

The possibility to use heavy ions for ADS was analyzed in some papers, through simulation with other Monte Carlo code (MCNPX, SHIELD), as in Ref. [7,8]. However, we consider that the energy cost was not correctly estimated. When we estimate the energy cost it is necessary to take into account that we accelerate charged particles. The energy spent to accelerate an ion with mass number A and charge Z depends on the ratio Z/A .

This remark, corroborated with another made in Ref. [9], where was shown that, for incident ion beams with the same energy per nucleon, the high energy part of neutron yield rise as a function of ion mass with a slope greater than unity, determined us to perform simulations with heavy ions. Ions with masses from ^4He to ^{157}Ba , at three energies (1, 4 and 8 AGeV) were simulated, and the results presented in fig. 6c. In these simulations bertini model was used for modeling of the hadronic inelastic interaction. It is seen from this figure that the rise in energy

becomes efficient for carbon beam and the efficiency increases with the ion mass. The slope of the curves is higher for energies from 1 to 4 AGeV.

During the second set of simulations, the energy deposited and the number of fission act in a target with radius 20 cm and length 200 cm, were registered for ion beams from proton to barium, and three initial energies (1, 4 and 8 AGeV). The results are synthesized in table 4 and figure 6. Figure 6 presents the ratio between the total number of fission acts (fig. 6a), or the energy deposited (fig. 6b) and the energy consumed for the acceleration of the charged particles (proportional with A/Z) and reported to the number of fissions obtained with protons with the same energy on nucleon, plotted as a function of nuclear charge. As can be seen from the figure, this ratio rises with the energy and the mass of the projectile. At the same energy per nucleon the curves show a quick rise for ions until Ca, followed by a slower rise for masses until Ba.

Table 4 Number of fission acts and the energy deposited in the target for different ion beams and energies

Particle	1 AGeV		4 AGeV		8 AGeV	
	N_{fis}	Edep, MeV	N_{fis}	Edep, MeV	N_{fis}	Edep, MeV
Proton	11.75	$2.652 \cdot 10^3$	40.68	$9.701 \cdot 10^3$	75.56	$1.841 \cdot 10^4$
Deuteron	18.82	$4.475 \cdot 10^3$	59.37	$1.487 \cdot 10^4$	113.28	$2.966 \cdot 10^4$
alpha	28.74	$8.352 \cdot 10^3$	113.17	$3.305 \cdot 10^4$	231.34	$6.449 \cdot 10^4$
^{12}C	58.64	$2.263 \cdot 10^4$	326.93	$1.112 \cdot 10^5$	634.19	$2.457 \cdot 10^5$
^{32}S	74.72	$4.978 \cdot 10^4$	739.73	$2.829 \cdot 10^5$	1403.76	$6.537 \cdot 10^5$
^{40}Ca	77.73	$6.021 \cdot 10^4$	859.61	$3.451 \cdot 10^5$	1914.18	$8.052 \cdot 10^5$
^{56}Fe	91.58	$8.204 \cdot 10^4$	1071.16	$4.649 \cdot 10^5$	2592.46	$1.117 \cdot 10^6$
^{137}Ba	125.5	$1.878 \cdot 10^5$	1751.95	$1.031 \cdot 10^6$	4257.23	$2.505 \cdot 10^6$

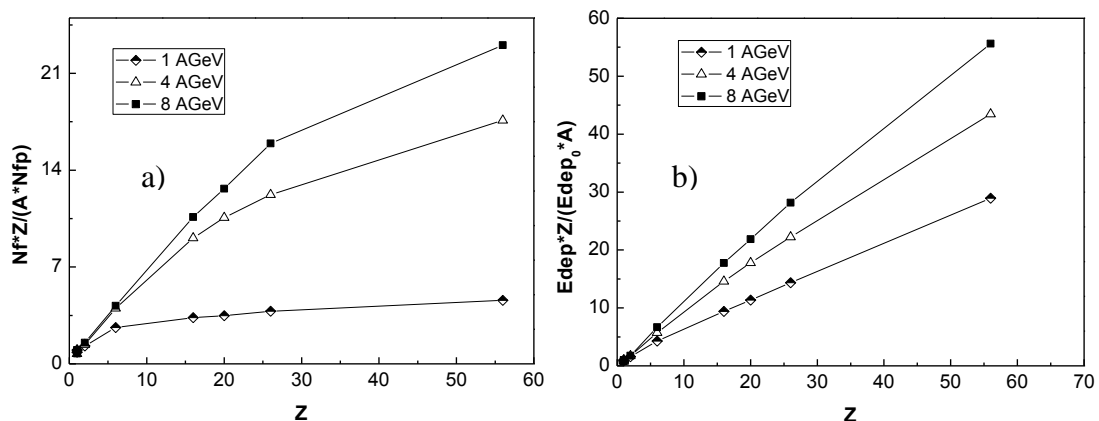


Fig. 6 The number of fission acts (a) and the energy deposited in the target (b), reported to the energy consumed for the acceleration of the charged particles (proportional with A/Z) and to the number of fissions obtained with protons with the same energy on nucleon

The simulation suggests that is more efficient, from energetic point of view, to accelerate ions than proton or deuteron. The aspect of curves shows an optimum region, for ions with masses between Ca and Fe. Present development of ion accelerator cannot ensure high intensity beams for ions in the optimal region. However, it can be seen from figure 6 that, even in the case of a lighter ion as ^{12}C the efficiency is higher than for proton, 2.5 times higher when the ions are accelerated to 1 AGeV, and 4 times when the kinetic energy is 4 AGeV. The use of carbon beams is possible because there are accelerators capable to give high intensity beams.

4. Conclusions

The analyze of available models in GEANT4 shows that, with a proper choice of them, it is possible to simulate the interaction of hadrons and ions in heavy targets, with an acceptable accuracy, similar with other Monte Carlo codes. In thin and medium thick targets binary cascade produces better results with respect to the neutron production in the interaction of hadrons with targets, in comparison with bertini model. In very thick targets binary cascade underestimate the yield of secondary neutrons with about 40 %. For this reason we conclude that in our simulations the use of bertini model is preferable. The modified model for the fission process induced by neutrons with low energy is in good agreement with the experiment.

The first set of simulations performed in uranium target shows that the ratio between the neutron yield and the initial energy per nucleon increases quickly for energies from 0.2 AGeV to 1 AGeV, followed by a slower decrease with the rise of the energy for protons and deuteron. For the ions with higher mass the curves have a different behavior, with a continuous rise, without a maximum. The rise is faster for energies between 1 and 4 AGeV, and slower for energies from 4 to 8 AGeV. From these results we can conclude that it is useful to increase the energy of the beam for ions with mass higher than deuteron.

The second set of simulation in uranium target demonstrates that the ratio between the total number of fission acts (respective the energy deposited in the target) and the energy spent to accelerate the particle compared with the ratio for protons with the same energy per nucleon rise with the ion mass, faster for ions until the region of Ca and Fe, and continues to rise slowly until Ba. This behavior suggests a possible optimum for the use of ions in ADS in the region around Fe. The use of ions with such high mass is difficult, because present accelerators cannot produce beams with high enough intensity. But for carbon beam situation is different. The simulations shown an efficiency higher than for proton (2.5 times higher for the energy 1 AGeV, and 4 times for the energy 4 AGeV), and there are accelerators capable to realize high intensity beams.

The results obtained in this work give arguments to plan experiments with carbon beams.

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