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Benchmark Study on the Computational Model in the Accelerator-Based Transmutation Simulation Code

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Abstract

Recently it is often said that there are some disagreemennts in the computational results between spallation reaction simulation codes such as NMTC,HETC and their modified versions. We examined the difference of product yields in the high energy fission reaction calculation between NMTC/JAERI and HETC/KFA2, which was pointed out by PSI at the first OMEGA Meeting at 1990. Our calculation results showed that the difference is mainly due to the estimation of the width of post-fission yield curve. We also discussed the influence of the difference on the number of neutrons generated in the high energy reaction procedure, which is the most important factor in the design study of accelerator-based transmutation system.

I. Introduction

According to the OMEGA project JAERI are performing the baisic research and development for " Proton Accelerator-based Transmutation in the following items,

*(1) development of design code system including the spallation cascade code,
(2) proton-induced spallation integral experiment,
(3) conceptual design study of minor actinide transmutation system and
(4) development of an intense proton accelerator.

It is important to use computer codes with high precision for analyzing the physical processes in an intense neutron source induced by the high energy proton beam and designing the accelerator-based transmutation system. In this report our study work is restricted on the development of the simulation codes, especially, the spallation cascade code. It has been recently said that there are some disagreemennts in the computational results obtained using the spallation cascade codes such as NMTC,HETC and their modified versions (ORNL version, BNL Version, NMTC/JAERI, HETC/KFA2, HETLAT etc.). In particular there seem some problems between High Energy Fission (HEF) calculation models which were not involved in the original NMTC and HETC. The discrepancy between the predictions by different HEF models was pointed out by the PSI researcher at the first OMEGA Meeting at 1990. We started the calculation study to find out the main cause for the discrepancies on fission products predicted from the spallation and cascad ecodes NMTC/JAERI and HETC/KFA2 by changing the parameter values such as fission probability and σ of Gaussian distribution curve determining the yield of fission products.

In this proceeding paper at first we would like to explain the JAERI code system developed for the conceptual design study of accelerator-based transmutation. Next brief descriptions for the calculational model of high energy fission model are given. The several mass yield curves of products are shown for the some cases set up to a thick and a thin ^{237}Np targets irradiated by 1 GeV and 590 MeV protons. By comparing these calculation results discussions about the causes giving the discrepancies are carried out. At last we summarize the results obtained at t-he present research step and describe the calculation plan in the near future.

II. Simulation Code System

Figure 1 is the flow chart showing the mutual relations among the simulation code systems developed at JAERI. As Nuclear Reaction Simulation Codes, NMTC/JAERI-NMTA and NUCLEUS codes are prepared for the energy range above 15 MeV and MORSE-DD, SP-ACE and TWOTRAN II for the range below 15 MeV. ORIGEN-2 and SPCHAIN calculate the time evolution process of TRU transmutation products in the lower and upper energy ranges respectively. The High Energy Nuclear Reactions and Nucleon-Meson Transport Code NMTC/JAERI is the main code in this code system. The codes included in the right part of this figure can simulate the high energy nuclear reactions above 15 MeV and ones in the left part carry out the neutron transport calculation below 15 MeV.

(a) NMTC/JAERI 1)

The NMTC/JAERI code is used for the Monte Carlo simulations of nuclear spallation induced by incident particles(proton, neutron, pion) from an external source in a heterogeneous medium. The subsequent internuclear transport processes is also calculated in the energy' range of 15 MeV to 3 GeV. In the JAERI version, the fission process (JAERI HEF model) has been incorporated as a competing process with particle evaporation. The range of mass number A of nuclides in the target has been extended from[A=1;8< A< 239] to [A=1;6< A < 250 1. The major part of NMTC is almost the same as the old version of HETC. The detail descriptions about NMTC/JAERI had given by Nakahara at the former conference ICANS-IV. 2) This code's main purposes are to perform the design study of transuranium nuclides(TRU) transmutation target-core system driven by a proton accelerator and analyze the data measured in spallation experiments. Analyses of the beam window on the spallation target and accelerator strucutral materials irradiated by high energy particle beam will be carried out using this code also.

(b) NMTA/JAERI 3)

In the improved version of NMTA, which is named to the routines analyzing statistically the Monte Carlo events in the NMTC/JAERI computation, the new subroutine HEATDP have been installed. HEATDP was developed at JAERI to calculate the energy-deposition and its spatial distribution for each component such as ionization loss energy and recioling energy of fission and spallation products without 7 -day heating of excited residual nuclei in the high energy range.

(c) NUCLEUS 4), 5), 6)

The NUCLEUS code has been developed by modifying and combining the Monte Carlo codes NMTC/JAERI and a routine in NMTA/JAERI. This code includes the statistical routine PROCES (poducts, particle emission) but the part calculating the internuclear cascade is rejected. The Uno & Yamada's mass formula routine revised by the recent measured data, has newly been equipped as another option. The NUCLEUS simulates the nuclear spallation reaction between a single target nucleus and a projectile in order to make direct evaluations of physical and computational models efficiently. The results obtained with this code can also be compared directly with the data of thin foil spallation experiment, in which the internuclear multiple scattering have little effects.

(d) Other codes 7),8),9),10),11),12)

For the whole energy range less than 3 GeV, a simulation code system, ACCEL had been developed by connecting NMTC/JAERI with the neutron transport code TWOTRAN-II or MORSE-DD. This code system was often used for the actual design computation of the transmutation system which consists of an intense proton accelerator and a TRU alloy fuel led core at the subcritical state. The SPCHAIN code, which is being developed on the base of the depletion code DCHAIN2 for the decay and built-up of fission products in a nuclear reactor, can calculate the time evolution process of spallation products SP. The new nuclear data have been compiled in SPCHAIN data file for about 1100 nuclides needed for TRU 'spallation calculation .

III. Calculational Model of High Energy Fission 13),14),15),(6)

Since the theory and calculational formulation of High Energy Fission model were described in detail in references (1) and (13), the brief descriptions is given in the present report only for parameters, of which the effect on the HEF prediction are examined.

As well known, the fission probability Pf is given based on the statistical theory in the folowing equations,

$$Pf = 1/(1 + \Gamma n/\Gamma f), \tag{1}$$

$$rn/rf = 4A^{(2/3)} af(E - Qn)/K0af\{2af^{1/2}(E - Ef)^{1/2} - 1\} \times \exp\{2an^{(1/3)}(E - Qn)^{1/2} - 2an^{1/2}(E -- Ef)^{1/2}\}, \tag{2}$$

where

A = Mass of fissioning nucleus,
E = Excitation energy of fissioning nucleus,

Q_n = Neutron binding energy,
K_0 = $h^2/(8\pi^2 m r_0^2) \sim 13$ MeV,
E_f = Fission barrier height,
a_n = Energy level dendity parameter for neutron evaporation,
a_f = Energy level dendity Parameter for fission.

The Evaporation Probability of particle x, which makes the direct contribution to the HEF prediction through the particle evaporation from the fisson fragment, was formulated by Weisskopf as

$$P_x = (2S_x + 1)\, m_x\, \varepsilon\, \sigma_{cx}(\varepsilon)\, \omega(E), \qquad (3)$$

where

S_x = Particle x's spin
m_x = Particle x's mass
& = Particle X's energy
Q_x = Particle x's binding energy
σ_{Cx} = Cross section for the inverse reaction
E = Excitation energy of residual nucleus after x emission
= (Excitation energy of compound nucleus) $- \varepsilon - Q_x$
$\omega(E)$ = Energy level density of residual nucleus.

< Hurwitz& Bethe Expression>

$$\omega(E) = \omega_0 \exp(2(a(E-\delta))^{1/2}) \qquad (4)$$

<LeCouteur Expression >

$$a = A/B0\cdot(1 + Y\cdot\Delta^2/A^2) \qquad (5)$$

$A = A - 2Z$
$BO = 8,\ 14$ MeV $\quad Y \sim 1.5$

The masses of fission fragment after fission is randamly selected from the Gaussian distributions with the mean value A_m and the appropriate σ-value. In JAERI HEF model the mass number of a frament produced in the fission of target nucleus(massnumnber A_0) is determined for actinides from the three peak Gaussian distribution (two or one peak approximation in actual computations) with mean values of $A_{m1}=0.4A_0$, $A_{m3}=0.6A_0$),($A_{m2}=0.5A_0$) and for subactinides from the one peak Gaussian with $A_{m2}=0.5A_0$.

When Ex and Ef denote the excitation energy of fissioning nucleus and the fission barrier height respectively, the σ- value is given according the following Neuzil and Fairhall's equation,

$$\sigma_J = 0.849321(U + 7), \qquad (5)$$

where

$$U = Ex - Ef. \qquad (6)$$

It is assumed that every Gaussian curve has the same a-value.

On the other hand in RAL HEF model the mass number of a fragment produced in the fission of a target nucleus(mass numnber AO) is determined for $Z^2/A_0 > 35$ from the symmetric or asymmetric (two peaks) Gaussian distribution with the mean value $A_{m3}=140$, $\sigma_R = 6.5$ and the asymmetric probability $=F/(1+F)$, where $F=4870\exp(-0.36Ex)$, and for $Z^2/A_0 \leqq 35$ from the symmetric (one peak) Gaussian with $A_{m2}=0.5A_0$ and the σ-value calculated by the following equation,

$$\sigma_R = 3.97+0.425U - 2.12\times10^{-2}U^2. \qquad (7)$$

The flow chart for calculating the fission probability in HETC/KFA2 is shown in Fig. 2 and almost the same to one in NMTC/JAERI. Figures 3 and 4 are copies of the calculation examples representing the large difference in the yield curve obtained from the diferent calculation models of high energy fission, which was presented by the participant from PSI at the OECD/NEA Information Exchane Meeting held in Mito in 1990. The mass yield distribution of products in a thin ^{237}Np pellet for proton energies of 1 GeV and 590 MeV are represented in Fig.3 and one in a thick ^{237}Np target for 1 GeV proton energy in Fig.4. Although comparing with JAERI results in the original figures we replaced them by the new clear images shown in the next session since the copY of our distribution images was very poor. In the present report our study work is focused on the intercomparison of results calculated by JAERI and RA1 models.

Iv. Calculation Results and Discussion

To search the cause for the difference described above we set up the calculational problems in the following items,

(1) mass yield distribution of products in a thick cylinder target(552 cm ϕ x 500 cm) and a thin pellet(10 cm ϕ × 2 cm), which are made of ^{337}Np metal with 1GeV and 590 MeV of incident protons,

(2) mass yield distribution of Products and number of evaporated particles from a “Fe nucleus with 1 GeV and 590 MeV Protons,

(3) mass yield distribution of Products from a ^{237}Np nucleus with 1 GeV and 590 MeV incident protons for some combinations of HEF parameters,

(4) number of spallation neutrons generated in the thick cylinder.

Our first approach to the problem is to certify the real differnece between mass yield predictions by recalculation using the NMTC/JAERI and HETC/KFA2 codes. The item (2) are calculated and checked as an example of the high energy reaction in a light nucleus with few fission. Next we are searching the cause by trying the reproduction of the HETC/KFA predictions using the NMTC/JAERI or NUCLEUS code with the change of some parameter values such as BO, Pf and σ in the HEF model. At last the uncertainty of spallation neutron production are examined for estimating the influence on the conceptual study of accelerator-based transmutation system.

Mass yield distributions of products in the thin ^{237}Np pellet irradiated by 1 GeV and 590 MeV protons were recalculated using the JAERI code with BO=8 MeV as seen in Figs. 5 and 6 respectively. These histograms represents the distributions of fission products with the relatively lower height over the wide range of mass number, compared with the corresponding curves given by the PSI code. Conversely for the mass yields of non-fission products near the target nuclide the JAERI code gives the value larger than the PSI code. In Fig.7 the mass yield distribution in the thick ^{237}Np target irradiated by 1 GeV protons was calculated using the NMTC/JAERI code for the case of BO = 14 MeV. Apparently the discrepancy of both distribution shapes near the maiximum height has been reduced considerably. However the BO is not considered to be the main parameter causinig the discrepancy because of the large remainig difference. Mass yield distributions of products from the spallation reaction in a ^{56}Fe nucleus were compared among the cases of a) 1 GeV and 590 MeV with HETC/KFA2 and b) 1 GeV and c) 590 MeV with NUCLEUS. Table 1 summarizes also the number of particles emitted from the ^{56}Fe reaction for NUCLEUS and HETC/KFA2(THIN) calculations with BO= 8 MeV and proton energies of 1GeV and 590 MeV. As seen from these results the product yield in t-he high energy reaction in a light nucleus with few fissions agrees each other within statistical errors. So it is not neccesary to check the part calculating the spallation reaction without high energy fission in both codes.

For the parameter Pf the concrete data used in both codes were checked up. Figure 9 shows the dependence of fission probability on the mass number of some actinide and subactinide nuclei with excitation energies of 20, 50 and 100 MeV, which is written on the code manual of HETC/KFA2. The Pf-values was directly compared with one computed by the NMTC/JAERI code for each excitation energy of fissioning nucleus in Fig.10. The solid lines with the square symbol and with no symbol denote the variations of Pf on the mass number A of fissioning nucleus by NMTC/JAERI and HETC/KFA2 respectively. At the excitation energy -20 MeV Pf for actinides ($A \geqq 225$) varies only in the range above 0.1 and both curves is almost in agreement. At the excitation energy above 50 MeV the Pf value by NMTC/JAERI is in avarage larger than one by HETC/KFA2 for actinides but HETC/KFA2 gives some peaks representing the high fission probability for subactinides. The following approximate condition has been defined instead of HETC/KFA2 curves as

$225 \geqq A \geqq 215$ $Ex \geqq 50$ MeV	Pf = 0.95,
’$211 \geqq A \geqq 209$ $Ex \geqq 50$ MeV	Pf = 0.3,
other cases	Pf JAERI values.

For convenience we call the condition “ Approximate RAL Fission Probability (ARFP)”, which is set temporarily in NMTC/JAERI when the calculations are carried out for comparion.

As described above, the mass yield distribution of products is determined through the sampling of Gaussian random number characterized with σ, which is given in Eq.(5) or Eq. (7). In the HETC/KFA2code(RAL model) all the value of σ_R at the excitation energy above 100 MeV is assumed to be equal to the value calculated by Eq. (7) at 100 MeV. In the NMTC/JAERI the equation (5) have been used to cauculate the value σ_J over 100 MeV. In this work we made the modification so that all the value of σ'_J at the excitation energy above 50 MeV is assumed to be equal to the value calculated by Eq. (5) at 50 MeV, taking into account the range where there exist the original measured data to be fitted.

As shown in Figs. 11~14 the mass yield distributions of products per ^{237}Np nucleus were computed using the NUCLEUS code for following cases to compare them with the corresponding distributions computed by HETC/KFA2(THIN),

(1) proton energy : 1 GeV, Pf : ARFP, $\sigma : \sigma_R$,

(2) proton energy : 590 MeV, Pf : ARFP, σ : σ_R,
(3) proton energy : 1 GeV, Pf : JAERI, σ : σ_J',
(4) proton energy : 590 MeV, Pf : JAERI, σ : σ_J'.

Here the Solid line denotes HETC/KFA2 calculations and the histogram the NUCLEUS ones. As seen in Figs. 11 and 12 for the cases of 1 GeV and 590 MeV, the histograms calculated with ARFP and σ_R can reproduce the HETC/ KFA2 curves relatively well and there are some disagreements in the yield distribution of spallation products at A = 160-200 and near the target nucleus. In Figs. 13 and 14 for 1 GeV and 590 MeV protons, there remain small discrepancies of their maximum heights between the histograms with σ_J' and the HETC/ KFA2 curves. For spallation products there are disagreements similar to the former cases. -

To examine the influence of HEF model in the design study of accelerator -core hybride type transmutation system, the dependence of number of neutrons emitted in the ^{237}Np thick target on the proton energy was calculated in the Fig.15, using both codes. Although the number increases linearly (not saturate), the line has the different gradient for each code. The line with the triangle symbol is the result calculated using the NMTC/JAERI with σ_J' and ~10 % more than the line with the cross symbol when the non-modified σ_J is used. For calculations using the HETC /KFA2 the number of neutron with B0=8MeV(closed circle) is also larger by a factor of 1.1 than one with B0=14MeV(open square). Here the HETC/ KFA2calculation showed that total neutron productions with and without the elastic scattering agree each other within statistical errors.

From these results we conclude that the discrepancy is mainly attributed to the esitamation of σ determining the width of Gaussian curve on the base of the excitation energy deposited in compound nucleus before fission. The FP distribution in JAERI model seems to cover the range of mass number wider than one in the RAL model. It is assumed that the equation calculating σ can be applied to the excitation energy above 100 MeV in JAERI model, while the σ is set to the value at Ex = 100 MeV for all fissioning nuclei wtih Ex >100 MeV in RAL model. However as apparent from calculations using HETC/KFA2, the high energy fissin rection, in the RAL model, is dominant in the medium energy range and the spallation reaction minor. The trend is forced us to change the idea that the spallation reaction with emissions of many particles is main one in the range. Presumably it seems for some part of the code to give a little over-estimation to the fission probability which has to be examined on the comparison with the measured data. Also is it reasonable for the present fission calculation models, which were fitted only to the measured data in the Ex range below 100 MeV, to be used in calculating the nuclear reaction of nucleus with Exof several hundreds of MeV ? Further discussions and studies about this applicability are necessary.

V. Summary

We examined the difference of product yields distribution in the high energy fission reaction calculation between NMTC/JAERI and HETC/KFA2 codes. Our calculation results showed that the difference is mainly due to the estimation of the width of post-fission yield curve, and the contribution of B0 and fission probability minor. It wa-s found that the discrepancy of predictions from the JAERI and RAL HEF models becomes small by adjusting the parameter σ. The range of exciation energy applicable to the width estimation equation seems to be less than 50 MeV for JAERI model and less than 100 MeV for RAL model respectively. In the real computation using both codes, however, it occures often for the compound nucleus to generate with the excitation energy above 100 MeV in the high energy nuclear reaction. It is the unresolved problem whether the present fission model can represent exactly the nuclear reaction of compounds with these high excitation energies or not. We also discussed about the influence of the difference on the number of neutrons generated in the high energy reaction procedure, which is the most important factor in the design study of accelerator-based transmutation system. The number of spallation neutrons in the thick target increses by a factor of 1.1 uniformly by modifying the parameter σ in the JAERI high energy fission model.

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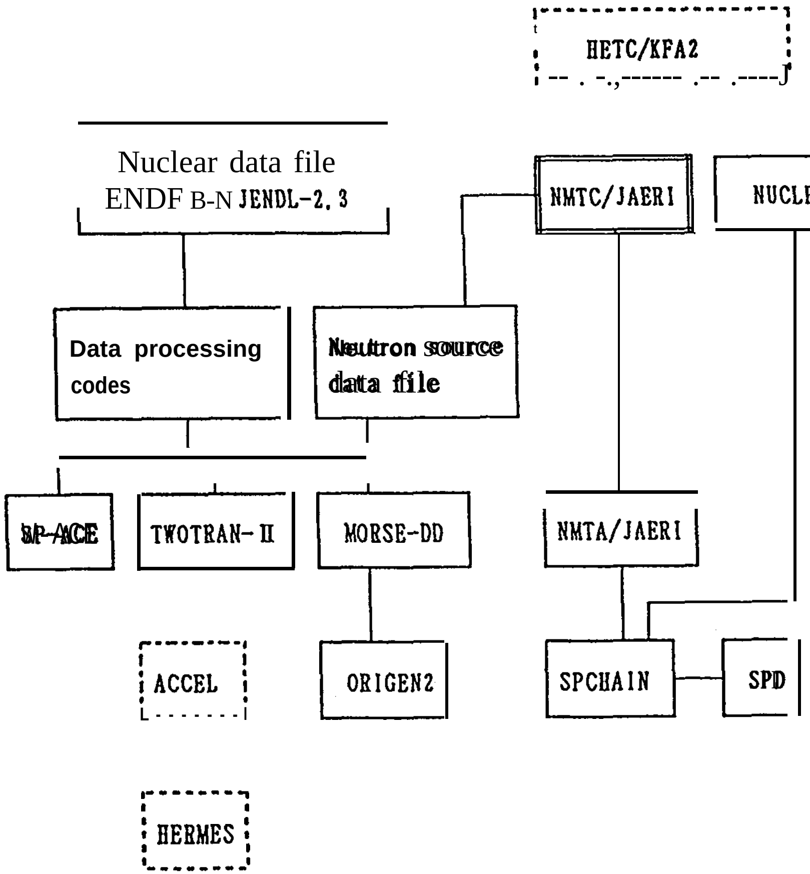


Fig. 1 Code system for designing the accelerator-based transmutation system at JAERI

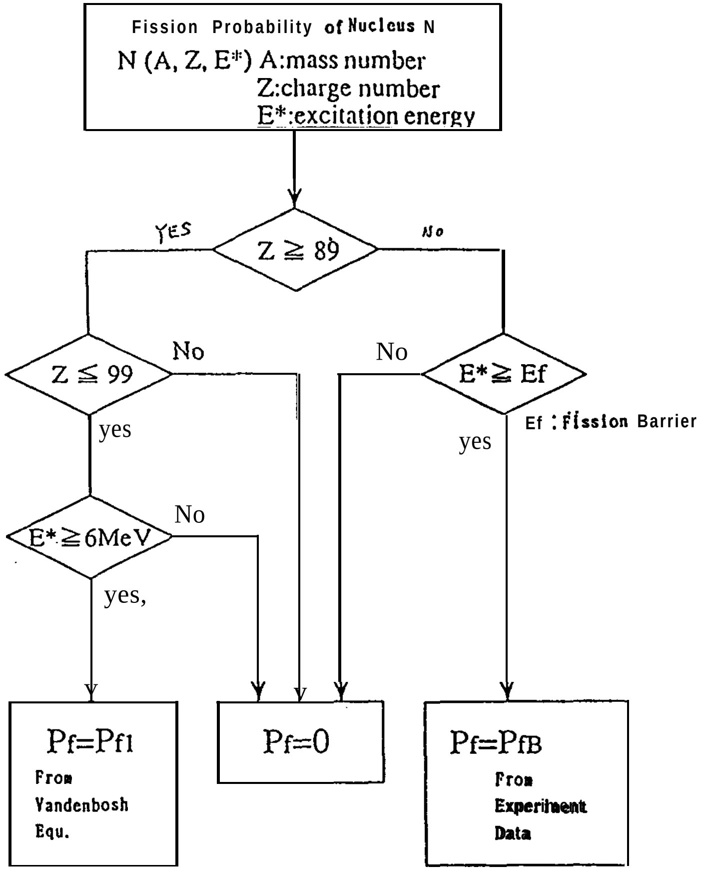


Fig. 2 Flowchart for calculating the fission probability

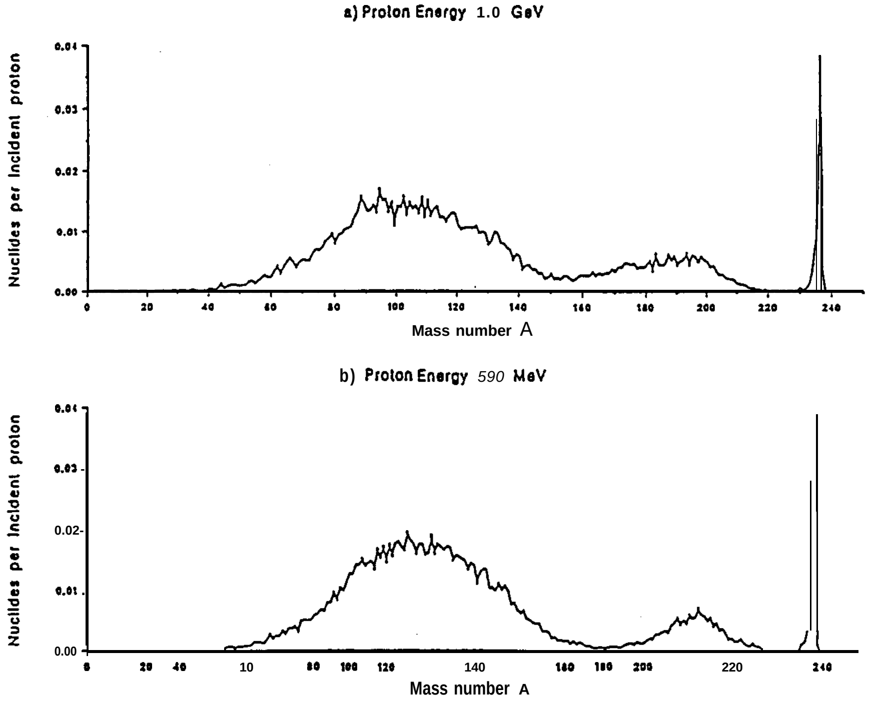
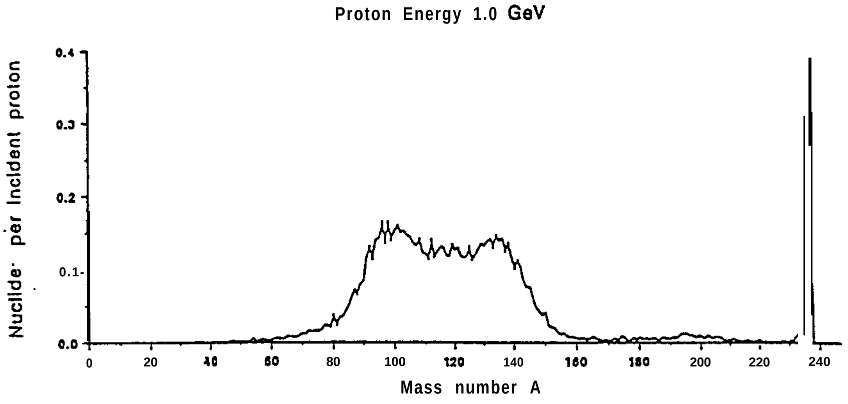


Fig. 3 Mass yield distribution in a thin ^{237}Np pellet presented by a PSI scientist at OMEGA meeting in 1990 proton energy : a) 1 GeV b) 590 MeV



Mass yield distribution frombombardment of a quasi-infinite Np-237 target

Fig. 4 Mass yield distribution in a thick ^{237}Np target presented by a PSI scientist at OMEGA meeting in 1990 proton energy : 1 GeV

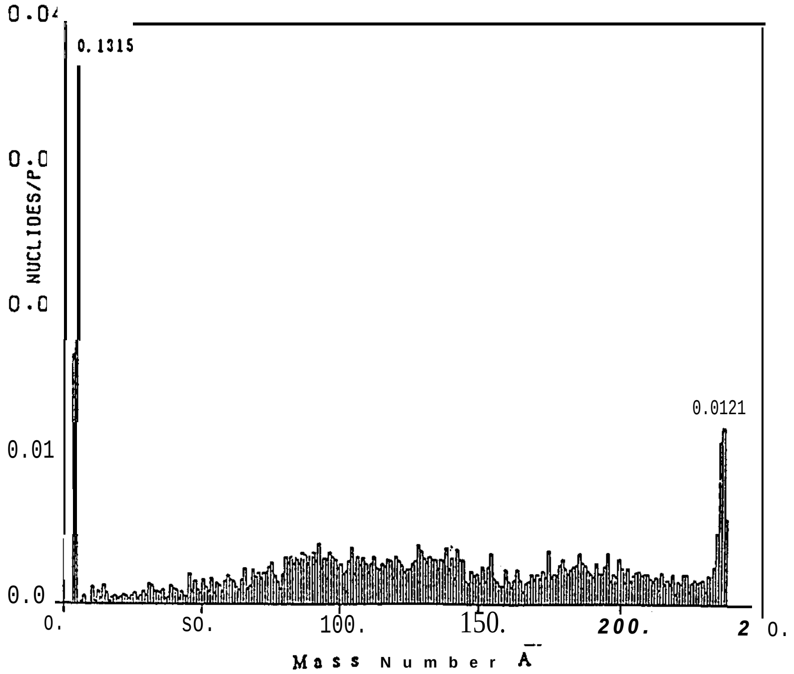


Fig.5 Mass yield distribution in a thin ^{237}Np pellet
(using the NMTC/JAERI code)
proton energy : 1 GeV, BO : 8 MeV

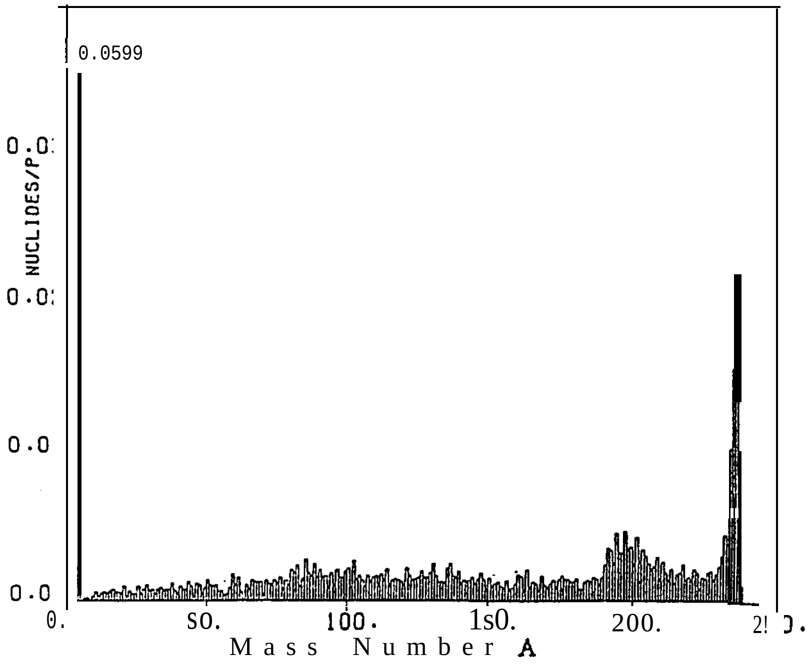


Fig.6 Mass yield distribution in a thin ^{237}Np pellet
(using the NMTC/JAERI code)
proton energy : 590 MeV, BO : 8 MeV

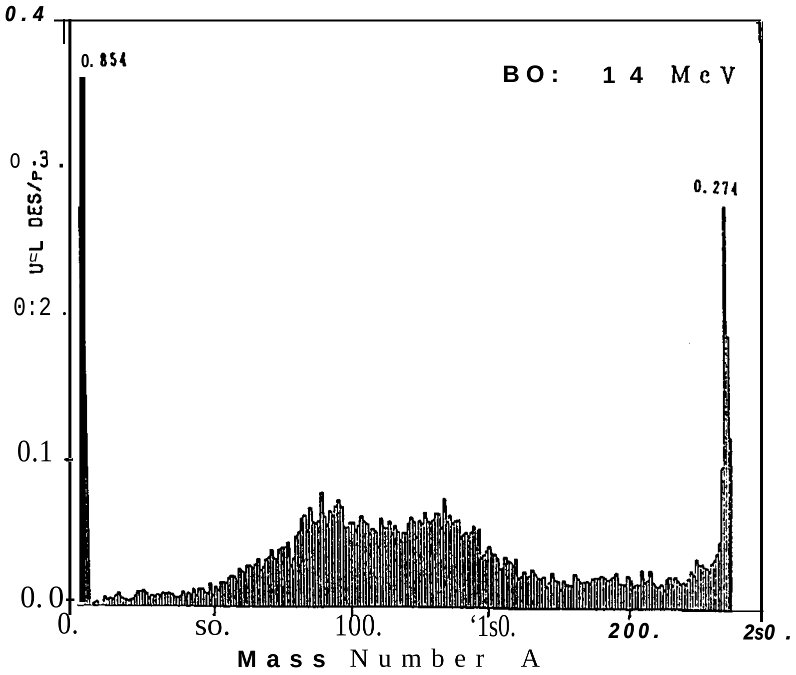


Fig. 7 Mass yield distribution in a thick ^{237}Np target
(using the **NMTC/JAERI** code)
proton energy : 1 **GeV**, **BO** : 14 **MeV**

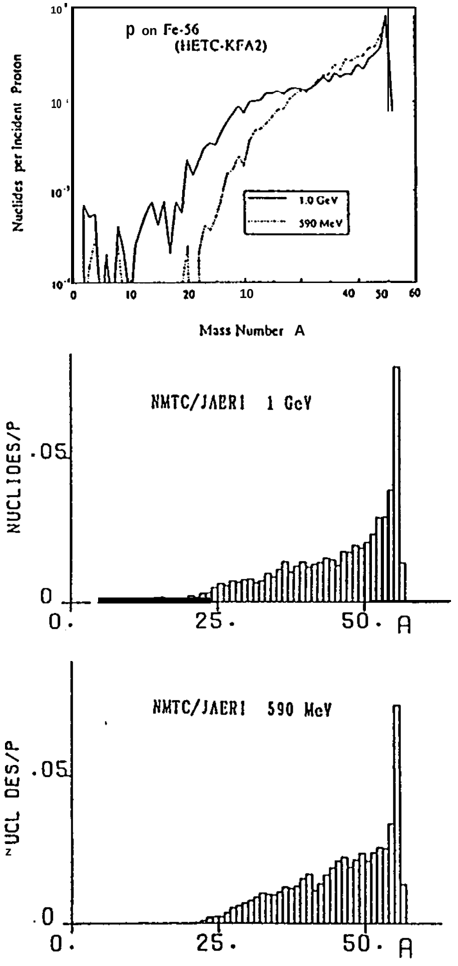


Fig. 8 Mass yield distribution of products from the
spallation reaction in a ^{56}Fe nucleus
(using the NUCLEUS code with **BO** = 8 **MeV**)
a) 1 **GeV** and 590 **MeV** with **HETC/KFA2**,
b) 1 **GeV** with NUCLEUS, c) 590 **MeV** with NUCLEUS

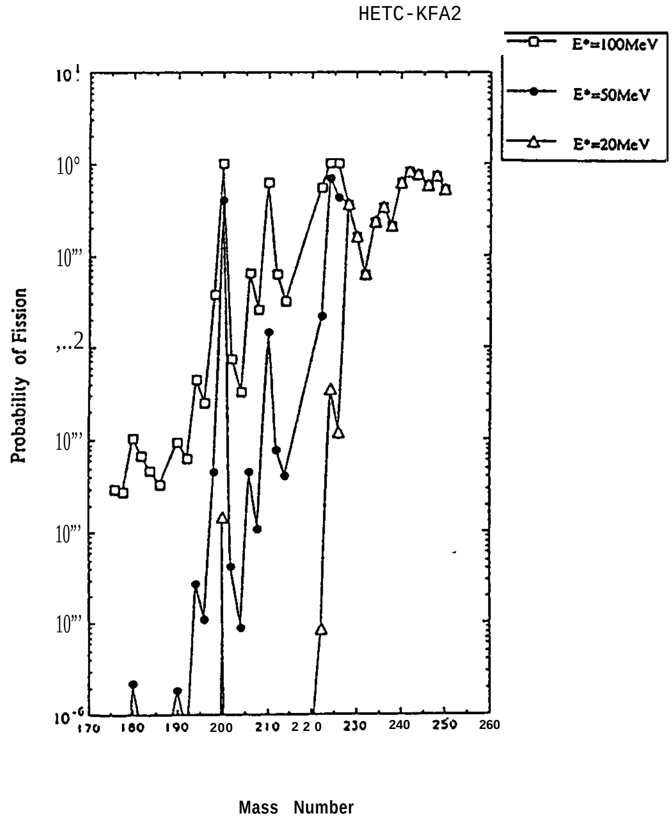
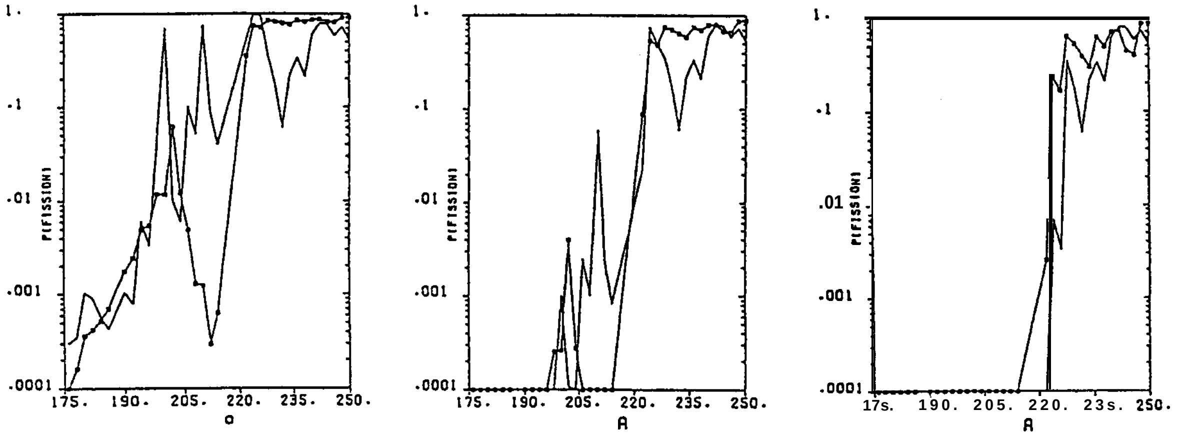


Fig. 9 Dependence of fission probability on the mass number of some **actinide** and subactinide nuclei by **HETC/KFA2** with excitation energies of 20, 50 and 100 **MeV**



a) Ex=100 MeV

b) Ex=50 MeV

c) Ex=20 MeV

Fig. 10 Comparison of fission probabilities given by both **NMTC/JAERI** and **HETC/KFA2** codes with excitation energies of a) 100 **MeV**, b) 50 **MeV** and c) 20 **MeV**

Line with no symbol : **HETC/KFA2**

Line with the square symbol : **NMTC/JAERI**

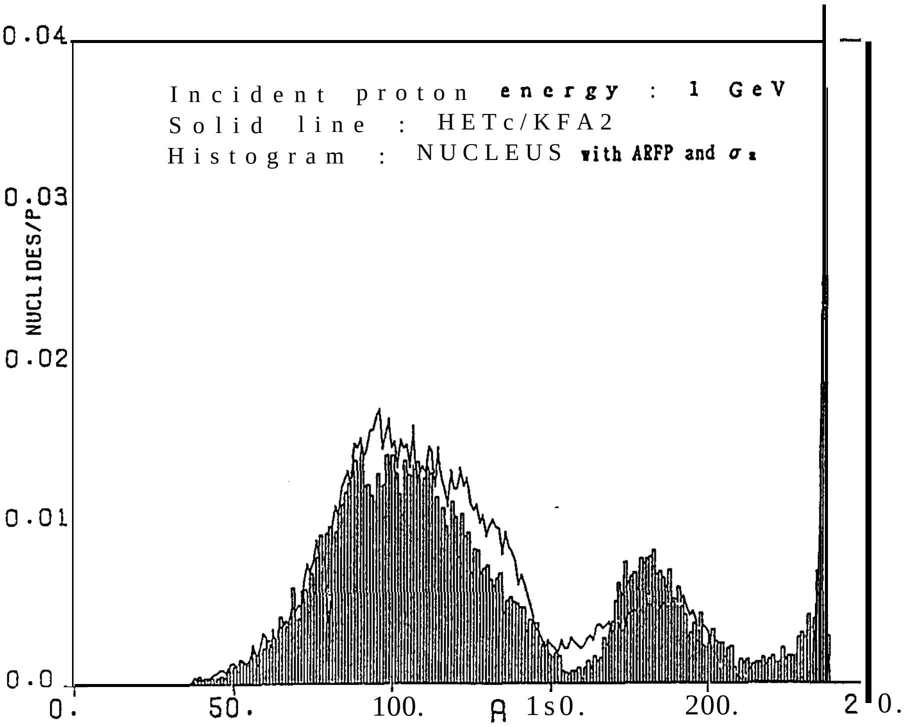


Fig. 11 Comparison (1) of mass yield distribution of products from the nuclear reaction in a ^{237}Np nucleus bombarded by a 1 GeV proton

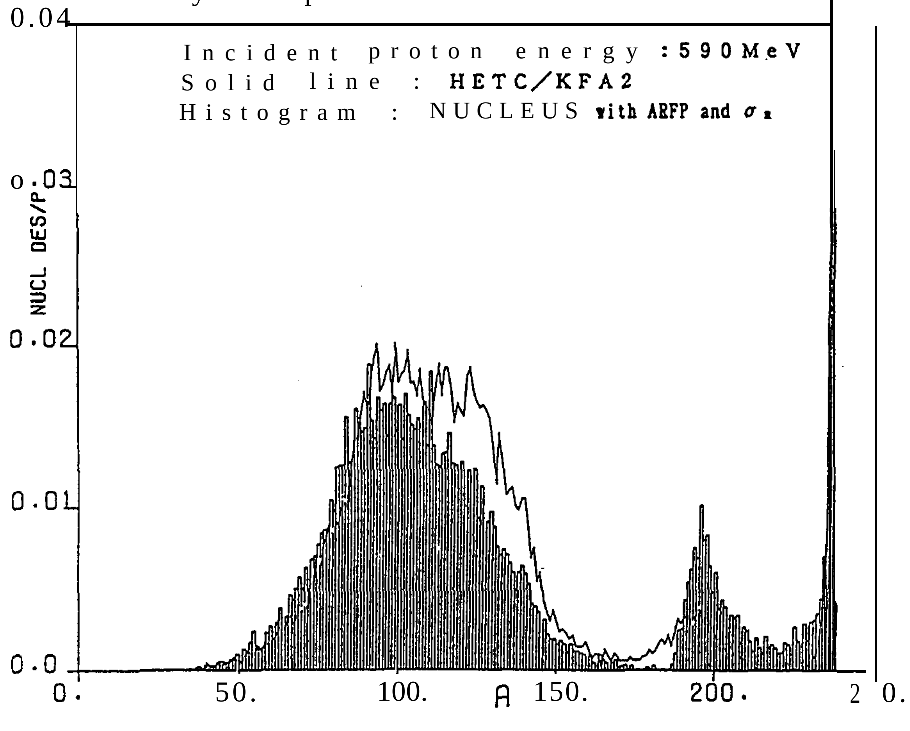


Fig. 12 Comparison (2) of mass yield distribution of products from the nuclear reaction in a ^{237}Np nucleus bombarded by a S90 GeV proton

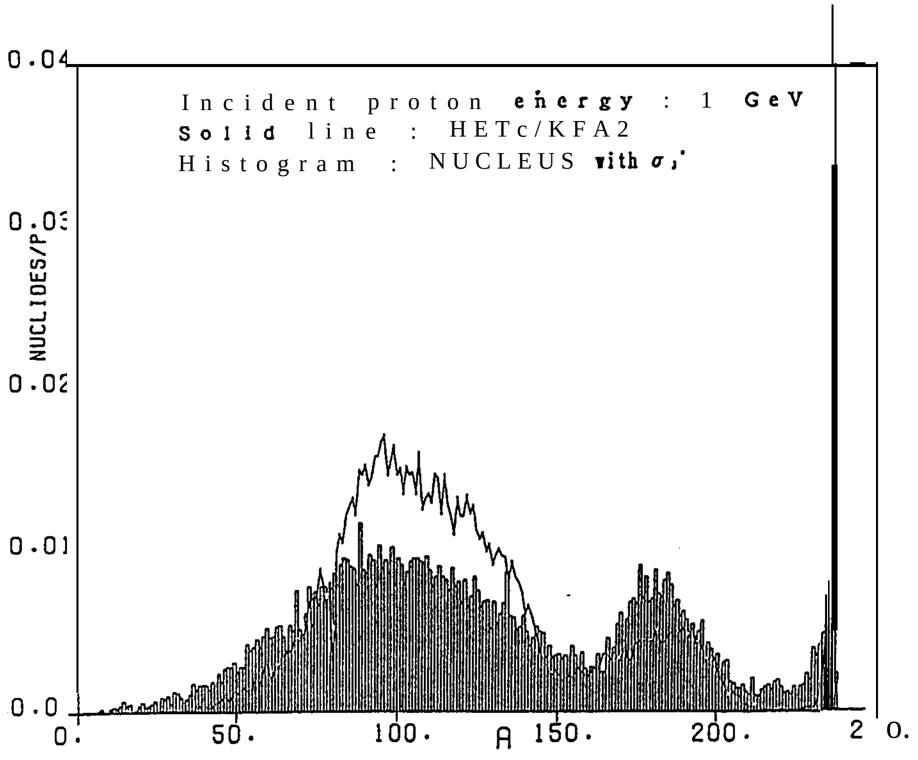


Fig. 13 Comparison (3) of mass yield distribution of products from the nuclear reaction in a ^{237}Np nucleus bombarded by a I GeV proton

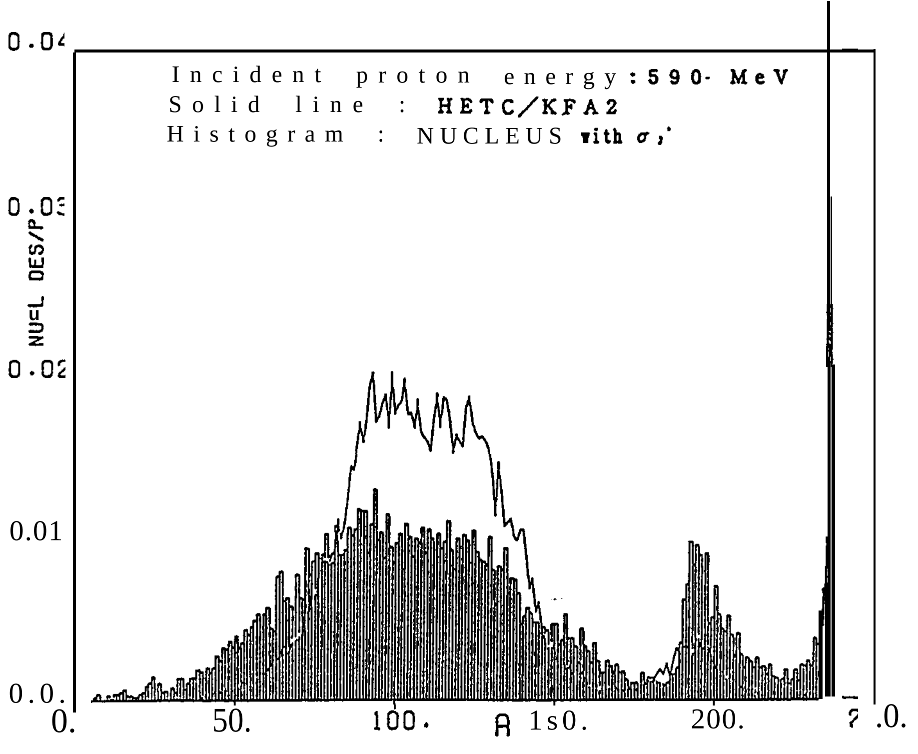


Fig. 14 Comparison (4) of mass yield distribution of products from the nuclear reaction in a ^{237}NP nucleus bombarded by a 590 GeV proton

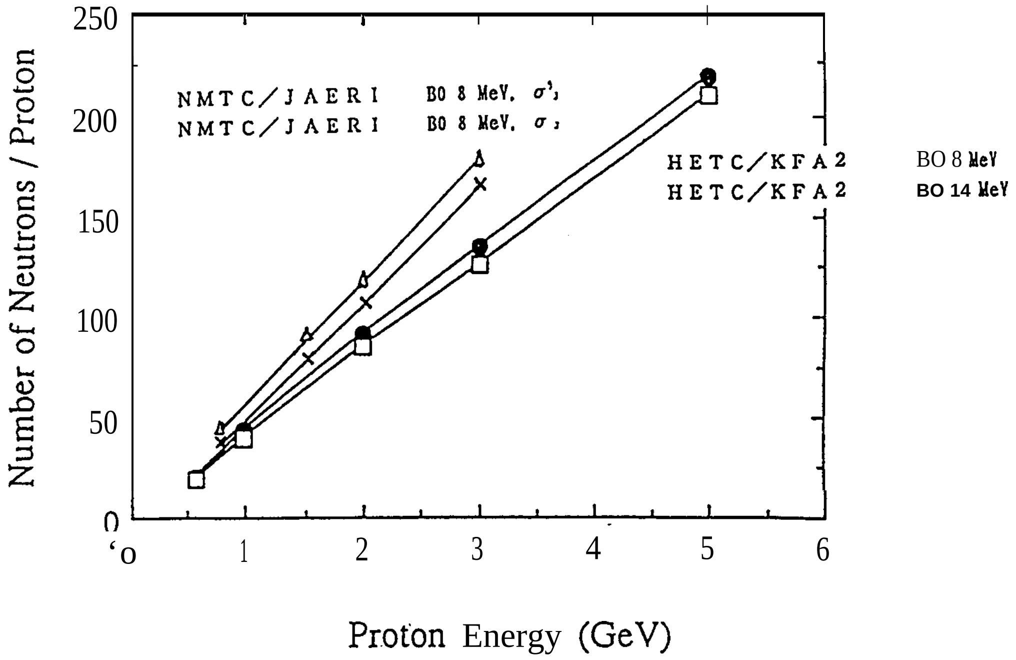


Fig. 15 Dependence of number of neutrons emitted in the ^{237}Np thick target on the incident proton energy

-△- : NMTC/JAERI with BO=8 MeV and σ

- x - : NMTC/JAERI with BO=8 MeV

--- : HETC/KFA2 with BO=8 MeV

-cl- : HETC/KFA2 with BO=14 MeV

Table 1 Comparison on the number of particles emitted from the *'Fe reaction between NUCLEUS and HETC/KFA2 with BO = 8 MeV for proton energies of 1 GeV and 590 MeV

Evaporated particles A : Mass number		Incident proton energy					
		1.0GeV			590MeV		
		NUCLEUS	HETC-KFA2	NUCLEUS HETC-KFA2	NUCLEUS	HETC-KFA2	NUCLEUS HETC-KFA2
A≦4	P(A=1)	1.389E+00	1.344E+00	103.35%	1.316E+00	1.006E+00	130.85%
	N(A=1)	1.999E+00	1.501E+00	133.18%	1.661E+00	1.085E+00	153.09%
	D(A=2)	2.578E-01	2.078E-01	124.06%	2.030E-01	1.104E-01	183.88%
	T(A=3)	5.100E-02	3.355E-02	152.01%	4.360E-02	1.815E-02	240.22%
	HE-3(A=3)	3.680E-02	3.410E-02	107.92%	2.160E-02	1.610E-02	134.16%
	HE-4(A=4)	1.478E-01	1.323E-01	111.72%	1.328E-01	8.185E-02	162.25%
	Total	3.881E+00	3.253E+00	119.31%	3.378E+00	2.318E+00	145.78%