NEA CODE INTERCOMPARISON FOR INTERMEDIATE ENERGY NUCLEAR REACTIONS : APPLICATIONS TO TRANSMUTATION OF LONG LIVED REACTOR WASTES

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Abstract

We summarize results of an international code intercomparison designed to test codes which may provide the necessary nuclear data to evaluate schemes for the accelerator driven transmutation of long lived reactor wastes. This comparison of intermediate energy nuclear reaction codes has been organized by the OECD - NEA Nuclear Science Committee. Results are presented for thin target double differential (p, xn) and (p, xp) cross sections on ^{90}Zr and ^{208}Pb targets at incident energies of 25 to 1600 MeV. We give indications of the degree of dependability of these codes for thin target measurements by use of a few comparisons of calculated and experimental yields. Broader comparisons are presented in the final NEA report published in 1994.

1. Introduction

Consideration is being given to the incineration/transmutation of long lived reactor wastes using high flux reactors,' or by secondary spallation neutrons produced by high intensity intermediate energy (800 to 1600 MeV) charged particle beams.[2] These feasibility studies involve the bumup of both transactinide and long lived fission products. If the schemes were successful, they would provide a permanent solution to the long term storage problem by reduction of long lived wastes to short lived or stable isotopes.

Evaluation of these proposals requires a very large body of nuclear data, much of which goes beyond present power reactor needs. This includes fission probabilities of transactinides for neutrons of up to a few MeV, and excitation functions for interaction of energetic neutrons with long lived fission products and reactor components. In this work we are concerned with data needs for proposals using intermediate energy accelerators to produce copious spallation neutrons to drive the transmutation processes. The first consideration is the flux and spectra of neutrons produced when an intermediate energy beam is stopped in a spallation target (e.g. Pb or W); a second question is the distribution of yields formed from the interaction of the primary beam with the spallation target, and by the secondary reaction products interacting both within the target and with surrounding materials.

The present experimental data base is inadequate for the needs of these proposals. Furthermore, the number of facilities and physicists with which additional measurements could be made is steadily decreasing. We will have to depend largely on nuclear modeling codes to generate the cross sections and spectra necessary for these design studies. With this in mind the NEA/OECD has been charged with conducting a code inter-comparison to assess the uncertainties associated with such nuclear reaction codes. The exercise has been conducted in two parts. The first requests calculation of double differential cross sections for thin target ^{90}Zr, ^{208}Pb (p, xn) (p, xp) reactions for incident energies of 25, 45, 80, 160, 256, 800 and 1600 MeV.[3] This exercise will test the microscopic nuclear physics in the different energy regimes. The second part of the exercise requests calculation of neutron spectra and product yields from 800 MeV protons on stopping length Pb and W targets.[4] This will test the combined microscopic nuclear physics and transport aspects of the codes in giving integral results.

While this intercomparison was motivated by the very important needs of ATW, the applications of intermediate energy nuclear data, and the needs in technological applications are very broad. Areas include radiation oncology (especially neutron and proton therapy), microelectronics (single and multiple event upsets, latchups), influence of cosmic rays on fly-by-wire guidance and on telecommunications equipment, dosimetry/shielding for commerical air travel and for space exploration, calorimeter design for high energy physics, etc.

In the present report we summarize participation in part 1 of this exercise, thin target yields, and make some preliminary analyses of the reliability and limitations of the codes. The participation and codes used are summarized and discussed in section 2; preliminary results are given in section 3, with conclusions in section 4.

2. Codes Tested In This Exercise

The nuclear models to be tested in this project are (1) intranuclear cascade (INC)[5-7] plus evaporation (EVAP)[8-9], (2) INC plus pre-equilibrium[10] (PE) plus EVAP[11], (3) PE + EVAP (4) quantal PE (using Feshbach, Kerman and Koonin theory)[12] plus EVAP, and (5) quantum molecular dynamics (QMD)[13]. In some cases more than one participant used either the same code or minor variations of the same code. The different code categories and participants are summarized in Tables 1 and 2.

The QMD model[13] is an INC approach for nucleon collisions. It differs in that between collisions nucleons each interact with all other nucleons via a two body force. This causes curved, rather than linear trajectories between collisions, and orders of magnitude increase in computation time. This approach may await massively parallel computers to become a practical tool. The quantal approaches on the other hand are starting to be useful tools for predictive nuclear modeling exercises. They retain one (energy dependent) free parameter, the strength of the nucleon-nucleon potential, and still require some work in treatment of multiple precompound decay. But steady progress is being made on making this a viable new method for prediction of precompound emission. All other codes listed in Table 1 should give predictive double differential cross sections (DDCS) using programmed global parameters. Questionnaires were returned with most entries giving details of the calculations and references to the literature for more complete discussions of the relevant physics of the various codes. These are available in the NEA report on Part 1 of this code intercomparison exercise.[14]

Table 1
Participation in Intercomparison by Code Name and Physics Employed

Code Name	Physics	Reference	Lab Designation
HETC / MECC7 + EVAP-F	INC+EVAP	1	PSI ▽
GEANT	INC+EVAP	2	CDF ▼
HERMES (HETC - KFA2)	INC+PE+EVAP	3	JUL ▶
LAHET	INC+PE+EVAP	4	B N L 2 D
LAHET	INC+PE+EVAP	5	LAS1 ×
HETC-3 STEP	INC+PE+EVAP	6	KYU □
CEM92M	INC+PE+EVAP	7	DUB ✱
CEM92	INC+PE+EVAP	8	IAE △
NUCLEUS	INC+EVAP+FERMI STATISTICS	9	JAE2 ⬠
ALICE92	PE+EVAP	10	LNL ■
ALICE87 MOD	PE+EVAP	11	CJD ●
ALICE F	PE+EVAP	12	JAE1 ●
PEQAQ2	PE (EVAP VIA MASTER EQ)	13	SBA ●
GNASH	EXCITON+HAUSER-FESHBACH EVAP	14	L A S 3 ∢
FKK-GNASH	FKK+EXCITON+EVAP (H-F)	15	L A S 2 ○
KAPSIES+GRAPE	FKK+EVAP	16	ECN ▲
QMD	INC+2 Body Forces Between Collisions	17	FRA ◁
SYSTEMATIC	SYSTEMATIC	18	BNL1 +

Table 2
Sources of Experimental Data

Experimental Data		Symbol	Source
^{208}Pb (p, xn)[a]	25 MeV, 45 MeV	●	R. R. Doering, D. M. Patterson and A. Galonsky, Phys. Rev. C12 (1975) 378.[27]
^{90}Zr (p, xn)[a]	25 MeV, 45 MeV		
^{90}Zr (p, xn)[b]	80 MeV	●	M. Trabandt et al., Phys. Rev. C39 (1989) 452.[28]
^{208}Pb (p, xn)[b]	80 MeV		
^{90}Zr (p, xn)[b]	160 MeV	●	W. Scobel et al., Phys. Rev. C41 (1990) 2010.[29]
^{208}Pb (p, xn)b	160 MeV		
Zr, Pb (p, xn)	256 MeV 800 MeV	◆	S. Stainer et al., Phys. Rev. C47 (1993) 1647.[30]
Pb (p, xn)	800MeV	a	W. B. Amian et al., Nucl. Sci. and Eng. 112 (1992) 78.[31]
Pb (p, xn)[c]	256 MeV	◁	M. M. Meier, C. A. Goulding, G. L. Morgan and J. Unman, Nucl. Sci. and Eng. 104 (1990) 339.[3a]
^{90}Zr (p, Xp)’	80 MeV	◁	A. A. Cowley et al., Phys. Rev. C43 (1991) 678.[33]
9$_{\%}$ (p, xp)[d]	160 MeV	◁	J. J. Lawrie et al., (Jan. 1993), to be published; W. A. Richter, R. Lindsay, A. A. Cowley, J. J. Lawrie, G. C. Hillhouse, S. V. Foertsch, J. V. Pilcher, R. Bonetti and P. E. Hodgson, NAC Annual Report, 92-01 (1992) 26.[34]

a) Data at 35 MeV and on other targets also available
b) Data at 120 MeV and on other targets also available.
c) Data at 113,597 MeV and on other targets also available.
d) Dara at 120 MeV and on other targets also available.

3. Results and discussions

The experimental data used are summarized in Table 2. An average of six angles for both neutron and proton exit channels were requested for each incident energy, for ^{90}Zr and ^{208}Pb targets. This led to around 170 figures for DDCS. Most of these are contained in the summary report. We show only several illustrative examples here.

In fig 1 we show the neutron and proton emission multiplicities calculated by many of the codes for different incident proton energies. The differences predicted in the various contributions may be seen to be quite large. This reflects both large variations in the total reaction cross sections generated within the codes, and from the nuclear physics models used to treat the subsequent de-excitation processes.

In fig 2 we show the ^{90}Zr(p, n) DDCS at 20° for 25 MeV incident energy. The end point energy comes at 18 MeV due to a -6.9 MeV Q value. We note that the INC codes show spectra to 25 MeV. This is due to the use of neutron and proton binding energies averaged over nuclides rather than use of thermodynamic values for each nuclide (as in the LAS and LNL results). While the PE + EVAP (or FKK + EVAP) models enjoy this advantage over the INC models at lower incident energies, they become inappropriate to use above 260 MeV because, unlike the INC codes, they lack pion and other particle production channels.

At incident energies of 80 and 160 MeV, for ^{90}Zr, both n and p emission channels have been measured at the same angles. This allows a test of the treatment of n and p emission branching and of the isospin physics in the different models . At forward angles many of the models are in quite good (within a factor of 2) agreement with experimental results. We show results for 69° in figures 3 and 4 for 160 MeV incident proton energy. At this angle the Dubna and PSI INC codes are in good to outstanding agreement with data; other codes may be seen to have significant deviations. Which codes do better changes with angle and incident energy; the conclusion at one angle and energy is not valid at all angles or incident energies. The comparisons of figs 3-4 are less favorable e.g. for 80 MeV incident energy.

In fig. 5 we present results for 800 MeV ^{90}Zr(p, n) spectra at 7.5° to illustrate one historic problem of the INC codes overprediction of the quasi-elastic nucleon - nucleon scattering peak at very small angles. At the larger angles for which data are available (30, 60, 120, 150°) some of the INC codes do an outstanding job of predicting the DDCS. An example is e.g. fig. 6, for 800 MeV incident energy and at 60° exit angle.

4. Conclusions

We have outlined the code intercomparison recently completed by the NEA/OECD for codes relevant to spallation targets for actinide/long lived fission product transmutation projects. In particular we have sketched the scope of part 1 of this exercise involving thin target double differential cross sections in reactions induced by 25-1600 MeV projectiles. Experimental data are available only up to 800 MeV, data at higher energies must be extrapolated from results at lower energies and estimates of reliability will have to be subjectively drawn from lower energy data.

A small sample of the results from the final report has been presented to point out some of the problems in the existing codes. practical space limitations do not permit a presentation of many of the most successful comparisons. These may be seen in the final NEA/OECD report.[14] Subjectively the overall reliability of codes over broad ranges of incident and exit energies is at present no better than to within a factor of two, and in many cases poorer. Scrutiny of results of this intercomparison should help identify problem areas in the models involved, and we hope lead to an overall improvement in the predictive power of the codes. In this summary we have discussed DDCS results. The final report also has summaries of single differential cross sections, reaction cross sections, neutron and proton multiplicities, and product yields for many of the codes used. Part 2 will illustrate the combined nuclear reaction and radiation transport capabilities of certain of the codes for thick target applications.[15] These are precisely the conditions relevant to the ATW proposals which prompted this exercise.

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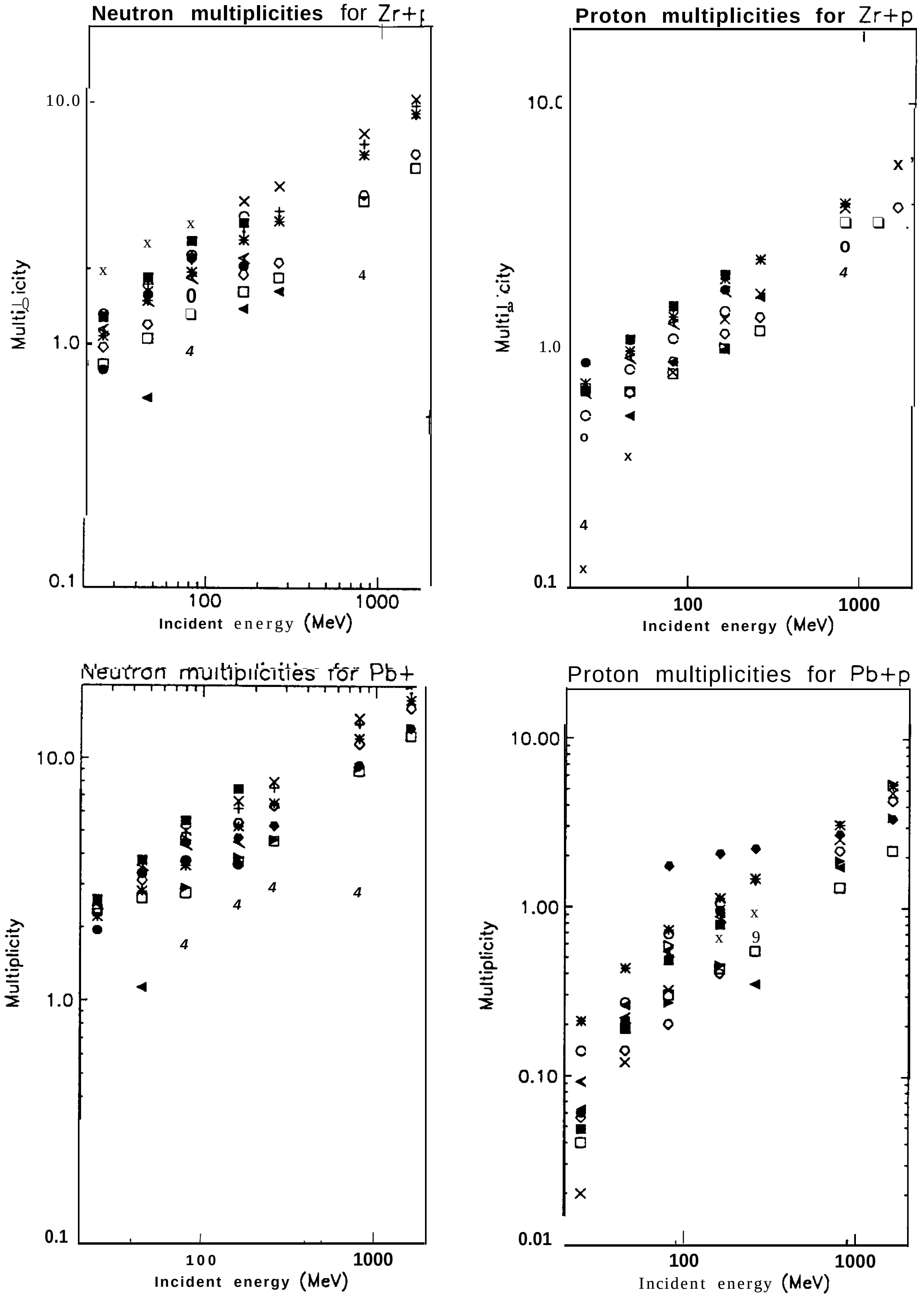
Fig 1 Neutron and proton emission multiplicities versus incident proton energy on ^{90}Zr and ^{208}Pb targets as predicted by several codes. Symbols for different calculations are identified in Table 1.



Neutron multiplicities for Zr+

Proton multiplicities for Zr+p

Neutron multiplicities for Pb+

Proton multiplicities for Pb+p

Fig 2 Calculated end experimental ^{90}Zr (p, xn) spectra at 20” for 25 MeV incident protons. Experimental results are connected by straight *line* segment. Calculated contributions are identified in Table 1. Sources of experimental data are identified in Table 2.

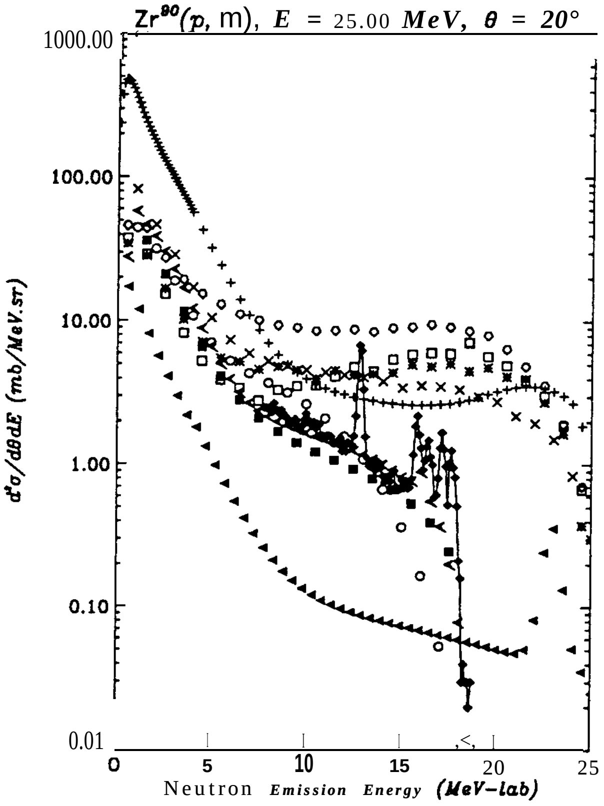


Fig 3 As in fig 2 for% (p, xn) spectra.

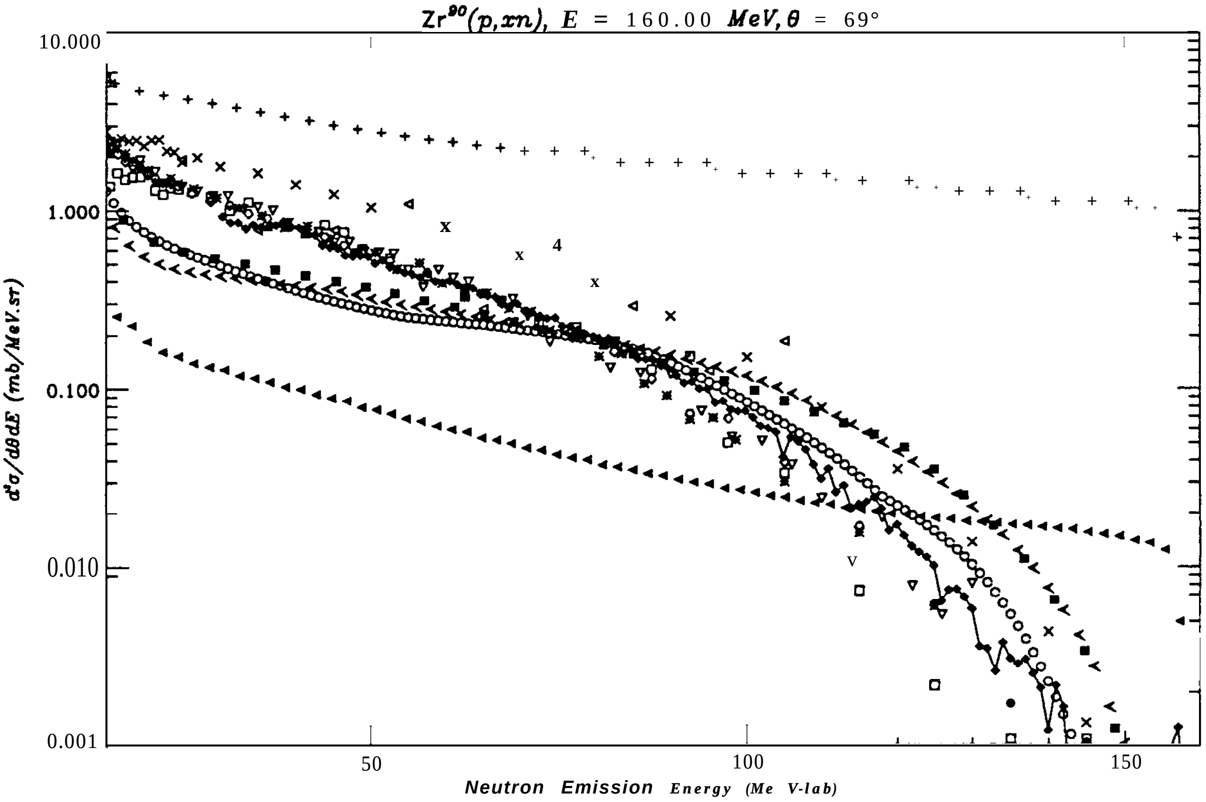


Fig 4 As in Fig 2 for ^{90}Zr (p, xp) spectra at 69° for 160 MeV incident protons.

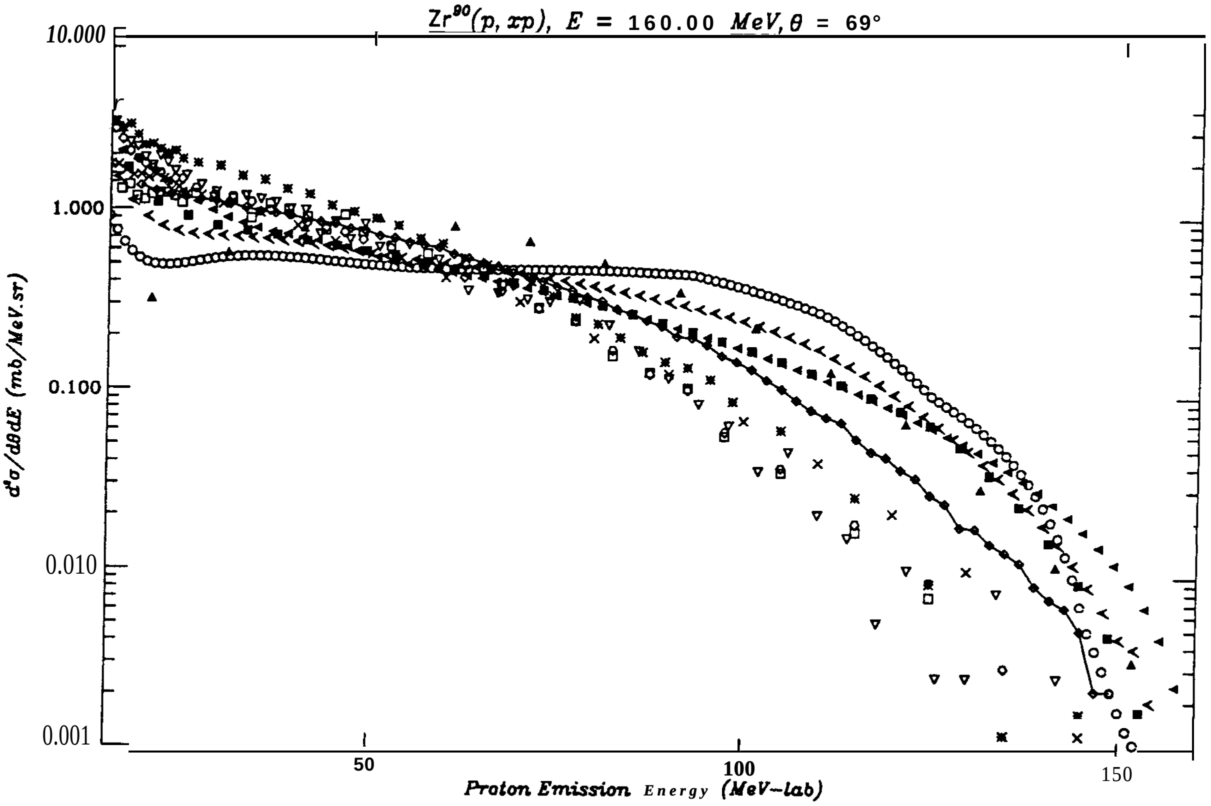


Fig 5 ^{90}Zr (p, xn) spectra at 7.5° for 800 MeV incident proton energy.

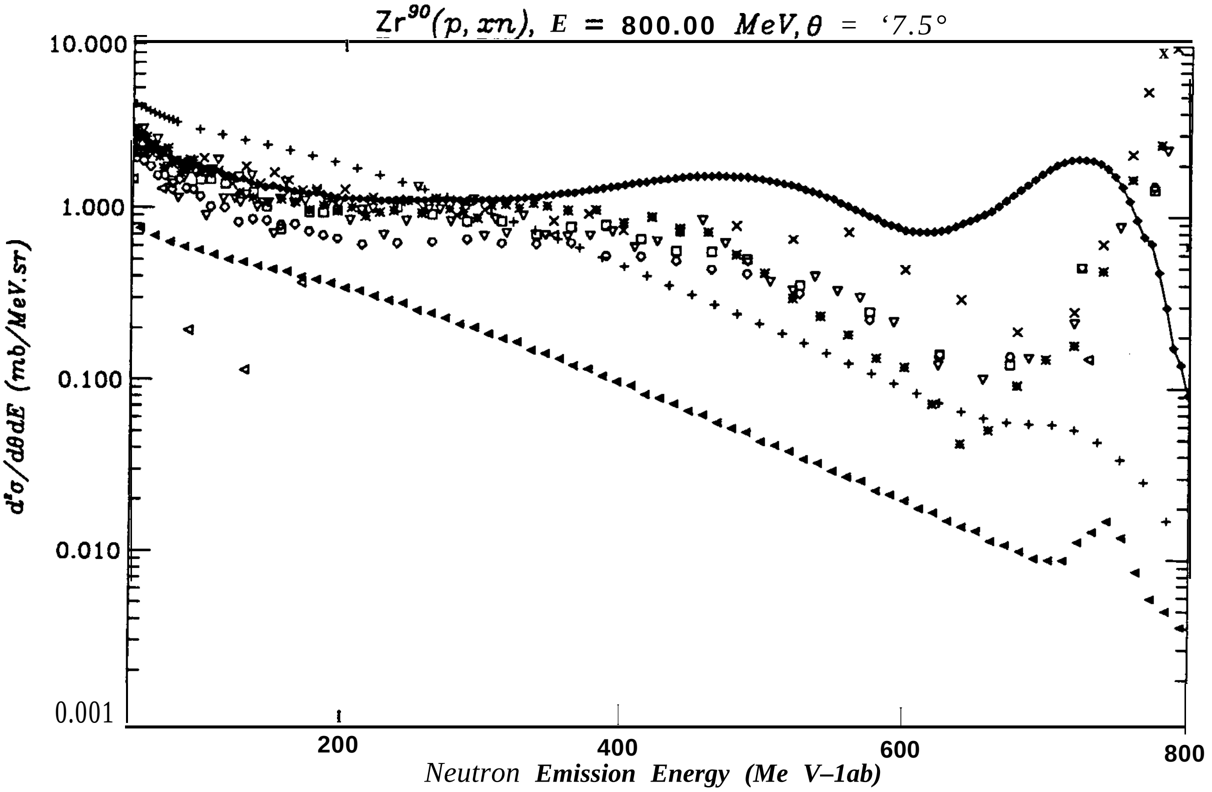


Fig 6 ^{90}Zr (p, xn) spectra at 60” for 800 MeV incident proton energy.