The HERMES System of Beam Materials Interactions and Systematics of INCE Calculations of Double Differential Cross Section Measurements of Neutron Production by Protons between 100 MeV and 800 MeV

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Abstract

There is still considerable interest in medium energy proton reaction data because of applications in astrophysics, neutron sources, materials research, accelerator technology, space research and high energy physics. Regarding accelerator technology, a new generation of spallation neutron sources has come into operation. The economic design and operation of new high current proton accelerators is strongly dependent on the accurate knowledge of neutron, pion, and radioisotope production, since these reaction products cause the main problem related to shielding, radiation damage, safety, and maintenance aspects. Much of the needed data has to come from nuclear model calculations. Such calculations require computer codes capable of multi particle emission.

INTRODUCTION

There is still considerable interest in medium energy proton reaction data because of applications in astrophysics, neutron sources, materials research, accelerator technology, space research and high energy physics. Regarding accelerator technology, a new generation of spallation neutron sources has come into operation [1]. The economic design and operation of new high current proton accelerators is strongly dependent on the accurate knowledge of neutron, pion, and radioisotope production, since these reaction products cause the main problem related to shielding, radiation damage, safety, and maintenance aspects. Much of the needed data has to come from nuclear model calculations. Such calculations require computer codes capable of multi particle emission [2-4]. A suitable code package is the HERMES system, which ist described below [2].

Some basic features of the physical models used in the codes, however, can be tested and validated in relatively simple experiments with clearly defined boundary conditions and excluding any contributions of secondary particle induced reactions. Experiments of this kind are called code validation experiments. Earlier neutron measurements at incident proton energies above 100 MeV are rather scarce and cover only a few points in the double differential scale [5-9].

Systematics studies and measurements were started as part of a study project for a new spallation source [10] by S. Cierjacks and co workers [11] in 1981. The publication and the discussion of those measurements (see Refs. 12-15) led then to a collaborative effort between LANL Los Alamos and KFA Jülich to measure double differential neutron production cross sections at the LAMPF WNR facility in 1984-1990. The measurements and validations have been published in several conference proceedings and journals [16-22]. After more than one decade of these measurements based on S. Cierjacks' measurements at the PSI proton cyclotron beam, a complete list of the status of the thin target (p,xn) measurements may be found in Table 1.

Table 1: Thin Target (p,xn) Measurements

Energy (MeV)	Target Materials	Angle (degree)
113	Be,C,O,Al,Fe,W,Pb,U	7.5,30,60,150
256	Be,C,O,Al,Fe,Pb,U	7.5,30,60,150
318	C,Al,Ni,Ta,W,Pb,U	7.5,30
597	Be,B,C,N,O,Al,Fe,Pb,U	30,60,120,150
800	Be,B,C,N,O,Al,Cd,Fe,W,Pb,U	30,60,120,150
800	C,Al,Ni,Ta,W,Pb,U	7.5,30
160(a)	Al,Zr,Pb	0,11....145
597(b)	C,Al,Fe,Nb,In,Ta,Pb,U	30,90,150
800(c)	Al,Cu,In,Pb,U	0,30,45,112

(a) Scobel et al. [23], (b) Cierjacks et al. [13], (c) Howe [6]

MEASUREMENTS

Measurements of neutron spectra were performed via the time of flight technique utilizing the unique conditions for this type of experiment at the Los Alamos WNR facility. The flight path lengths were between 30 m and 60 m at several distinct angles. The time resolution was 200 ps, mainly due to the favourable pulse structure of the proton beam, and at a reasonable intensity of about 10^8 protons per micropulse. Other sources of time uncertainty could not be determined. But it is probable that they exist and reduce the accuracy, which can be estimated with the above machine parameters.

Another source of uncertainty, which has to be considered in neutron time of flight measurements, is the energy dependent efficiency of the neutron detector. Several efficiency curves for scintillator materials exist, which differ considerably at energies above 400 MeV (see Refs. 20 and 22). Details about the experimental arrangement and the analysis procedure are given in Refs. 16-18.

THE HERMES SYSTEM

The HERMES code (High-Energy Radiation Monte Carlo Elaborate System), as described in full detail in the HERMES report [2], is used at KFA Jülich to perform Monte Carlo simulations.

To calculate the production, interaction with matter and transport of highly energetic particles, the latest state-of-the-art radiation transport codes and event generators are used in HERMES. All the codes employ Monte Carlo techniques with 3-dimensional geometry description. Therefore it is possible to treat in detail the reaction mechanism and the transport of high-energy particles as well as of the low-energy particles created.

The problems that can be solved with the aid of the HERMES system cover a wide range of incident particle energies and a set of different particle types. Therefore the computational work has to be shared between several Monte Carlo codes, each solving a specific part of the total problem. Currently three Monte Carlo codes are implemented, namely HETC [24/25], MORSE-CG [26] and EGS4 [27], besides some auxiliary codes. Off-line coupling of the codes is used, due to practical and scientific reasons:

- With off-line coupling it is much easier to implement additional Monte Carlo codes. Thus, HERMES can be extended in an easy way to represent the state of the art without need for extensive changing of programs.
- Some problems that require a large amount of computer power, in terms of storage and CPU time, can be partitioned into steps.
- The results of each step can be examined to find out errors as well as statistical and physical quality of intermediate results. Subsequent steps can be tailored according to the statistical properties of the prior steps.
- Intermediate results may also improve the understanding of the problem.

The coupling procedure controls the flow of particle data through the system and the collection of results. A general data structure was designed to be used by all programs of HERMES:

- to accept particle sources generated in other programs;
- to submit particle data for further treatment in other programs;
- to submit detector results at the end of each independent batch and at the end of a run.

An important subroutine package of HERMES is the Combinatorial Geometry CG-L2 which was implemented in HETC, MORSE-CG and EGS4. Therefore, the geometry description of a problem may be made only once for all these codes. The Combinatorial Geometry was considerably increased in its capabilities. A test program has been developed to provide extensive testing of the geometry set-up prior to the Monte Carlo runs. Additionally a package of routines is available, named STATLIB, to be used in the analysis part of all programs. To get final results the STATIST code is used to combine the outcome of different Monte Carlo codes working on the same problem. An overview of the main physics and auxiliary codes is given in the following.

The HETC/KFA

HETC (High-Energy Transport Code) is implemented in a version based on the original coding given in ref. [25]. The particles treated by HETC are n, p, $\pi\pm$, $\mu\pm$, D, T ^{3}He, α and heavy ions with $A < 20$.

The physical model of HETC consists of mainly two parts, the intranuclear cascade model and the evaporation model performing

- production of residual nuclei and residual excitation energy;
- charged-particle ionization energy loss (dE/dx);
- primary-particle small-angle multiple Coulomb scattering;
- automatic parameter update for nonelastic collisions above 3.5 GeV (limited energy range for scaling for protons and neutrons with $E_{\text{max}} \leq 25$ GeV and for $\pi\pm$ with $E_{\text{max}} \leq 15$ GeV);
- elastic collision for proton- and neutron-nucleus collisions up to 20 GeV;
- high-energy fission in the evaporation model;
- automatic parameter update for B_0 in the level density equation used in the evaporation model; and
- anisotropic angular distribution of evaporated particles.

The MORSE-CG/KFA

MORSE-CG (Multigroup Oak Ridge Stochastic Experiment with Combinatorial Geometry) was implemented in a KFA version based on the original code [26]. MORSE-CG is a multigroup particle transport program to simulate the histories of neutral particles, which may originate from fixed neutron- or γ-sources or fission feedback or from submitted neutron- or γ-source distributions in phase space. MORSE-CG simulates the following physical process:

- elastic neutron-nucleus collisions including hydrogen collisions, nonelastic neutron-nucleus collisions, capture and fission, γ-production and -transport;
- productive nuclear collisions (n,2n, etc.); and

- analysis of fluxes and reaction rates in phase space, and light production in scintillator materials.

The EGS4/KFA

The EGS4 (Electron Gamma Shower) code was implemented in a KFA-version based on the original code. The EGS computer codes provide a Monte Carlo simulation of the coupled transport of electrons and photons with energies from a few keV up to several TeV [27]. The particles treated by EGS4 are e^+, e^- and γ, which may originate from fixed sources of these particles or from submitted electromagnetic particle sources (e^+, e^-, γs in phase space).
EGS4 simulates the following physical processes:

- small - and wide-angle scattering;
- bremsstrahlung, pair production, Compton scattering, Möller effect, Bhabha effect, photoelectric effect;
- annihilation; and
- continuous e^+, e^- energy loss.

The Deexcitation module NDEM

The NDEM code is used to generate a γ-ray source from the deexcitation of residual nuclei. The assumption is made that all particle decay modes have been exhausted. Thus, γ-emission does not compete with particle emission. The NDEM formalism is taken from the Los Alamos PHT code [28]. The input to NDEM is a data file containing the residual nuclei information recorded by HETC. The γ-ray source generated in return on a file can be input into MORSE-CG or EGS4.

The general-purpose analysis module SIM

We have implemented an on-line-analysis subroutine package into HETC, which is used to provide scoring of the physical results of the HETC run. This package, named SIM, includes routines to read in user analysis request, to compute the contributions of an event to detector signals, to provide estimates of the statistical errors of detector signals and to interface HETC to the final processing code STATIST. The currently available detector types are:

- yield of secondary particles from the intranuclear cascade;
- yield of secondary particles from evaporation and fission;
- yield of secondary particles;

- energy deposited by various deposition schemes;
- scintillation light generated by various schemes;
- forward particle current through given surfaces;
- particle fluxes on given surfaces;
- particle track-length flux in given regions;
- particle energy streaming through given surfaces:
- material damage analysis.

The statistics module STATIST

STATIST has been created to combine the results of correlated Monte Carlo runs. It reads the detector results stored on files at the end of each Monte Carlo batch. Arithmetical and logical operations can be applied on the loaded data to derive additional information from the detector output. Detector logic, like coincidence or veto, can be simulated. Finally a set of physical quantities is available for each batch. Frequency distribution functions of these variables can be requested. A set of statistical moments is computed for each frequency distribution function, including the mean value, the fractional standard deviation, skewness and kurtosis.

The variable set derived from the loaded detector results can be stored on a file for further processing in more advanced statistics modules like SAS [29].
The HERMES scheme is shown in Figure 1.

MONTE CARLO SIMULATIONS

The present calculations are based on the intranuclear cascade-evaporation model originally developed by Bertini [24], and implemented in the high-energy nucleon-meson transport code [25] developed at Oak Ridge National Laboratory (ORNL). This Monte Carlo code for particle production and radiation transport has been modified several times in the past. Various code modifications of HETC have been made at the Forschungszentrum Jülich (KFA). All the modifications relevant to the included nuclear model refer to the evaporation model, which involves the Ewing-Weisskopf formalism [30] without a contribution from preequilibrium processes. The changes contain an update of the atomic masses using the 1977 Atomic Mass Evaluation values of Wapstra and Bos [31]. The range of possible residual nuclei was extended by implementing the semi-empirical mass formula of Cameron [32] in case of masses not covered by those tables. Furthermore, the parameter B_0 in the formula of the level density is allowed to vary with A, using data compiled by Baba [33]. A new kinematic calculation involving the recoil momentum of the residual nucleus allows non isotropic evaporation. At last the high energy fission model (RAL-model [34]) has been included in the evaporation model based on the statistical model of Fong [35]. In the actual update this modified HETC has been implemented into the framework of the HERMES code system [2], resulting in the actual version HETC/KFA 2.

The calculational predictions of proton induced neutron emission presented were made by using the so-called "thin target"-setup of HETC/KFA-2. In this setup only the included nuclear models of HETC are taken into account. Starting an on-line analysis of emitted nucleons directly after their emission from the nucleus, time consuming extranuclear transport algorithm are switched off. This procedure is somewhat different from previous published calculations [14] avoiding the writing of large event histories on computer storage devices. Physically this setup can be understood as an ideal thin target consisting of only one nucleus. This method is valid because the "geometrical" cross section of the bombarded nucleus is known by the code [2]. This method results in significantly shorter computing times than another method simulating the geometry of a real thin target used in experiments. For U and Pb targets the RAL fission model [34] with a constant value of B_0 =8 MeV and isotropic emission of secondary particles during evaporation in the laboratory system were used. For all other target nuclei the fission model was excluded and the variable B_0-option was selected, while non-isotropic emission of evaporation particles was allowed.

To achieve optimum comparison, identical energy intervals as used in the experimental analysis were provided in the HETC calculations. Depending on target material, emission angle and incident proton energy, the number of spallation events varied from $2.5 \cdot 10^5$ to $6.0 \cdot 10^5$ to achieve reasonable statistics in the calculations.

EXPERIMENTAL RESULTS AND COMPARISON WITH MONTE CARLO SIMULATIONS

The predictions of the HETC-INCE model were compared to the experimental data. The total uncertainties of the experimental results (combining statistical and systematic errors) were determined as 10-15%, and thus are of the order of the data point sizes. Theoretical cross sections were calculated with typical statistical uncertainties between 1% and 5% (one standard deviation), except for a few of the highest energy group.

Some examples of the measurements given in Table 1 were simulated and are partly given in Figs. 3-8 as examples of (p,xn) cross sections. Comparisons of calculated and experimental cross sections are commonly displayed in a double logarithmic scale using units of barns/(MeV·sr). The kind of presentation (per unit of lethargy) was chosen here to pronounce discrepancies between experimental and simulated curves. The respective conversion is given by the relation:

$$\frac{d\sigma_i}{d\Omega \cdot dU} = \frac{d\sigma_i}{d\Omega \cdot dE} = \frac{E_{i+1} - E_i}{\ln E_{i+1} - \ln E_i}$$

where $d\sigma_i/d\Omega\, dE$ is the double differential cross section in the energy interval $[E_i, E_{i+1}]$. For this purpose in Fig. 2 an illustrative example is given.

Measurements of proton induced neutron production cross sections are available now for a wide range of target masses, incident energies and neutron emision angles. Discrepancies between earlier measurements and INCE simulations are considerably smaller with the latest measurements. A detailed analysis of the state-of-the-art of accuracy of neutron cross section measurements and validation simulation will be published in Ref. [36].

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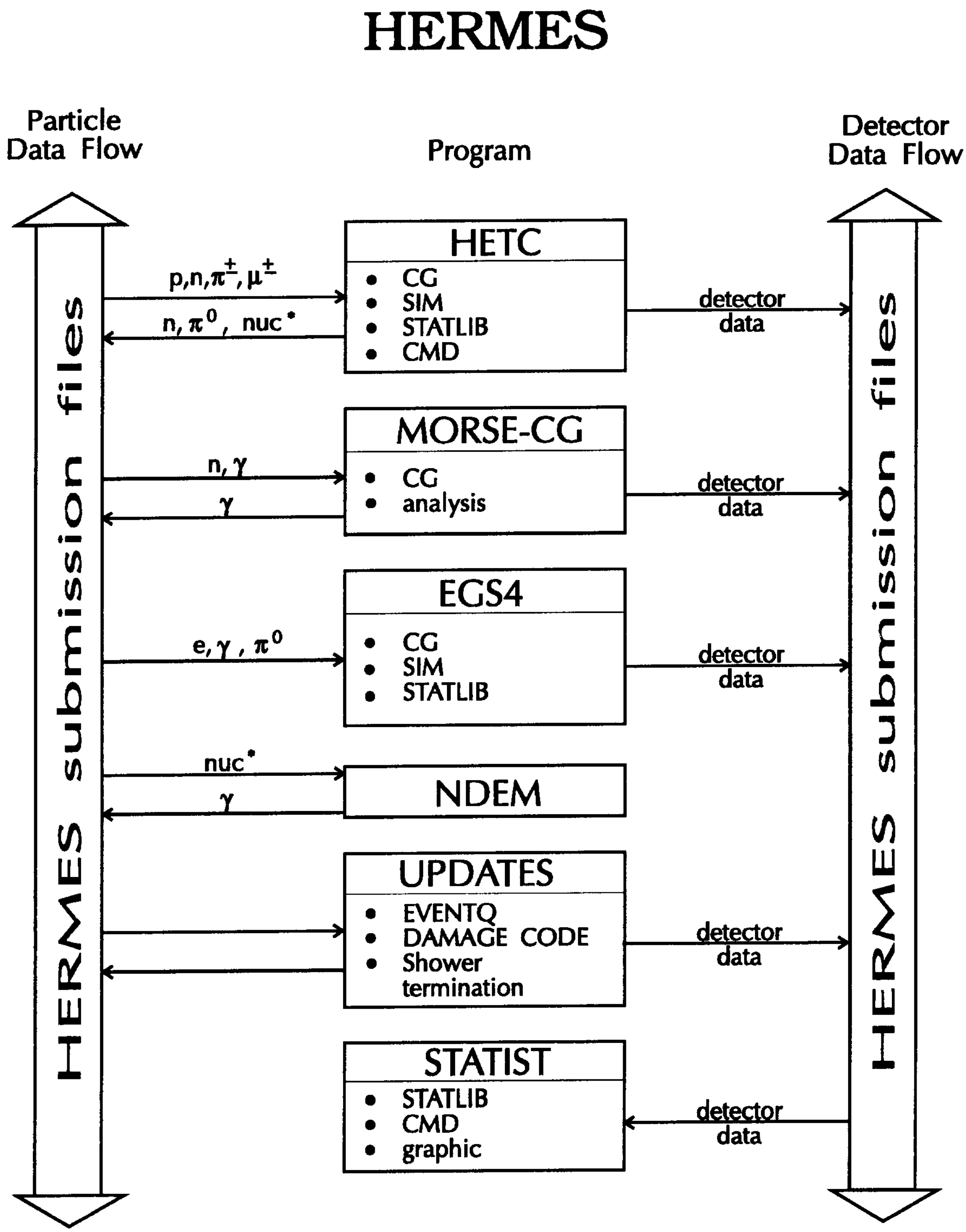
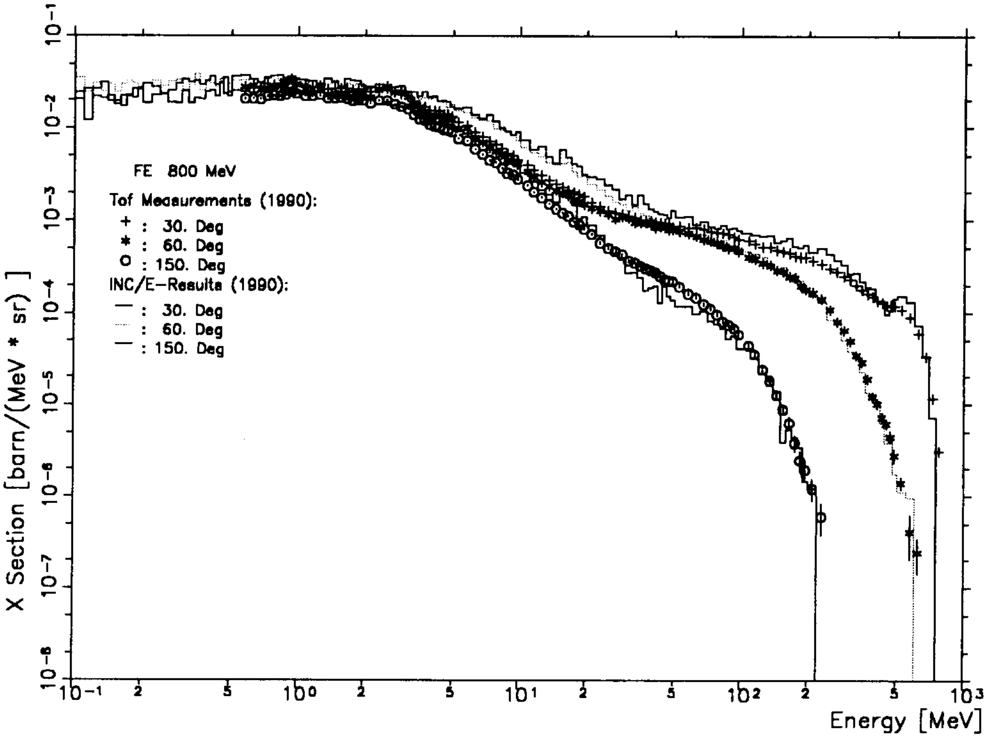


Fig. 1: The HERMES System



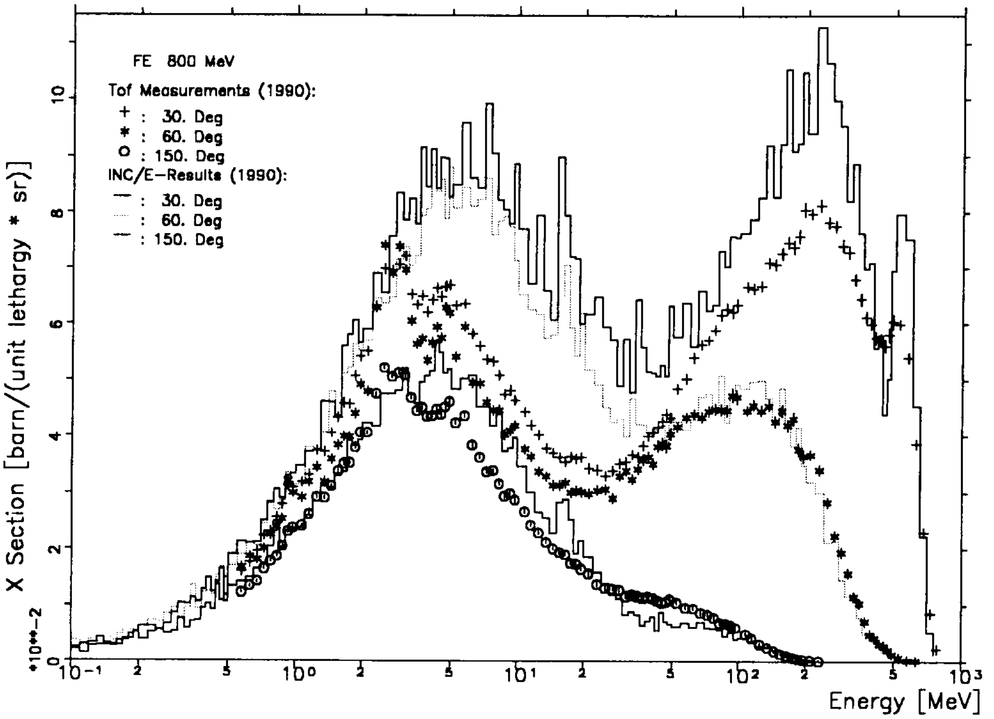


Fig. 2 : Example for the presentation of double differential cross sections of neutrons from 800 MeV protons on iron (above: double logarithmic scale [barns * sr^{-1} * MeV^{-1}]; below: linear-logarithmic scale [barns * sr^{-1} per unit lethargy])

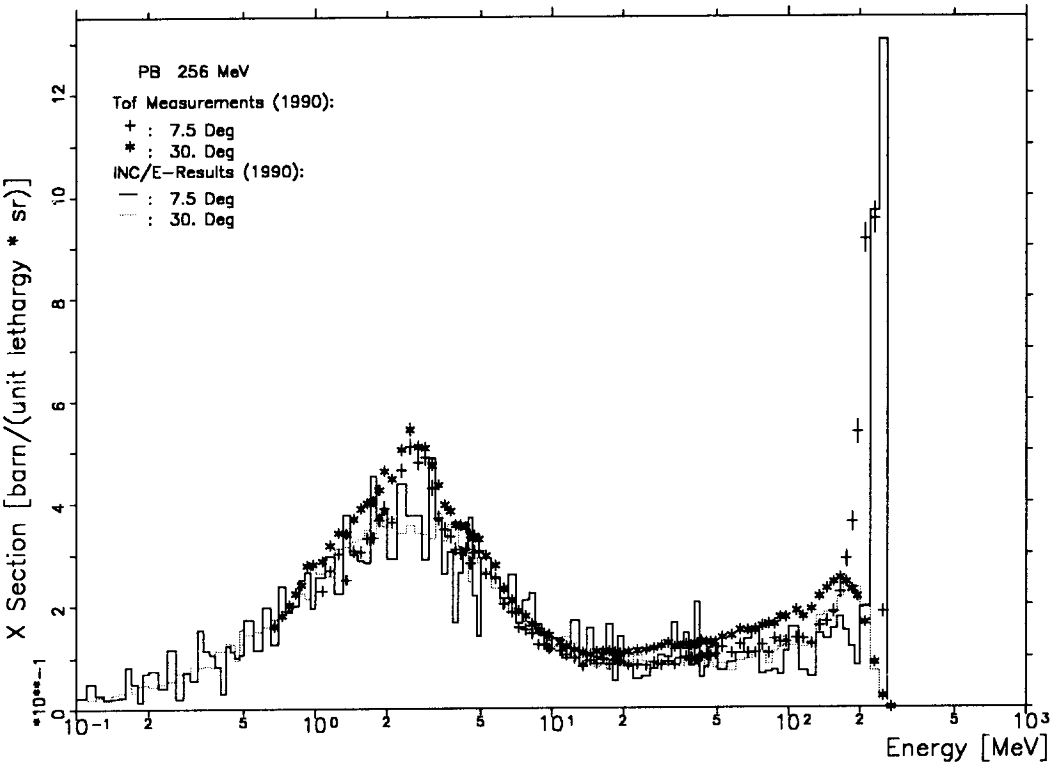


Fig. 3a : Neutrons from 256 MeV protons on lead

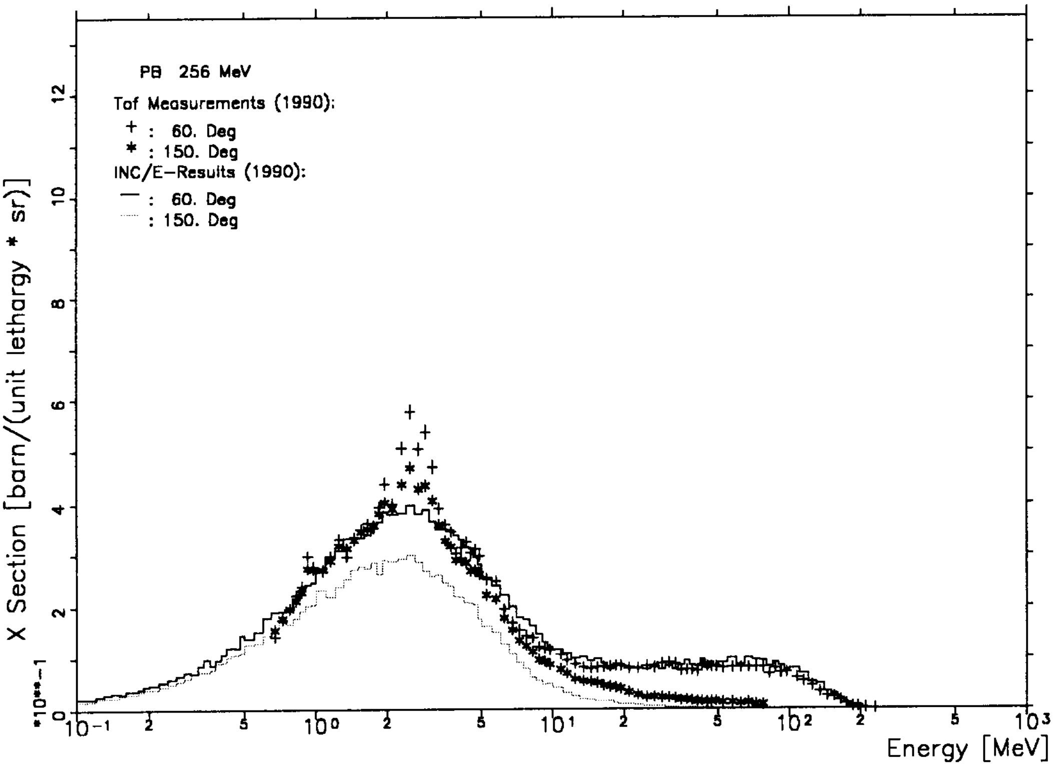


Fig. 3b : Neutrons from 256 MeV protons on lead

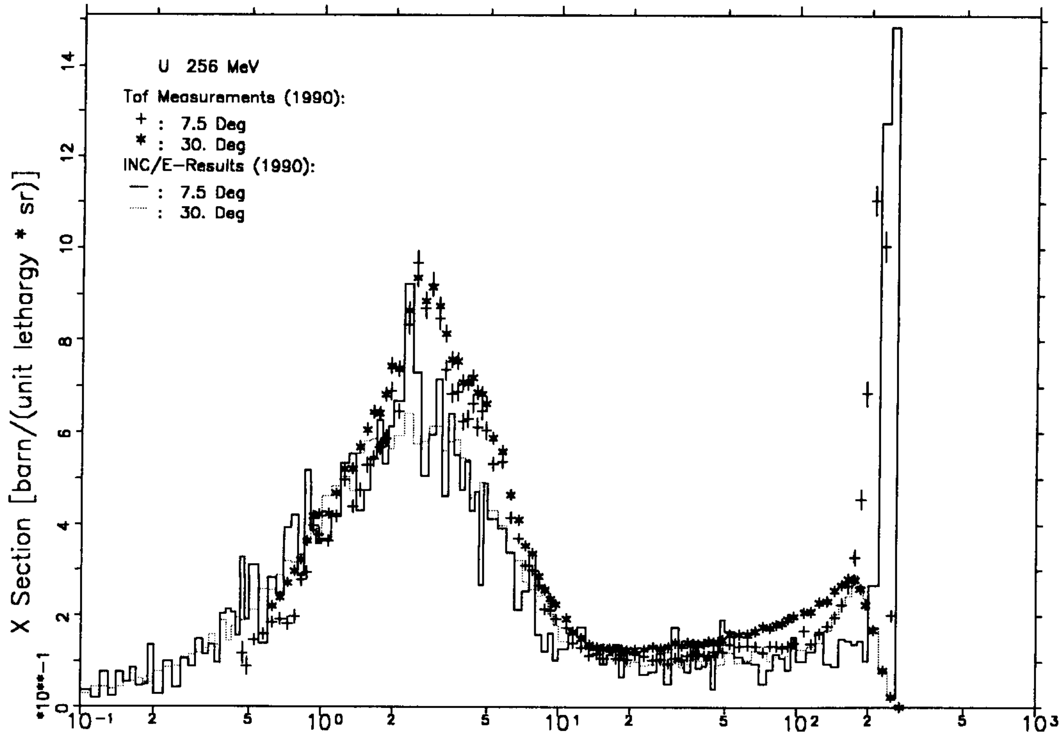


Fig. 4a : Neutrons from 256 MeV protons on uranium

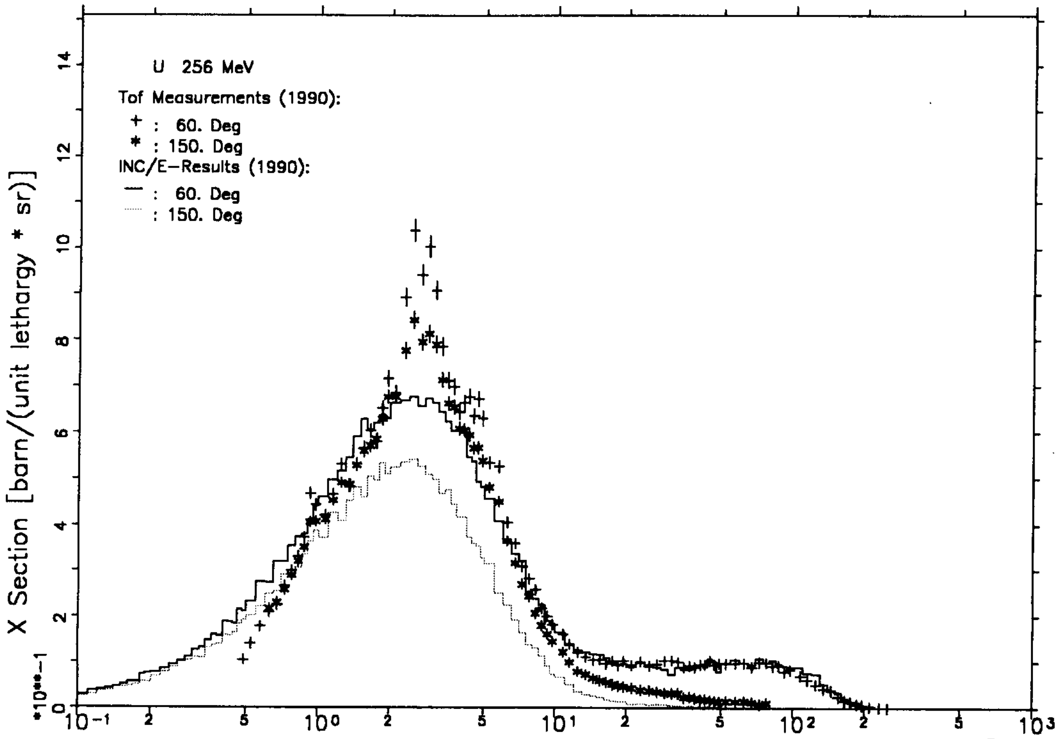


Fig. 4b : Neutrons from 256 MeV protons on uranium

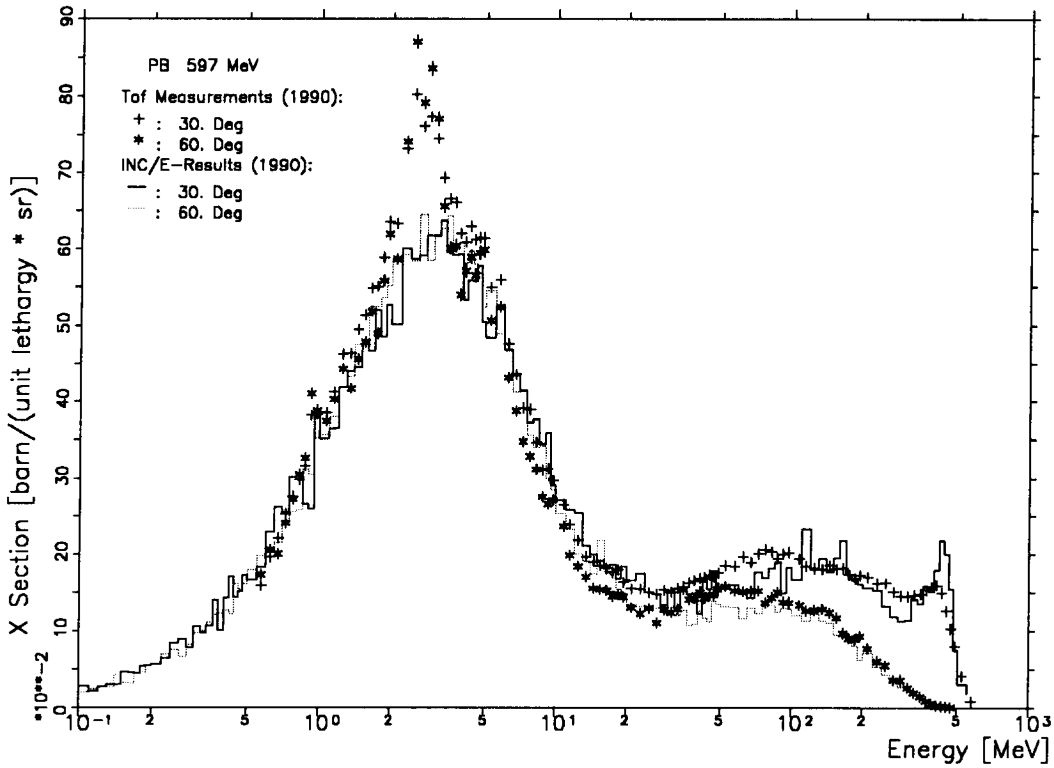


Fig. 5a : Neutrons from 597 MeV protons on lead

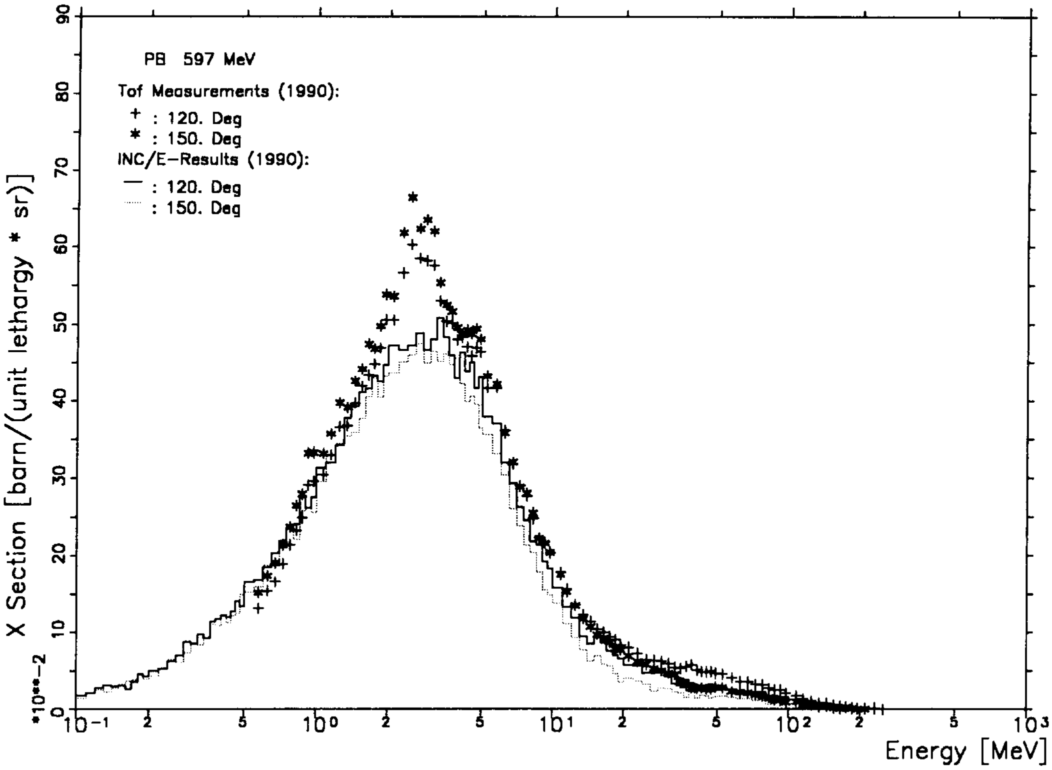


Fig. 5b : Neutrons from 597 MeV protons on lead

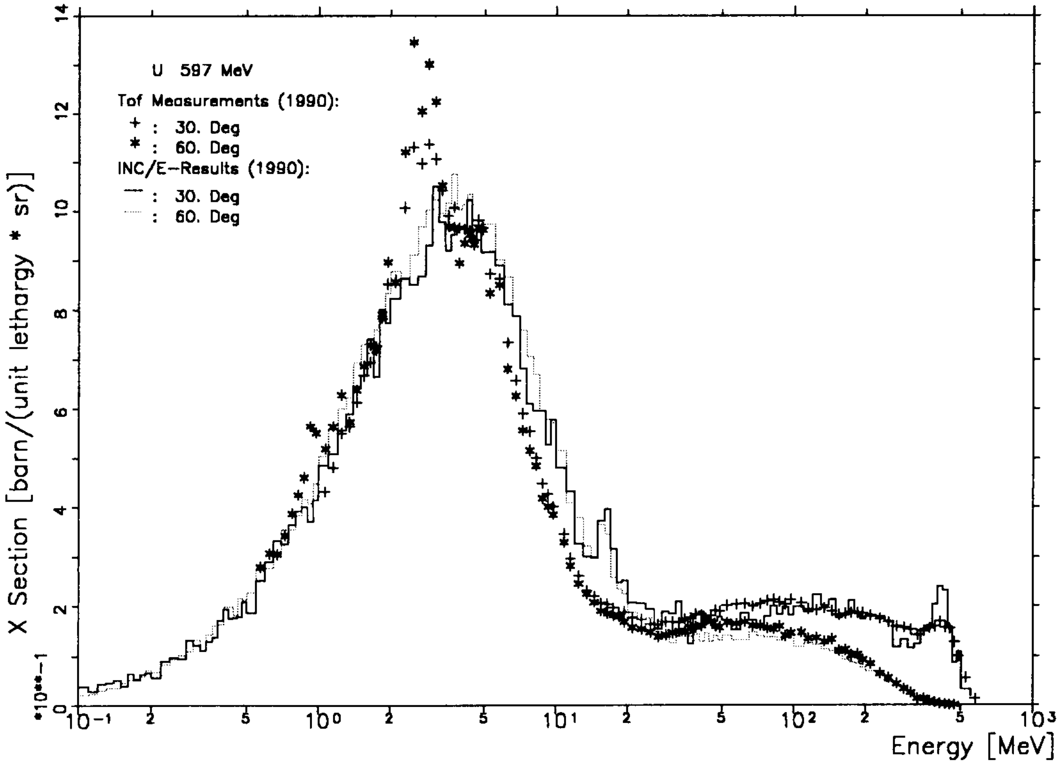


Fig. 6a : Neutrons from 597 MeV protons on uranium

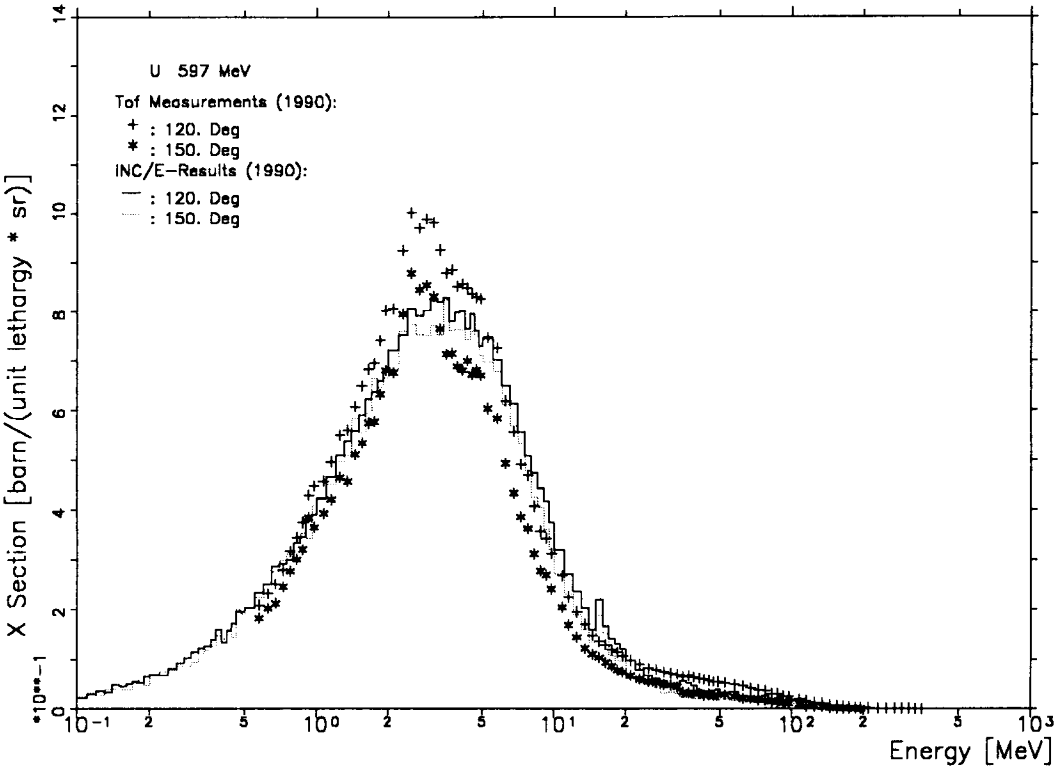


Fig. 6b : Neutrons from 597 MeV protons on uranium

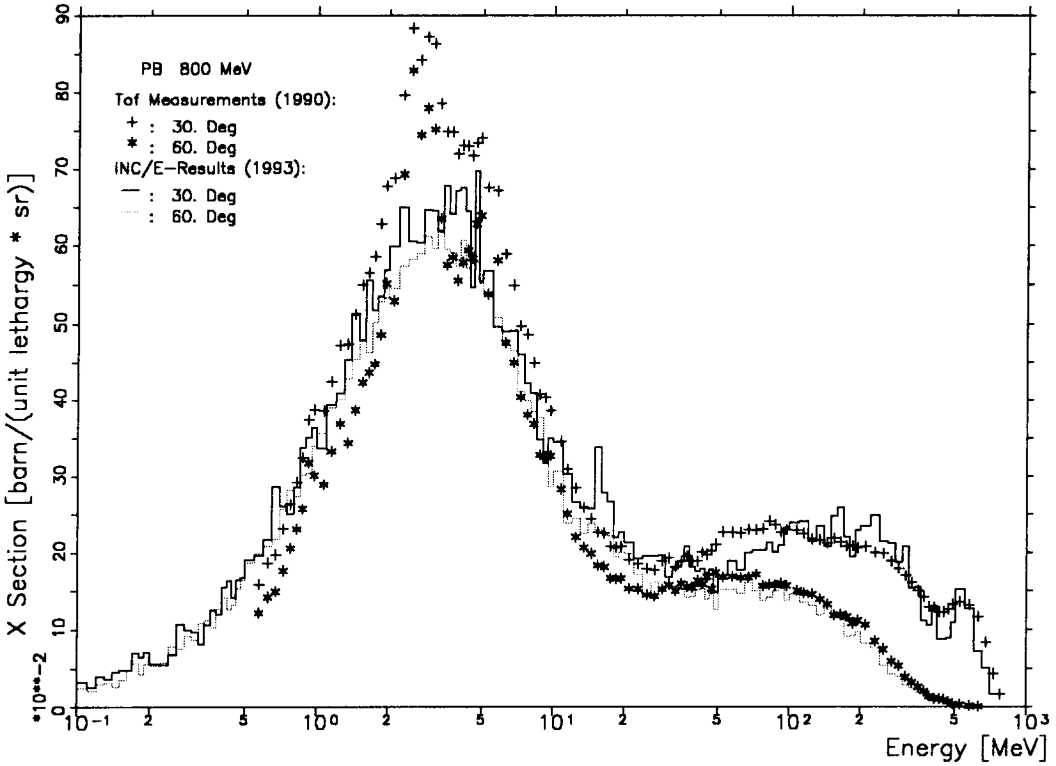


Fig. 7a : Neutrons from 800 MeV protons on lead

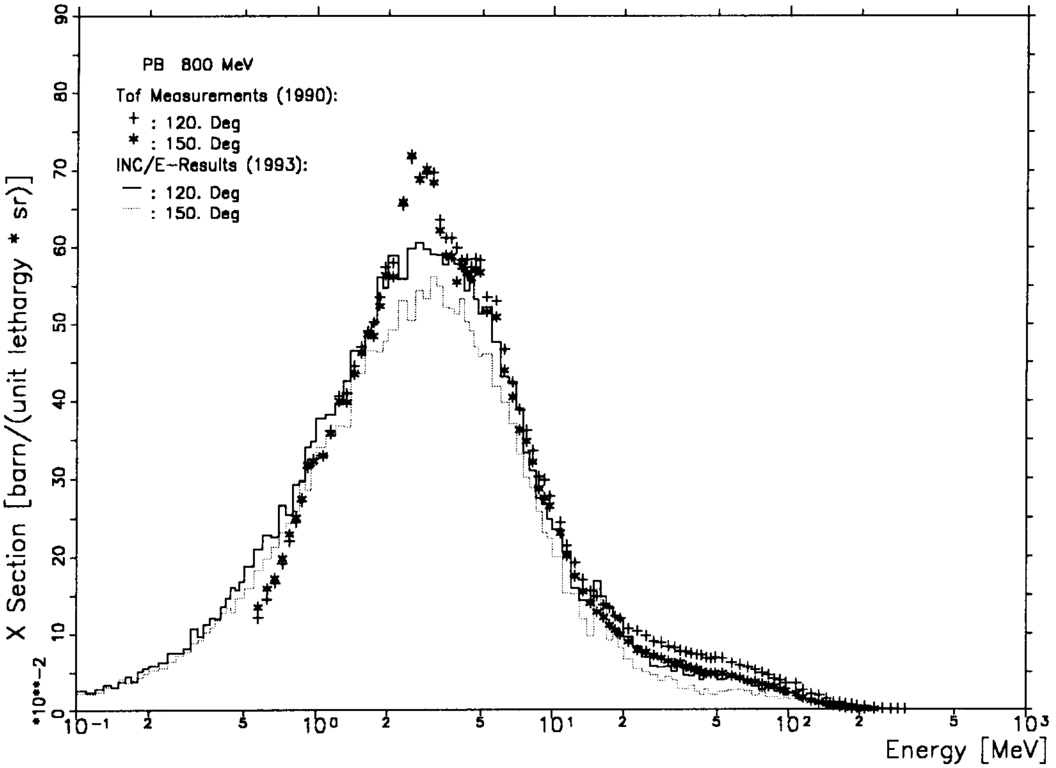


Fig. 7b : Neutrons from 800 MeV protons on lead

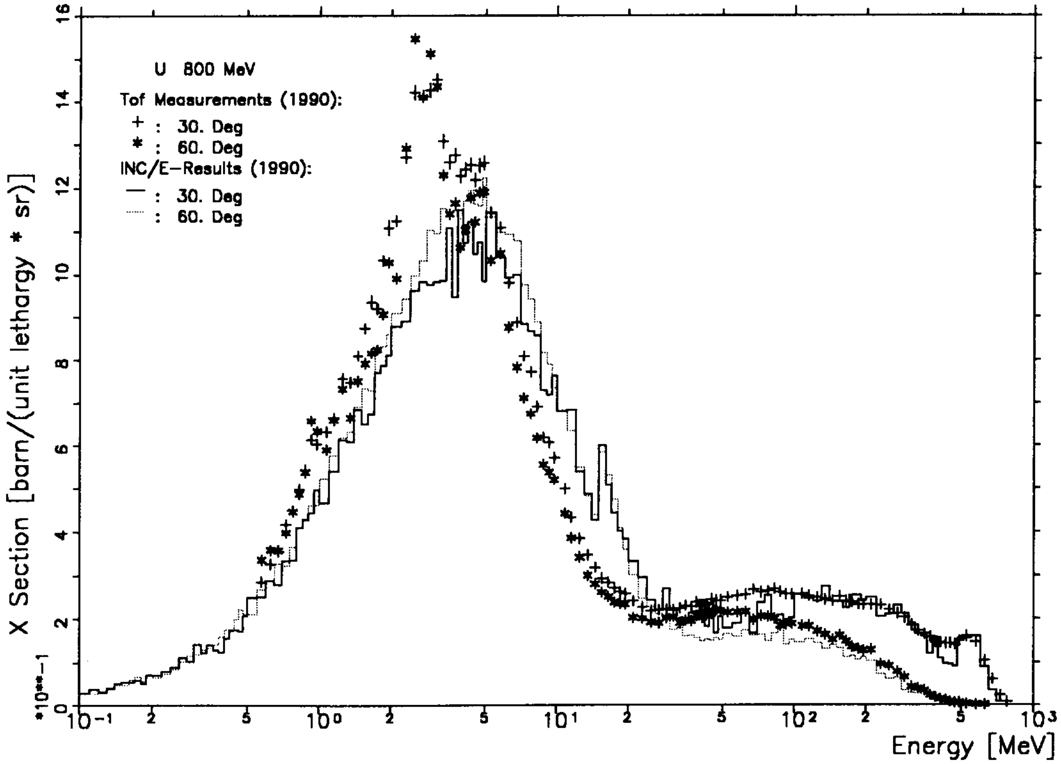


Fig. 8a : Neutrons from 800 MeV protons on uranium

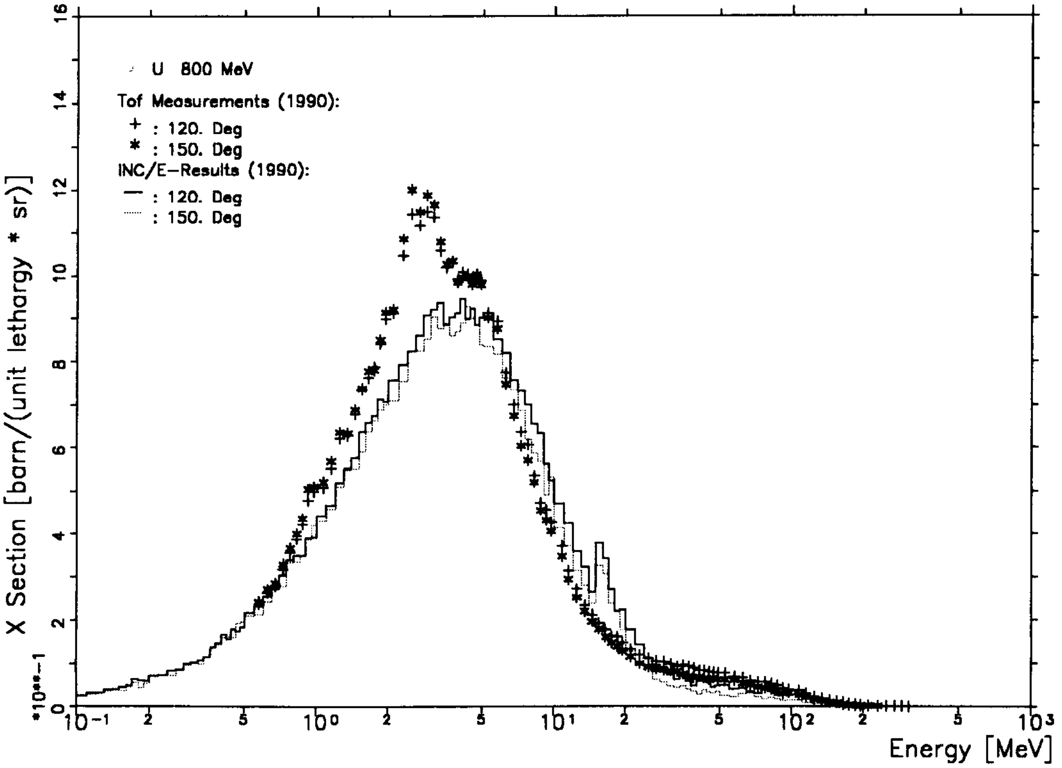


Fig. 8b : Neutrons from 800 MeV protons on uranium