MEDIUM ENERGY NUCLEAR DATA FOR APPLICATIONS

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<u>Abstract</u>: The types of medium energy nuclear data required for applications are discussed. Features of analysis tools, consisting of both detailed nuclear model codes and simple formulas based on nuclear systematics are presented. The activities of the Medium Energy Nuclear Data Working Group (MENDWG) are described including the recent benchmark comparison of nuclear model codes.

Introduction

Many applications, that include space science, spallation neutron sources, ion therapy, isotope production, radiation damage and accelerator shielding, need medium energy nuclear data. The medium energy range for applications extends from above fission and fusion energies, say tens of MeV to about 1000 MeV. The boundaries are not fixed. Nucleons and light nuclei through alpha particles, form the main primary beams and, together with photons, the secondary radiations encountered. Heavy ions, which are used for producing new isotopes and form a small but significant fraction of cosmic rays are also important. Primary electrons and photons will not be considered here.

The data types of most interest include total; elastic; nonelastic; photon and particle emission and residual nuclide production cross-sections. These cross-sections may be needed as doubly or singly differential energy and angular dependent data or in wholly integrated form.

This paper presents a brief survey of the data base available, examples of analysis methods and describes the international cooperation of the Medium Energy Nuclear Data Working Group.

Bibliography

Specialized indexes to bibliography help the scientist to keep up with his field and catch up with new subjects of interest. Several indexes are relevant to medium energy nuclear data. These are the INIS-ATOMINDEX/1/, The Computerized Index to Neutron Data (CINDA)/2/, Nuclear Structure References (NSR)/3/, Integral Charged Particle Bibliography (ICPND)/4/, and Heavy Ion Reactions (HIR)/5/. In addition, these data are covered in several reports/6,7,8/ not issued on a regular basis.

Experimental Data Base

The long standing importance of neutron data to basic research and nuclear power programs resulted in the rather complete compilation and distribution/9/ of neutron data files in an international exchange format, EXFOR. More recently, charged particle data, on a limited basis, is also contained in these files. Atlases containing the results of several measurements of the same quantity in tabular or in graphical form, possibly combined

with eye guides, evaluations, or nuclear model calculations, are useful to show what and how well nuclear data are known. The neutron data contained in EXFOR extends above 1 GeV. A recent atlas containing data to 200 MeV, Neutron Cross Sections, Volume 2/10/, has just been published and will be discussed at this conference. More than 4000 charged particle data sets extending above 20 MeV have been compiled and are available in EXFOR. However, most atlases/11,12,13,14/ containing charged particle are very dated and contain few medium energy data.

Nuclear Systematics

Before discussing model codes that calculate nuclear data from first principles and few if any empirically determined parameters, trends observed in the experimental data that can be described by simple physical or parametric models will be presented. These facts are called nuclear systematics.

Experimental data and eye guides/15/ for the proton nonelastic or reaction cross-section are shown in Figure 1. The reaction cross-section over a mass range from A=9 to 208 has a giant resonance peak around 30 MeV and a slight minimum around 300 MeV. The proton nonelastic cross-section as a function of mass A and energy E (in MeV) above 20 MeV can be closely fit by the equation/16/

$$\sigma_{ne} = 45A^{0.7}f(A)f(E)$$
 mb, where (1)
 $f(A) = 1+0.016 \sin(5.3-2.63 \ln A)$
 $f(E) = 1-0.62e^{-E/200}\sin(10.9E^{-0.28})$

At energies above the coulomb barrier the neutron nonelastic cross-section is about the same as the proton nonelastic cross-section. The total neutron cross-section, comprised of the nonelastic plus elastic scattering cross-section, as shown in Figure 2, shows a systematic shift in energy of the giant resonance for different atomic masses due to the nuclear Ramsauer effect/17/. A semi-empirical formula, similar to Equation 1 can be used to fit the neutron total cross-section over a wide energy and mass range as shown in Fig. 2/18/.

Semiphysical evaporation shapes/19,20/ can be used to fit experimental neutron emission spectra from proton induced reactions. These data are observed to vary nearly monotonically with increasing energy, mass, and angle. The

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computer code PNEM/21/ parameters were empirically determined/22/ for the energy range about 590 MeV as shown in Figure 3 for Fe. Using simple extrapolations good agreement between calculation and experiment was also found at 318 and 800 MeV as shown in Figure 4.

Energy and mass dependent parameterizations have recently been developed for the nucleus-nucleus/23/ nonelastic or absorption cross-sections that agree to within 10 percent of a more detailed model/24/. The equation for the absorption cross-section of a projectile p bombarding a target t is

$$\sigma_{abs} = \pi r_0^2 \beta(E) (A_p^{1/3} + A_t^{1/3} - \delta)^2$$

$$\beta(E) = 1 + 5/E$$

$$\delta = 0.2 + 1/A_p + 1/A_t - 0.292e^{-E/792} \cos(0.229E^{0.453})$$

$$r_0 = 0.126 \times 10^{-12} \text{ cm}$$

$$E = \text{MeV per nucleon}$$
(2)

For large incident energies the equation assymptotically becomes energy independent. An example comparison of calculations with experiment for carbon-carbon collisions is shown in Figure 5.

There are also recent semi-empirical models developed to estimate the isotopic product yields from proton/25/ reactions and from heavy ion fragmentation/26/ reactions. The latter approximates the results from a detailed optical model reaction theory/27/.

Nuclear Model Codes

Medium energy nuclear model codes generally consist of two types, (1) a closed form preequilibrium plus evaporation model, and (2) an intranuclear-cascade and evaporation model. An example of the first type of code is ALICE/28/ which uses Weisskopf-Ewing evaporation, Bohr-Wheeler rotating drop fission competition and the excition preequilibrium models to describe nuclear reactions. Another example is GNASH/29/. Examples of the second type of code are various versions of the high energy transport code HETC/30/ which are extensions of the Bertini/31/ model. Both ALICE and HETC attempt to physically model nuclear reactions and rely on very few empirically determined parameters.

The algorithm solution for ALICE is deterministic, for which a given set of input produces a unique answer, and the algorithm solution for HETC is stochastic, for which a given set of input produces a statistically determined answer whose convergence improves as the number of trials is increased. Several nuclear models/32/ of these types are used to calculate nuclear data. These codes and others may be referred to in several abstracts/33-36/.

The nuclear modelling of intranuclear

The nuclear modelling of intranuclear cascade codes like HETC includes more particle-particle kinetics than preequilibrium codes like ALICE. The development of HETC has been primarily based on physics data above 100 MeV whereas the development of ALICE has been primarily based on nuclear reaction physics data below 100 MeV. The HETC model calculations are expected to be valid only above 150 MeV where the nucleon de Broglie wave length is lower than the mean free path in the nucleus. However, when measured high energy spallation neutrons

with experiment as indicated by the Fe-56(p,n) data in Figure 6.

from the reaction of 590 MeV protons with Fe are

compared with intranuclear cascade calculations, the high energy neutrons in the backward and in

ALICE calculates cross-sections up to 300 MeV. If its algorithms are extended to higher energies with empirical corrections to the optical model nonelastic cross-section, the code

can be used for high energy calculations. ALICE

also underestimates back angle neutrons emitted from proton induced spallation reactions but calculations of activation products can agree

some cases the forward directions are underestimated by calculations/37/. The code

For deuteron induced reactions, a projectile stripping model was added to the GNASH code resulting in favorable comparisons between calculation and experiment for neutron emission data/38/.

Data Files

A nuclear data file is useful in two ways. Cross-section data are stored and accessed as needed instead of being calculated on demand by lengthy deterministic or Monte Carlo nuclear model calculations. This cannot only save time, but also yield unique cross-section values compared to Monte Carlo cross-section calculation methods. The file of reference cross-sections can also be used for sensitivity studies where the effect on calculated results due to discrete changes in input data are observed. This aids cost-benefit analysis since only those data that significantly effect applications need to be seriously reviewed and improved where necessary.

Preliminary evaluations of neutron and proton cross-sections for Fe-56 are available/21/ in the new ENDF-6 formats for review of the adequacy of both data and formats. The data cover the energy range to 1000 MeV. The evaluations contain cross-sections of the following types: total (neutron induced only); elastic scattering (nuclear); nonelastic; product yields; and neutron (double differential), gamma, proton, deuteron and alpha production.

International Cooperation

In 1986, the National Nuclear Data Center at Brookhaven National Laboratory was sponsored to organize the Medium Energy Nuclear Data Working Group (MENDWG) in order to benefit from inter-laboratory, interagency, and international exchange of information. The Summary and Recommendations/38,39/ of the two meetings held so far have been issued. The Summary and Recommendations are divided into four parts:

1) Applications and Data Requirements, which serve as the driving force for determining what information is needed; 2) Codes and Models, which when validated, generate data libraries or

are used directly in transport calculations; 3) experiments, which can be used directly as a source for evaluated data or as benchmarks for the validation of nuclear model codes that generate nuclear data; and 4) Data Files, which store information in computerized formats for

repeated use.

In 1987, MENDWG selected five medium energy proton reaction cases for benchmarking nuclear model codes. The quantities calculated are isotopic activation yields for 180 MeV protons on Al and 40-200 MeV protons on Co, and double differential neutron emission spectra from Al, Zr-90 and Pb-208 for 35, 80, 160, 318, and 800 MeV proton bombardment. An example of the results/40/ for 160 MeV proton induced neutron emission at 30° is shown in Figure 7. There is very close agreement between two revisions of the HETC code, one is labeled HETC-F or TIERCE from Bruyeres-le-Chatel and the other is labeled HETC-H or HETC-KFA-2 from KFA in Juelich and there is fair agreement among all the codes in this case. For other cases, particularly for back angle emission, the code results can be widely different. Important for consideration is that codes based on nuclear systematics have running times of the order of seconds, deterministic nuclear model codes of the order of minutes and stochastic codes of the order of

REFERENCES

ATOMINDEX, INIS Issued semimonthly. Available from Division of Publications, International Atomic Energy Agency, P.O. Box 100, A-1400 Vienna, Austria. In the U.S., from UNIPUB, P.O. Box 1222, Ann Arbor, MI 48106

CINDA, the Index to Literature and Computer

Files on Microscopic Neutron Data. Availability same as Ref. 1. Nuclear Structure References, S. Ramavataram. Supplements published 4monthly as Recent References issues of the Nuclear Data Sheets journal published by Academic Press. See also the Reaction Index, same publication.

Integral Charged Particle Nuclear Data Bibliography, N.E. Holden, S. Ramavataram, and C.L. Dunford. See BNL-NCS-51771. Information is derived from Ref. 3. Annual

supplements.

Heavy-Ion Reactions, A Current Awareness Bulletin. Updates to the US-DOE Energy Data Base. Issued semimonthly on heavy-ion (A>4) reactions. Available from National Technical Information Service, Springfield, VA 22161 as PB87-900500.

Sections Proton-Nucleus Cross of Interactions at High Energies, NRL Report 7593, Dec. 21, 1973 - R. Silberg and C. H.

- Annotated References on Neutron and Photon Production from Thick Targets Bombarded by Charged Particles, Atomic Data and Nuclear Data Tables 32, 471 (1985) - T. Nakamura
- and Y. Uwamino.

 Bibliographic Survey of Medium Energy
 Inclusive Reaction Data E. D. Arthur, D. M. McClellan, and D. G. Madland. LA-10689-PR (1986).
- Data compiled and exchanged in the international exchange format, EXFOR, are available to requestors from the following

regional centers or national centers within regional centers.

U.S. and Canada: National Nuclear Data Center, Brookhaven National Laboratory,

Building 197D, Upton, NY 11973 OECD Countries: Nuclear Energy Agency Data Bank, 91191 Gif-Sur-Yvette, Cedex, France USSR: For Charged Particles- CAJaD, Inst. Atomnoi Energii I.V. Kurchatova, 46 Ulitsa Kurchatova, Moscow, D-182, USSR For Neutrons- CJD, Inst. of Physics &

Energetics, Obinsk, Kaluga Region, USSR Others: IAEA Nuclear Data Section

P.O. Box 200, A-1400 Vienna, Austria V. McLane, C. Dunford, P. Rose, "Neutron Cross Sections," Volume 2, The Book of

- Cross Sections," Volume 2, The Book of Curves. Published by Academic Press 1988.

 N. Jarmie and J. D. Seagrave. "Charged Particle Cross Sections." LA-2014 (1956).

 D. B. Smith, N. Jarmie and J. D. Seagrave. "Charged Particle Cross Sections, Neon-Chromium." LA-2424 (1961).

 F. K. McGowan, et al. "Nuclear Cross Sections for Charged-Particle Induced Reactions Mn, Fe, Co. ORNL-CPX-1 (1964).

 Also, Nuclear Cross Sections for Charged-Particle Induced Reactions Ni. Cu. ORNL-Particle Induced Reactions Ni, Cu. ORNL-CPX-2 (1964).
- H. Muenzel, et al. "Karlsruhe Charged Particle Reaction Data Compilation". Physik Daten 15-Index (1979-1982).
- 15. P.U. Renberg et al., Nucl. Phys. A183, 81. (1972).
- J. L. Letaw, R. Silberberg and C. H. Tsao. Astrophys. J. Suppl. Ser., 51, 271 (1983). J. J. Peterson, Phys. Rev. 125, 955 (1962). Proceedings of the Conference on High Energy Radiation Background in Space, Sanibel Island, Florida-Nov. 3-5, 1987. In
- Press. T. Nakamura, Nucl. Instr. Methods Phys. Res. A240, 207 (1985).
- K. Tsukada and Y. Nakahara. Atomkernergie <u>44</u>, 186 (1984).
- 21. S. Pearlstein, Brookhaven Laboratory, Private Comm.
- S. Pearlstein, Nucl. Sci. Eng. 95, 116 (1987).
- L. W. Townsend and J. W. Wilson, Radiation Res. 106, 283 (1986).
- L. W. Townsend and J. W. Wilson, NASA Reference Publication No. RP-1134, 1985.
- R. Silberberg, C.H. Tsao and J. R. Letaw, Astrophys. J. suppl. Ser., 58, 873 (1985).
- J. W. Wilson, L. W. Townsend and F. F. Badavi, Nucl. Inst. Meth. <u>B18</u>, 225 (1987).
- L. W. Townsend et al. Phys. Rev. C34, 1491 (1986).
- M. Blann, Phys. Rev. <u>C28</u>, 1475 (1983) and LLNL Report UCID 20169 (1984).
- P. G. Young and E. D. Arthur, LANL Report LA-6947 (1977).
- HETC, Code package CCC-178, ORNL-4744, Radiation Shielding Information Center, Oak Ridge National Laboratory.
 - H. W. Bertini, Phys. Rev. <u>188</u>, 1711 (1969).
- S. Pearlstein, Chairman, Summary of the Medium Energy Nuclear Data Working Group, Informal Report BNL-NCS-38404 (1986).
- National Energy Software (enter: Software ANL-7411 Abstracts (1986),periodically.
- Nuclear Program Abstracts, Nuclear Energy Agency Data Bank, Regularly Revised. Ref. 9.

- 35. Abstracts of Digital Computer Codes, ORNL-
- RSIC-13, See Ref. 30. 36. Computer Codes, A Bibliography, DOE/TIC-3386 (1985).
- 3386 (1985). 37. D. Filges et al., Phys. Rev. <u>C36</u>, 1988 (1987).
- 38. E. D. Arthur, LANL Progress Report, LA-10915 PR (1987).
- 39. S. Pearlstein, Chairman, Summary of the Medium Energy Nuclear Data Working Group., Informal Report BNL-NCS-40070 (1987).
- S. Pearlstein, An Intercomparison of Medium Energy Cross-Section Codes. In Press.

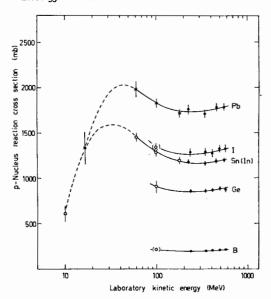


Fig. 1 Proton nonelastic cross-sections. The lines are eye guides.

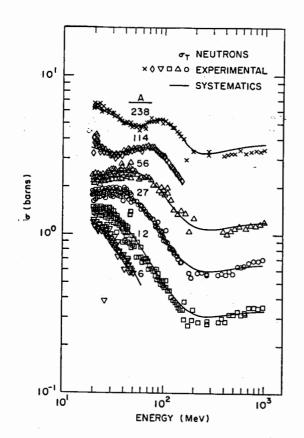


Fig. 2 Neutron total cross-sections. The lines are parametric fits to the data.

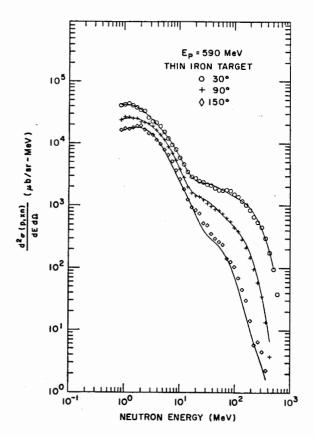


Fig. 3 Neutron emission spectra from 590 MeV proton bombardment of a thin Fe target. The lines are parametric fits to the data.

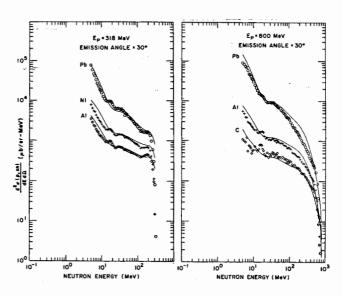


Fig. 4 Neutron emission spectra from 318 and 800 MeV proton bombardment of thin targets. The lines are extrapolated from nuclear systematics.

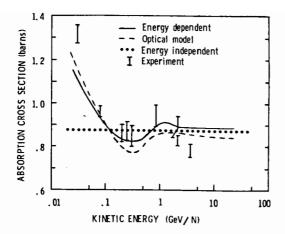


Fig. 5 Absorption cross-section for carboncarbon collisions.

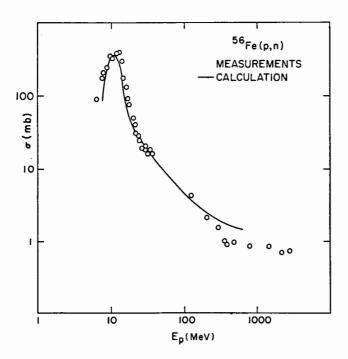


Fig. 6 Comparison between modified ALICE calculations and experiment for the Fe-56(n,p) cross-section.

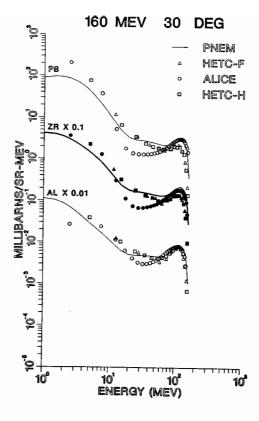


Fig. 7 Benchmark calculation results of neutron emission spectra at 30 degrees from 160 MeV proton bombardment of thin Al, Zr and Pb targets.

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