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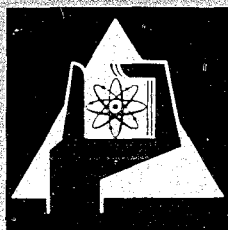
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Organizational and Technical Aspects
in the Field of Neutron Nuclear Data Evaluation

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THE HISTORY OF THE CITY OF BOSTON

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A B S T R A C T

In the field of neutron nuclear data a worldwide organizational and technical effort has developed in the last ten years in the measurement, compilation, and evaluation of all information pertinent to the development and calculation of nuclear reactors. Supraregional committees like the European American Nuclear Data Committee (EANDC) and its various Subcommittees and the International Nuclear Data Committee (INDC) have made substantial contributions to the international organization and coordination of this effort, which resulted in an almost exponential increase of experimental information. The critical judgement and comparison of this vast amount of information and its conversion to unique "best" sets of data is the basic technical problem in neutron nuclear data evaluation. Particular difficulties in the evaluation process are connected with gaps in the experimental information, which have to be closed by reasonable interpolation, by use of some nuclear systematics or by parameterisation of nuclear theories and models, and the often large systematic errors and discrepancies between different experiments, which, for their resolution often involve uncomputerisable human experience, judgement and selection of information. It is only recently that the development of semi-automatic methods of evaluation has been started.

In this report I shall try to give a brief outline of organizational and technical aspects involved in the evaluation of neutron nuclear data. Let me begin with some general explanations of what is meant by evaluation of neutron nuclear data.

The field of evaluation of neutron nuclear data has its origin in the development of nuclear reactors. The neutron physical behaviour of nuclear reactors is described by the Boltzmann neutron transport equation. In this equation neutron cross sections for various scattering and absorption processes and energy and angular distributions of scattered neutrons as functions of the neutron energy occur which have to be known and for which values have to be inserted before a solution of this equation in each particular case can be given.

The question at which neutron energies these data have to be known is most easily answered by considering the neutron energy distributions occurring in nuclear reactors. The source of reactor neutrons is the fission process and the hardest possible spectrum encountered in a reactor or in a reactor experiment is close to the fission neutron spectrum, i.e. the energy distribution of the neutrons liberated in the fission process. This distribution has a convex shape, its maximum lies at a neutron energy of about 0.7 MeV and its average at a neutron energy of about 2 MeV, less than one percent of the neutrons have energies above 10 MeV. The opposite extreme is encountered in so-called thermal reactors, in which the neutrons starting from fission energies have been completely slowed down to those very low energies at which they reach thermal equilibrium with the surrounding nuclei obeying thus nearly a Maxwellian distribution in the meV and eV range. All other reactors populated by intermediate energy or fast neutrons, so-called intermediate or fast reactors, have neutron energy spectra somewhere inbetween the fission and the thermal spectrum. Thus, the total domain of energies covered by reactor neutrons ranges from about 1/10 of a meV to about 15 MeV.

In nuclear physics terms this means that one has to do with the various decay properties of excited quasi-stationary compound nucleus states ranging in position from neutron binding energy ($5 \lesssim E_B \lesssim 10$ MeV) to $E_B + 15$ MeV. Almost coincident with E_B is the thermal energy range in which, beside energy dependent absorption, fission and elastic scattering cross sections, one has to consider chemical binding effects and in particular inelastic energy exchanges between neutrons and the phonon spectrum of the crystal lattice structures of the surrounding medium. Just above the thermal region compound nucleus states are encountered which are still so long living, i.e. whose half widths are still so small compared to their distance that they can be clearly discerned experimentally. These states are called neutron resonances. In light and medium weight nuclei they extend to a few 100 keV, in heavy nuclei to a few 100 eV or a few keV. These resonances decay essentially by γ -ray or elastic neutron reemission, in fissionable nuclei in addition by fission. With further increasing neutron energy the widths and the number of the decay channels and the energy density of the compound nucleus levels increase; this leads to an increased broadening and mutual overlapping of the resonances. In the MeV range of neutron energies the resonances become experimentally indiscernible; only a more or less smoothly energy dependent cross section structure can be observed. The new decay channels that open belong mostly to inelastic neutron scattering to various rest nucleus states, to various endothermic neutron absorption processes like (n,p) or (n,α) and, at higher MeV energies, to three and more particle break-up processes like $(n,2n)$, (n,np) and others.

These few remarks let understand that for a solution of the various reactor physical problems not only energy dependent neutron cross sections, but also individual and average properties of neutron resonances like quantum numbers, half widths for the various decay modes and distribution functions are needed, furthermore nuclear level schemes with regard to neutron inelastic scattering, then various types of data connected with the fission process like numbers of prompt and delayed neutrons liberated in fission and their energy distributions as a function of the neutron incident energy, fission product yields and so on.

It still remains to define what is meant by the term evaluation. In the field of neutron nuclear data it has become usual to make a difference between compilation and evaluation, two notions which in other domains of physics have about the same meaning and are interchangeably used. Compilation means the gathering of experimental references and nuclear data contained in these references for a certain neutron reaction with a given nuclide in a given energy range. Evaluation denotes the critical judgement, comparison and occasionally selection of this compiled information and its elaboration by some averaging procedure into a complete easily interpolable unequivocal set of so-called best or recommended data for further use in reactor physics calculations. The requirement of completeness involves the necessity of using appropriately parameterised nuclear theories or models and nuclear systematics considerations in the case of gaps and inconsistencies of the available experimental information. It also involves, as the neutron, in a given energy range, do not leave out any of the physically possible processes, that all neutron reactions occurring in that range have to be considered. The idea of making a difference between compilation and evaluation is essentially born out by the manner in which the whole process of gathering the required nuclear data information is organized today. Some historical remarks will help us to understand this organisation, its origin and its problems, more clearly.

In the beginning of the reactor development in the fiftieths the interest was centered on thermal reactors and rather crude calculational methods; at that time essentially only the rather small nuclear data information in the range of thermal and low resonance energies was needed. Since the beginning of the sixtieths the interest became more and more focussed on the development of fast and intermediate reactors and thus on the much larger energy range between eV and MeV energies. Simultaneously the modern computer development allowed and forced steadily increasing refinements of the reactor theory methods; these went parallel with and were also provoked by the increasing refinements of the measurement techniques used in experimental reactor physics. These refinements in reactor theory and experiment opened the possibility of much more detailed and reliable predictions of reactor physical properties under the almost only condition that the neutron nuclear data involved be known to sufficient completeness, detail

and reliability over the whole energy range of reactor neutrons. Since then it became indispensable that an evaluation of neutron nuclear data for a given element or isotope had to cover the whole neutron energy range of more than 10 decades from almost 0 to 15 MeV and all possible neutron reactions occurring in that range.

It is particularly to be emphasized that the accuracy, to which the knowledge of neutron data is requested by the reactor physicists, is quite unusually high and makes very high demands on accurate experimental techniques and careful evaluation. As a typical illustration let us quote a 1% inaccuracy in the number of fission neutrons and a few % inaccuracy in the fission cross section of a typical fissionable material like Pu²³⁹ over the most important neutron energies. From the experimental point of view these inaccuracies must already be considered as very small. On the reactor physics side, however, they may involve an inaccuracy of, say 3% in the neutron multiplication factor of a typical fast power reactor. This in turn means an uncertainty in the critical Pu²³⁹ mass of this reactor of about 150 kg or, for a 10 \$ per g price of Pu²³⁹, an uncertainty in the capital investment of 1.5 Mio \$. This is still a small quantity compared to the total capital cost of a fast power reactor and thus not the worst consequence. What may, however, happen, in the case of an underestimate of the critical mass, and what is much worse is that the reactor cannot be put into operation at all, because not enough Pu²³⁹ is available and because the technical design is fixed to the lower critical mass.

Already in the years around 1960 the requirement of a comprehensive nuclear data basis for reactor calculations became important particularly with the onset of the development of fast reactors, and first more comprehensive evaluation work began particularly at Livermore in the US, at Aldermaston in the UK and at Karlsruhe in Germany. In these first studies the necessary literature references and the data information contained in these references had to be collected in a very cumbersome procedure so to say by hand. At once huge gaps in the experimental information became apparent: for important nuclei the parameters of only few resonances were known, the knowledge of inelastic level excitation cross sections was still very sparse and that of elastic scattering angular distributions still insufficient, to give only a few typical examples. Simultaneously

there was still almost no coordination between reactor physicists, evaluation physicists and experimental and theoretical nuclear physicists: in particular the nuclear physicists did not know enough about the data needs of the reactor physicists.

In order to remedy this bad situation in 1959 the Tripartite Nuclear Cross Section Committee (TNCC) was founded in which the USA, UK and Canada participated. One year later in 1960 this committee was enlarged to the European American Nuclear Data Committee (EANDC) in which now all OECD countries participate. A similar increasingly important role is played by the International Nuclear Data Committee (INDC) which arose in 1967 from the International Nuclear Data Scientific Working Group (INDSWG). This committee works on a worldwide basis which comprizes not only the OECD, but also the Non-OECD countries. I would like to concentrate myself on the role the EANDC has played and still plays in the supraregional organization and coordination of nuclear data experimental, compilation and evaluation work. I should merely mention that the EANDC has regional subcommittees e.g. in North America, UK and Euratom countries which in their respective domains fulfill similar tasks as the EANDC and which report to the EANDC. The EANDC meets about all nine months, the Euratom Subcommittee for example every year.

One of the first and still continuing most important actions of the EANDC consisted in assembling after critical judgement the nuclear data requests from the reactor physicists in comprehensive lists and in making widely available these request lists among experimental nuclear physicists. These continuously updated request lists contain the neutron nuclear data to be measured for given elements and energy ranges, they specify in addition the desired experimental resolution, accuracy and priority according to the needs on the reactor physics side. In order to help to fulfill these requests the EANDC discusses and stimulates measurement techniques and the establishment of new experimental groups and apparatus; it states and helps in satisfying isotope and sample needs for measurements; it simultaneously tries to coordinate and distribute the experimental work along various research lines and according to the experimental capabilities and experiences of the various laboratories.

As a first result of these efforts of the EANDC during the last years new experimental facilities, particularly electron linear accelerators and Van de Graaff machines, were built in many laboratories, and the experimental conditions, in particular the energy resolution, were very much improved. The consequence of this large progress on the experimental side was a very rapid, almost exponential increase in the amount of data produced.

Let me give some typical examples in order to characterize this situation. With a strong neutron source like a modern electron linear accelerator and high resolution experimental techniques like the neutron time-of-flight method one resolves of the order of a few 100 resonances in individual nuclei. A single such measurement commonly yields several 1000 data points; for the more important nuclei like e.g. Au¹⁹⁷ or Pu²³⁹ a whole series of such measurements is available. Typical inelastic scattering experiments cover the cross sections for excitation of, say, 10 different nuclear levels over a larger neutron energy range, typical elastic scattering angular distribution measurements cover of the order of 10 different angles at 20 or 30 neutron energies. This data explosion created a series of new problems as the on-line conversion of the experimental raw data like counts per channel into cross section data, the computerised parametric analysis of neutron resonance measurements by the experimenters themselves and in particular the question arose of how to make this vast amount of data available to the reactor physicists.

Firstly this latter question was a problem of how to get the data together and how to make them available in an appropriate form to evaluation physicists, i.e. a problem of data compilation. To make a long story short I would like to quote only the conclusion: the problem of compiling references and data on neutron nuclear interactions can be regarded as solved in principle on a worldwide basis by the creation and cooperation of four neutron nuclear data centres, i.e. the National Neutron Cross Section Centre (NNCSC) at the Brookhaven National Laboratory, which evolved from the old Brookhaven Sigma Center, the ENEA Neutron Data Compilation Center (CCDN) at the IAEA in Vienna and the Nuclear Cross Section Information Centre at Obninsk in Russia. Each of these centres is responsible for the collection

of data information including a reference index (CINDA = Card index of nuclear data) from laboratories in a certain region - the Brookhaven NNCS for US and Canada, the Saclay CCDN for the rest of the OECD countries, the IAEA NDU for the Non-OECD countries, the Obninsk Center for Russia - and to make available this information upon request in a form appropriate for further evaluation, e.g. on punched cards or magnetic tapes. Meanwhile about 10^6 data points have been accumulated particularly by the Brookhaven and Saclay Centres and 50000 references through a worldwide extended system of literature readers.

Secondly this was and is still the major problem of how to convert this huge and often diversified information into unique best data sets which then form the data input of reactor calculations, this means it was a problem of data evaluation and of the establishment of computer libraries of evaluated data. In order to reach this target the evaluation effort itself was much intensified in the already existing groups, and a series of new groups was created, partly working in close bilateral cooperation or contract with the already existing groups. Such cooperations developed between a French group at Cadarache and the British group at Aldermaston, between a group at the Technion Institute at Haifa in Israel and the German group at Karlsruhe, to give only two typical out of many examples. Computer formats for evaluated nuclear data libraries were developed particularly at Aldermaston in the UK, at Brookhaven in the US and at Karlsruhe in Germany. The organization of the evaluation effort in the US serves particular mention and is typical for the organization of this work also in other countries. In 1966 a Cross Section Evaluation Working Group (CSEWG) was founded at Brookhaven with members coming from about 15 different laboratories and industrial firms representing each small evaluation groups. Each of these groups got the task to evaluate or to take over from other data libraries complete neutron nuclear data sets and to store or convert them to the ENDF/B (Evaluated Nuclear Data Format B) format developed before at Brookhaven. Furthermore subcommittees were created for further physical microscopic testing of data evaluations, for evaluation of reactor shielding nuclear data, and for the testing of the reliability of evaluated data sets by comparison of reactor calculations based upon these data with the results of integral reactor physics experiments. The iterative feedback from those tests and comparisons are reevaluations and steady improvements of the already existing libraries.

Due to the extensive discussions and recommendations of especially created study groups like the EANDC Compilations Study Groups in America and Europe and the EANDC/EACRP^{##} Joint Subcommittee on Nuclear Data Evaluation also some supraregional cooperation and coordination evolved. I may particularly mention the systematic collection of evaluated nuclear data files in the Saclay and Brookhaven Compilation Centres, the exchange and distribution of these files upon request, furthermore the establishment and regular updating of a computer list of existing evaluation work with a very wide distribution.

This picture of organizational successes in the nuclear data field would not be complete without the explicit mention of several large conferences held upon the recommendation and/or with the sponsorship especially of the EANDC. I may mention particularly the Conference on Neutron Time-of-Flight Methods at Saclay in 1961, the International Conference on the Study of Nuclear Structure with Neutrons at Antwerp in 1965 both sponsored by the EANDC and the Conference on Nuclear Data for Reactors in Paris in 1966 organized by the IAEA. Also the two Conferences on Neutron Cross Sections and Technology in Washington in 1966 and 1968 found a wide attention and participation. These conferences, which more or less covered as well the fundamental as the applied aspects of neutron physics measurements and evaluation including the reactor physics points of view, were of great value in bringing nuclear, evaluation and reactor physicists together and helping them to understand each other's problems.

The largest and partly almost insolvable difficulties, however, reside in the evaluation process itself. This is by far not only a matter of the large amount of data to be handled, but still more a consequence of the large difficulties involved in neutron nuclear data measurements which in turn show up in often large systematic errors and discrepancies. Take as a typical example two different relative measurements of the same resonance fission cross section performed with different energy resolutions: these measurements may be differently normalized; they may show differences in the energy scales, in the number of resonances resolved, in the statistical scatter of the data and in the background of radioactive decay α -particles and of backscattered neutrons; they may differ in the corrections for

^{##}EACRP = European American Committee on Reactor Physics.

multiple scattering and neutron beam attenuation in the sample; they may finally differ in the theoretical interpretation in terms of resonance parameters. Whereas in the ideal case measurements performed under the same experimental conditions and being subject only to statistical errors can simply be averaged by least squares or other adjustment procedures, this is generally not possible with systematically discrepant measurements, when the sources of these discrepancies cannot be removed.

In the simplest case such discrepancies in relative measurements are due to a normalization to wrong standard values and may be resolved by correction of the standard values and renormalization of the measured data. However, in spite of a very large effort - I would like to mention here particularly the excellent work performed at the Central Bureau for Nuclear Measurements at Geel in Belgium - the cross section values for those reactions as $\text{Li}^6(n,\alpha)$, $\text{B}^{10}(n,\alpha)$ or $\text{U}^{235}(n,f)$ or the average number of neutrons liberated in spontaneous fission of Cf^{252} commonly used as standards in neutron nuclear data measurements are still not known to sufficient accuracy. Sometimes those systematic discrepancies can be univoquely resolved in favour of one particular measurement, if still other independent, easier measurable and therefore better ascertained information can be used for a decision. The use of experimental nuclear neighbour systematics is restricted in its reliability, because due to shell and even-odd nucleon effects the properties of neighbouring nuclei are not a smooth function of atomic weight and may show variances of the order of the discrepancies considered.

As a consequence evaluation is often not simply a mathematical averaging, but a more or less justified selection among given informations. The human judgement, physical imagination and long experience, which have to be brought into this selection in each individual case, can often not be expressed in logical terms and decisions and can therefore not be explained in a systematic way to a computer. Here much has still to be learned and this is also the main reason, why computerised automatic evaluation is still in the beginning.

Recently a group at Atomic International, in cooperation with IBM people, has begun to develop semi-automatic evaluation procedures in a program called SCORE [1]. This program uses graphical display units developed by IBM and allows continuous man-machine interaction during evaluation.

The experimental data information stored in the computer can be made visible in tabular or graphical form on a screen and can be changed, deleted, corrected and averaged in least squares or spline fits by light pen or typewriter manipulation in desired, programmed ways. This procedure, although still expensive in its present form, promises to replace successfully the eyeguide curves drawn previously through experimental data sets and in addition should speed up in appropriate cases the evaluation process considerably. Also at other places evaluation schemes are under development which try to computerise the main procedures normally used in different ranges of neutron energy and atomic weight [2].

Beside discrepancies still important gaps are encountered in the experimental information in spite of the large experimental progress; fortunately this generally represents not such a large problem. In the case of a smooth energy dependence of a cross section these gaps can easily and rather reliably be closed by mathematical or graphical inter- or extrapolation. Nuclear theories in their present development stage can be physically sensefully parameterised in order to describe successfully the given experimental information adjacent to the gap and can thus be used rather reliably for interpolation. A good example is the optical model which nowadays has been refined to a tool which with appropriate parameterisation allows the reliable prediction of total, total reaction cross sections and of elastic scattering angular distributions within experimental accuracy. The resolved and statistical resonance theories are capable of reproducing almost any measured cross section shape with inclusion of complex interference phenomena in the case of reactions with only one or a few exit channels like scattering and fission. Refined nuclear Fermi gas and evaporation models are available for prediction respectively interpolation of the spin and energy dependences of level densities and of energy distributions of inelastically scattered neutrons. Corresponding computer programs are increasingly developed and used in the evaluation field.

I would like to finish my talk with a few words on the actual status of evaluations and evaluated data libraries. Evaluated microscopic neutron nuclear data sets are now available for the most important elements or isotopes, they are mainly due to work done in the UK, US, Italy, France

and Germany. Not all of them are complete with regard to the reactions and energies covered, only part of them are really updated, because the neutron data compilation centres have only recently come into full operation and, because large amounts of new experimental information are still continuously flowing in. Thus, one is still far away from a complete up-to-date coverage of the periodic system.

Some of this evaluation work has been extensively documented in tables, graphs and physical descriptions. A comprehensive review of references for presently available neutron nuclear data evaluations may be found in the Newsletter No. 5 of the Saclay compilation centre [3]. Particularly illustrative examples are given by the comprehensive documentations of the Aldermaston/Winfrith (see e.g. [4]) and of the Karlsruhe [5] evaluations and data libraries. The well known BNL-325 and BNL-400 prepared by the Brookhaven cross section center [6] since many years are excellent examples particularly for a documentation of compiled experimental data. These works and documents have provided the field of neutron nuclear data compilation and evaluation a wider acknowledgement in the nuclear scientific community and have made it a new branch within applied nuclear science.

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