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ASPECTS OF CRITICAL EVALUATION OF NUCLEAR DATA INFORMATION

J.J. Schmidt
Nuclear Data Section
International Atomic Energy Agency

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Abstract

In this report some aspects of critical evaluation of nuclear data information are discussed particularly in relation to the data needs of nuclear reactor designers. These aspects comprise filling gaps in experimental data, establishing and guaranteeing inner consistency among evaluated data and detecting and removing systematic errors of experimental data.

Recently a unique computer format called EXFOR for the coding and international exchange of experimental neutron data information has been developed, in a cooperative effort of the four world neutron data centres at Brookhaven, Obninsk, Saclay (ENEA) and Vienna (IAEA). This system will not only contain the experimental data together with statistical and systematic errors and the pertinent bibliographic information, but also additional detailed physical information related to the measurement conditions. These should alleviate the critical assessment and comparison of experimental data, particularly as an auxiliary tool for the evaluator.

1. Why nuclear data evaluation?

At the First International CODATA Conference in Arnoldshain/ Frankfurt, reports were given which were concerned with the organizational aspects in the compilation and evaluation of neutron nuclear data. In the meantime a rather comprehensive account on the historical development in the field of neutron nuclear data has been published in Codata Newsletter No.3. Therefore, in my present talk I would not like to repeat the thoughts expressed in these papers but instead prefer to follow with you the patterns of the actual evaluation tasks in one of the many specialized fields which are treated at this Conference.

I feel obliged to do so by the very reason that this is not covered by most of the other papers at this Conference. Thus a gap should be filled here and I hope you will agree with me that it is beneficial for all of us if someone tries to describe in somewhat more detail what evaluation in actual practice means and why it is needed. This might enable us to appreciate better the intellectual, computer, manual and other efforts which go into the evaluated data content of a magnetic tape or a handbook.

Certainly I have to restrict my remarks to one specialized field and to a few of the problems encountered. However, I hope that these remarks can be made in such a way that you will be able, at least occasionally, to recognize the problems in your own field. I shall restrict myself for convenience to neutron cross sections as applied in the physical and technical design of nuclear fission reactors. There are certainly a number of other nuclear data like photon or charged particle induced data, nuclear structure data like level and decay schemes, etc. which are mainly needed in other applied nuclear fields like thermonuclear fusion, reactor and accelerator shielding or nuclear material safeguards. Regarding these fields my remarks will not represent a serious restriction of generality.

First I would like to ask the general question: Why is nuclear data evaluation needed at all? Certainly this question is not restricted to the nuclear data field. It arises with varying emphasis in almost any scientific discipline. The general simple reason for this is that there is an almost inevitable disaccord between the information as it is supplied by the information producer and the information as it is needed by the information user.

What are the reasons for this disaccord? The simplest reason is obviously that the purpose for which information is produced is different from the purpose for which someone else needs it. A reactor physicist who needs various kinds of cross sections over a large range of energies is certainly not satisfied by a single neutron capture cross section measurement at 25 keV performed to explain nucleosynthesis in stars. However trivial this sounds, it makes immediately clear that in order to avoid the disaccord mentioned above as a basic minimum condition information producer and user must have a common understanding of the purpose of the information concerned. In order to meet this target the information users must clearly define their information needs, look for suitable information producers and make them acquainted with their needs. The information producers in turn must be interested, willing and capable enough to supply the requested information. To establish such an active relationship between information producers and users is no more trivial at all; the whole history of formulation of nuclear data needs for nuclear reactor research and development and of the response to these needs by extensive nuclear data measurement programmes, is a lively illustration of the difficulties which have to be overcome to reach this goal.

Apparently evaluators are here in a key-position as mediator between the information producers and users. Specifying this position in the field of neutron data for reactors, evaluators have to understand the data needs of reactor physicists in very detail and have to communicate them by appropriate ways to neutron data measurers. In the opposite direction they have to make available to reactor physicists the measured neutron data in a form suitable for their purposes.

For the following we can assume that neutron data measurers and reactor physicists as neutron data users, to a reasonable degree, have reached a common understanding of neutron data purposes and needs. The experiences with conferences like the Second IAEA Conference on Nuclear Data for Reactors in Helsinki in June this year, which brought together reactor physicists, nuclear physicists and evaluators for extensive exchange of interests and achievements, allow to draw this conclusion. Most efficient instruments for establishing this understanding were the request lists for neutron nuclear data measurements, as stimulated and furthered by international nuclear data committees like EANDC and INDC. Thus we will only be concerned with the transmittal of information from the neutron physicist to the reactor designer.

This leads me back to the original question "why evaluation?" When there is a common understanding of the purpose of the information between reactor physicists and neutron data measurers, what reasons remain that make the intervening of evaluation indispensable? The answer to this question brings us into the middle of the problem.

Certainly, if instruments were available which yield the needed information to inner consistency and completeness in exactly the desired form, with a 100% confidence level, and this all on adequate economic conditions, no evaluation would be needed. Evaluation necessarily starts at a point where several of these requirements are not met by the data producer. As a matter of fact, almost none of these requirements are met; this is the much more difficult reason why evaluation of nuclear data is vitally needed.

2. Nuclear data needs for reactor design

In order to facilitate the understanding of some of the problems in neutron data evaluation, to be discussed further below, first the neutron data requirements of the reactor designer have to be defined in greater detail. The reactor designer needs the cross sections for all neutron induced absorption and scattering reactions in the energy range from 0 to about 15 MeV. He needs these cross sections pointwise in a very fine energy mesh which he can easily interpolate. At lower energies the neutrons still discern individual resonances when interacting with the nucleus. Thus the reactor physicist must also be provided with resonance parameters like widths and spacings. All this information is needed for a considerable portion of nuclei over the whole periodic table ranging from hydrogen to californium because of the large spectrum of reactor materials. This spectrum consists of the very heavy fissionable and fertile isotopes, heavy fission products with atomic weights ranging from 80 to 160, medium weight and heavy structural and shielding materials, light and medium weight cooling and moderator materials. Usually the reactor physicist needs not to learn from a graph or a table what the cross section value at what neutron energy is, he needs all the data in a well organized computer library from which he can retrieve any material and cross section selection he needs as data input in his design calculations and computer programmes.

3. First evaluation aspect: to complete the available information

Thus the primary requirement of the reactor designer is for a given nucleus to have complete data information, complete in neutron energies and reactions, in order to fill in the needed numbers in his equations. In practice this requirement is never fulfilled a priori; there are always gaps in the available information. These gaps can be purely coincidental: for example, so far nobody might have thought or has been asked to measure neutron capture in barium. These gaps can also be due to experimental difficulties or to the fact that the experimental methods are still not sufficiently developed; a typical example for this situation is the measurement of inelastic scattering in a fissile nucleus where it is very difficult to separate inelastic from fission neutrons. Finally it might not have been worthwhile or economically justifiable to do certain measurements. In some of these cases nuclear model calculations would be much easier and cheaper and as accurate as an experiment.

All these gaps, wherever they exist and whatever origin they have, have to be closed by the evaluator, because usually it takes too long or it is not worthwhile to wait for an experiment. In the simplest case gaps can be closed most efficiently and rapidly by graphical inter- or extrapolations. The reliability of this procedure depends upon the "prefixed shape" of the inter- or extrapolated parts and upon the experience and physical intuition of the evaluator. In more difficult cases recourse must be made to nuclear models and systematics for inter- and extrapolation of the known patterns of measured data and for the prediction of unknown data.

Let me consider this latter point to somewhat greater detail. Nuclear models basically suffer from the fact that they are not self-consistent. They all contain parameters which have to be fitted to some experimental results before they can be applied for reasonably reliable predictions. One of the most widely used nuclear models is the so-called optical model. It allows to differentiate the total cross section into a shape-elastic and a global reaction part. The successful application of the optical model presupposes a knowledge of parameters of the nuclear potential like its form and depth. This model has actually been fairly successful in reproducing known cross sections and thus guarantees, by suitable parameterization, some degree of reliability of prediction of unknown cross sections.

Let me illustrate this by methodically typical examples: Usually it is not necessary in the MeV range of neutron energies to measure elastic scattering angular distributions at many energy points. Optical model descriptions of measured angular distributions are usually very good and within experimental error. Thus the model can be fitted to known data at a few energies and then used for interpolation.

In all cases in which nuclear properties depend only weakly upon the atomic weight use can be made of nuclear systematics for interpolation between neighbouring nuclei. The fact that optical model parameters are only slowly varying as a function of atomic weight can be used to fix the parameters of the model by fitting known cross sections of one or more nuclei and to use these to predict unknown cross sections of neighbouring nuclei.

4. Second evaluation aspect: to make the available information consistent

A second important requirement is the inner consistency of the data information stored in a computer library of evaluated data.

The simplest requirement of this kind is that all cross sections have to be given at the same energies. This allows an easy computer check of the correctness of data input as, for example, a check whether the total cross section is identical to the sum of the partial cross sections. As the information for different cross sections usually has different sources and is thus given at different energies, this requires manual or computer curve plotting and reading off numbers for different reactions at the same energies.

Another requirement of a similar kind is that different representations of the same quantity must exactly correspond to each other. There might be some reactor physicists who need elastic scattering angular distributions as pointwise angular data, others prefer a representation in terms of coefficients of a Legendre polynomial expansion. Thus both representations must be present in an evaluated data library, and the stored Legendre polynomial coefficients must reproduce the point-wise angular data.

These interrelationships have particularly to be considered when data modifications are introduced in an already existing consistent evaluated data file. First one has to know what other changes are involved by a particular change according to the relationships between the various data and secondly in what order these other changes have to be made. These consequential modifications can usually be done by computer programmes.

A very simple example is the following. At a certain energy the following cross sections may be given:

$$\sigma_T, \sigma_X, \sigma_\gamma, \sigma_p, \sigma_n', \sigma_n, \sigma_a$$

which fulfill the following relationships:

$$\sigma_n = \sigma_T - \sigma_X$$

$$\sigma_X = \sigma_a + \sigma_n'; \quad \sigma_a = \sigma_\gamma + \sigma_p$$

Now let us assume that σ_p has been changed. This entails first a change in σ_a, then in σ_X and then in σ_n (for σ_T usually kept constant).

A much more difficult kind of consistency requirement is that different data must correspond to identical physical conditions under which they should have been obtained. If this requirement is not fulfilled by the available information, the evaluator has to reduce the available data to the same physical conditions as far as possible.

A typical case are measured resonance cross sections which can be described by individual resonance parameters. What an evaluator has to do in this case? The reactor physicist needs resonance parameters and resonance cross sections at different temperatures. Now any measured resonance cross section shows not only a temperature broadening of the natural resonance line shape, but also a broadening due to the finite energy resolution of the measurement. Also usually no two measurements of different quantities show the same resolution conditions. Here the evaluator has to reduce all measured cross sections to the natural line shape (for $T = 0^{o}K$). From this a reactor physicist can start and calculate those temperature broadened line shapes as he needs.

5. Third evaluation aspect: to remove systematic experimental errors

Let me now touch upon the most difficult aspect of neutron data evaluation - the detection and removal of systematic errors in experimental data. What the reactor physicist needs most of all is physically true data. Those inconsistencies as I described before introduce errors in his design calculations and may lead to disagreement with reactor experiments. However, in these cases the disagreement can still be traced back to the mentioned inconsistencies in the evaluated data. Part of the still existing discrepancies between reactor calculations and experiments are due to the fact that in the evaluated data used in the calculations unknown systematic errors persist. Unfortunately in the neutron data field in spite of an immense progress in experimental techniques in the last years, systematic discrepancies outside statistical errors between two and more experiments are still frequently encountered which reflect the pronounced basic difficulties in experiments with neutrons.

The most common systematic error consists in the choice of a wrong standard value. Most neutron cross sections are measured relative to one of a couple of standard cross sections which mostly have a particularly simple energy dependence. Examples are cross sections for the following reactions: $H^{1}(n,n)$, $He^{3}(n,p)$, $Li^{6}(n,\alpha)$, $B^{10}(n,\alpha)$, $Au^{197}(n,\gamma)$ and $U^{235}(n,f)$.

Relative measurements are particularly simple to perform since they avoid the determination of the incident neutron flux which is greatest possible accuracy. Because of this importance much work has been and is still being devoted to the development of suitable methods for their accurate determination. In spite of this the requested accuracies have not yet been attained. The requested cross section accuracies which could in principle be achieved without excessive labour are in the range of 1 - 3%, and the present confidence level achieved lies in the range of about 5 - 10%. As the statistical errors, due to the high intensity of present-day neutron sources, are generally much smaller than the confidence levels presently achieved, unknown systematic errors still persist even in standard cross section measurements.

However badly known the standards might be, the evaluator, in a given task of evaluating relative measurements, has first to assume consistent standard data and to renormalize the relative measurements to these assumed standard values. Then differences between groups of measurements based on different standards might still persist pointing to inconsistencies between these standards, and so on. These remarks should just illustrate a few of the problems connected with the role of standards in neutron data evaluation.

Another typical source of inconsistencies between different measurements consists in different neutron energy calibration. In cross sections with a weak energy dependence, differences in the energy scales are very difficult to detect and to interpret unequivocally. This task is obviously much easier in pronounced cross section structures as e.g. in the resonance range. For example the positions of prominent resonances can be used for energy calibration, for these positions consistent values have to be assumed and the one or other measurement to be recalibrated. Another typical error of this kind often occurs in the higher MeV range: in some experiments relativistic corrections for the neutron energy are taken into account, in others not. This leads to differences in energy scale to be corrected of the order of one hundred to a few hundred keV.

Errors in standards and energy calibration are the simplest examples of systematic errors. It must suffice here to mention briefly a few other sources of systematic error.

Every measurement sample has finite dimensions. Depending upon the reaction studied and upon the thickness of the sample used not only primary processes are measured but also secondary and higher order processes occurring after one or more scatterings of the incident neutrons. This fact has to be accounted for by so-called multiple scattering corrections.

Impurities of the sample are another source of systematic errors. Not always is the sample composition accurately known from a careful chemical analysis. It may even happen the inverse, namely that inconsistencies in some cross section data detected by an evaluator stimulate such an analysis of sample material which was assumed pure before. Again this is most easily detected in resonance measurements: resonances may show up in one measurement and are not seen in another one.

Another broad source of systematic errors consists in the various backgrounds. In many ways neutrons can be scattered within and by the surroundings of the experimental facility used and cause "wrong events". Obviously it is one of the most difficult tasks in evaluation to trace an inconsistency between different data sets back to an inconsistency or lack in the background determination. When many of the aforementioned systematic errors can be detected and accounted for by scientists not directly involved in the measurements concerned, here only the experimenter himself, who knows all the details of his facility, can help in correctly determining the various occurring backgrounds and in making sure that backgrounds he assumes negligible are really negligible.

6. EXFOR

From the above remarks on systematic errors it is obvious that an evaluator, whoever that is, an experimenter or a theoretician, must have available to the fullest possible extent and in a consistent way all the information he needs for a valid comparison and judgement of the measurements he is concerned with. More specifically he does not only need to have the data, but must also know the conditions under which the data have been obtained, i.e. all that information which allows conclusions to inconsistencies and systematic errors in the data which might not yet have been accounted for by the experimenter himself.

Generally it is true that not all the information needed can be gathered from the literature and that most experiments are documented incompletely or in inconsistent terms and units. Here the evaluator is faced with the problem of a lengthy correspondence with the data originators - and be it only for the purpose of getting the needed information together. Also the scanning of all the pertinent literature for a few items concerned can be a very cumbersome task. The evaluator would like, and is supposed, to start his work with all the data and pertinent information at hand, in a convenient medium and in a consistent way. This in turn requires complete and systematic compilation of all the data and physics conditions in neutron data experiments on a world-wide scale.

During the sixties this requirement has been more and more recognized and its fulfillment attributed, as one of the major genuine tasks, to the four world neutron data centres at Brookhaven, Obninsk, Saclay and Vienna. More recently, in order to cope with this requirement in a consistent way, the four centres have developed a computer-based exchange system called EXFOR. This system provides a unique computer format for the coding and transmission of neutron data information between the four centres. It might be worth mentioning that the EXFOR system includes a magnetic tape exchange with the USSR, a pioneering feature which might be of importance also for other fields of scientific exchange. The to be compiled has been agreed between the centres and a consistent classification and keywords scheme of the various kinds of data been developed. Secondly EXFOR contains bibliographic information documenting the source of the data. For this item open-ended keyword dictionaries for publication media like journals, books, conferences, reports, etc., for institutes and countries have been developed. Two important additional keywords are "history" and "status". The keyword history is used to document chronologically the handling of the particular data within the data centre, the keyword status specifies whether the data are preliminary, approved by the author, renormalized, etc. These two keywords are on the borderline to the third kind of information contained in EXFOR which allows to specify the physical conditions under which the data have been obtained by a well defined system of physical keywords like facility, method, standard, neutron source, sample, detector, corrections, error analysis and others.

Each entry in the EXFOR system contains these three categories of information. EXFOR does not replace a publication and is not intended to do so, but represents a compilation of most important information items from neutron physics experiments in computer retrievable and easily recognizable form. Thus EXFOR does not only serve the archival purpose of keeping a computer documentation of neutron physics experiments, it is hoped that it will serve the more imminent purpose of helping in the comparison and evaluation of neutron data information.