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# INTRODUCTION TO KFK 120 "NEUTRON CROSS SECTIONS FOR FAST REACTOR MATERIALS", PART I, "EVALUATION"*


by

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## 1. General Remarks

This report gives a short introduction to part I "Evaluation" of the three-partite report KFK 120 (EANDC(E)-35"U") entitled "Neutron Cross Sections for Fast Reactor Materials". In part I the neutron nuclear data evaluation at Karlsruhe since the beginning of the fast breeder reactor project in 1960 is documented. It is the third and last part of the cross section report KFK 120; part II "Tables" and part III "Graphs" were published in 1962 and 1963.

The general content of part I is as follows:

1. Part I documents the cross section data contained in KFK 120/parts II and III, thus also the original content of the Karlsruhe nuclear data file (KEDAK).
2. Since the publication of parts II and III new very valuable experimental and theoretical informations became available in an almost exponentially increasing amount, causing considerable changes to the originally recommended data. Therefore it became necessary to improve and update the tables of part II and KEDAK. Thus this more recent information is also discussed and evaluated in part I. Since the information material published between 1962 and 1966 is by far more comprehensive than the whole of the information before 1962, the discussion of this more recent information takes the largest place. At present KEDAK is going to be updated; after completion of this task a second edition of KFK 120/part II "Tables" is planned and a copy of KEDAK will be sent to the ENEA neutron data compilation center at Saclay.
3. Parts II and III contained only cross sections as a function of the neutron energy. But, as is well known, for Doppler coefficient and shielded cross section calculations also the parameters of resolved and statistical resonances and quantities characterizing the statistical distribution functions of the half widths are needed. Therefore part I gives also an extensive discussion and evaluation of the available experimental and theoretical results in the resonance range to tables of parameter "best"values. Also these parametric data are contained in KEDAK.

4. Among the most important theoretical foundations of the nuclear data evaluation we mention the resonance theory in the ranges of resolved and statistical resonances, the optical model, the evaporation model and the theory of fission. Several review articles do already exist on the subjects of the optical and evaporation models, which discuss also details of application. These models in spite of being applied have therefore not explicitely been treated in part I. Regarding the resonance theory, however, several basic articles exist, but no comprehensive presentation of all commonly used approximations. Therefore an own chapter was introduced, which reviews comprehensively those approximations, which are most commonly used in the interpretation of measured cross sections in the resolved and statistical resonance regions and in the calculation of Doppler coefficients and effective cross sections. As theoretical framework we chose the most commonly applied R-matrix theory and derived the following approximations:

   the one-channel, multi-level and one-level approximations, applicable to medium-weight nuclei with mostly elastic scattering, and

   the multi-channel,multi-level and one-level approximations, applicable to resonances of heavy and heaviest nuclei ($A \geq 80$).

   Characteristic for this latter approximation is the omission of interference terms between different resonances in fission and capture cross sections. Generally this omission is justified for the capture reaction with many exit channels, but no more for the fission reaction with only a few open channels. Approximations with consideration of such interference terms in the fission cross sections were not treated, since up to now we did not apply them in our evaluations. Out of the fission theory only some results of the evaporationtheory (for the fission spectra) and of the channel theory (for the energy and spin dependence of the average fission widths) were used.

Originally the title "Theory and Compilation" was foreseen for part I. This title should have indicated, that nuclear physics data evaluation is a composite of compilation and evaluation of experimental information, decision of discrepancies, closing of gaps and parametric interpretations of measured data by means of nuclear theory. Meanwhile for this activity "evaluation" has become the commonly used name. Therefore the original title was changed into "Evaluation".

## 2. Details of Organisation and Content of KFK 120/part I

Proceeding from light to heavy elements, part I is organised in six principal chapters:

I. Cross sections for light nuclei (H, He, C, O),

II. Resonance theory,

III. Resonance cross sections and parameters for medium weight nuclei (Na, Cr, Fe, Ni, Mo),

IV. Resonance cross sections and parameters for heavy nuclei (U 235, U 238, Pu 239),

V. Fast cross sections for medium weight nuclei (Na, Cr, Fe, Ni, Mo),

VI. Fast cross sections for heavy nuclei (U 235, U 238, Pu 239).

Generally the energy dependence of the cross sections for the light nuclei is smooth (H, He) or it shows a resonance character up to 10 MeV (C, O). Therefore for the light nuclei the whole energy range between 0.01 eV and 10 MeV was treated in only one chapter. For medium-weight and heavy nuclei the different energy dependences of the cross sections, the different types of experiments, the different theoretical interpretation and practical applications suggested a subdivision in separate sections on thermal, resonance and fast cross sections.

All reaction types and their cross sections occurring in the energy range of reactor neutrons (0.01 eV - 10 MeV) are discussed with only two exceptions. The one of these exceptions is the energy distribution of inelastically scattered neutrons in the range of almost continuously distributed rest nucleus levels describable by the nuclear evaporation model. However, the total inelastic scattering cross section between the lowest inelastic threshold and the excitation cross sections for separate rest nucleus levels up to several MeV are extensively discussed. Upper energy limits for the excitation cross sections are:

| | | | |
|---|---|---|---|
| Na: | 4 MeV | Mo: | 2.1 MeV |
| Cr: | 3.2 MeV | U 235: | 2.3 MeV |
| Fe: | 5 MeV | U 238: | 2 MeV |
| Ni: | 4 MeV | Pu239: | 0.55MeV |

For H and He inelastic scattering does not occur, in C and O for the few levels below 10 MeV inelastic excitation cross sections could be determined up to 10 MeV.

The second exception are the elastic scattering angular distributions. They are discussed, but evaluated only up to the mean cosine in the laboratory system, which is needed in diffusion theory. Meanwhile for all materials treated in part I elastic scattering angular distributions have been entered into KEDAK, the documentation is still missing.

Every principal chapter is subdivided according to the data types. Each individual data type for each nuclide is generally discussed in an own subsection. Each such subsection begins with a quantitative review of the available experimental and theoretical information. In most cases the literature was considered back to 1950, in some cases, e.g. for fissionable nuclei, back to the Manhattan-District-Project. The literature was then completely covered up to the EANDC conference on the "Study of Nuclear Structure with Neutrons" at Antwerp in July 1965. Furthermore the most important more recent references up to spring 1966 could be considered, but not more the results of the Washington conference on "Neutron Cross Section Technology" in March 1966 and of the Paris conference on "Nuclear Data for Reactors" in October 1966. Fortunately important results of these two conferences confirmed our evaluations.

In order to save space and time a more extensive discussion of the experimental methods had to be omitted. Moreover good review works are available on this subject as e.g. the two volumes on "Fast Neutron Physics" by Marion and Fowler. Measurement methods are discussed only, if this was considered necessary for the understanding of discrepancies between different experimental results. Generally only certain typical features of the experiments are given like e.g. energy resolution, experimental errors etc., which characterize their quality and reliability. At first then the different experimental results are extensively compared and discussed in the text. In order to have, in addition to these often lengthy discussions, in each individual case a short review of the information material to be evaluated, we inserted comprehensive tables with measurement characteristics for each nuclide, data type and energy range. Typically these tables contain the following informations:

> reference - year of publication - measured quantity - short indication of the experimental method used - energy range - experimental energy resolution - experimental accuracy - column for comments and additional information.

These tables contain the experimental results only in those cases in which only a few data are concerned as e.g. in the case of thermal capture cross sections or infinitely dilute resonance integrals.

Important measurement results are documented in the following way:

1. Important more recent measurements are tabulated if the number of data points did not exceed the order of $10^2$ - $10^3$.
2. For the resonance region tables are given with the measured resonance parameters in the ranges of resolved and statistical resonances and tables with infinitely dilute resonance integrals.
3. In the fast energy range the experimental information is quantitatively given in graphical representation together with the recommended curves. For U 235, U 238 and Pu 239 in addition, extensive tables for $\bar{\nu}$ with corrections of the experimental values and normalisation on common standards were compiled. Furthermore for all isotopes more recent experimental results on level schemes after 1961 were evaluated and tabulated, which are used in the calculation of inelastic excitation cross sections by means of the Hauser-Feshbach theory. The level scheme compilations of K. Way generally consider only references up to 1961.

Most of the mentioned tables simultaneously contain our recommended "best" data in order to enable an easy optical comparison. Occasionally also theoretical information is tabulated; this concerns e.g. the comparison of different calculated excitation cross sections for U 238.

The discussion of the available experimental and theoretical information is then followed by extensive explications of their evaluation. Thereafter in most cases a comparison with other evaluation work is given. These comparisons demonstrate the progress in knowledge and the open problems. Here we had to restrict ourselves to a few important evaluations of microscopic nuclear data. As a compensation at the end of chapter I, V and VI tables are given on the most important microscopic and group cross section sets for the materials treated in part I. These tables give information on the data content, the energy range, the application and the data content of the references concerned also for other nuclei. When one needs group or microscopic cross section references for other materials than those treated in part I, one is easily informed by these tables.

In important cases for comparison purposes also the results of other evaluations are quoted in the tables and graphs. For example, different fission cross section curves recommended by Aldermaston, YOM etc., between 1 keV and 10 MeV are compared in one figure for Pu 239.

Each coherent subsection for a nuclide is followed by a list of all references concerned, subdivided according to reaction type and energy range. As a consequence one and the same reference may be quoted several times in different places. This drawback was admitted in order to make possible a rapid comparison with CINDA.

Finally we mention three tables in the final chapter, which summarise the results of part I:

1. The first of these tables contains the uncertainties of the recommended "best" data for all materials and reaction types treated for the whole energy range. With few exceptions these figures are physical, not mathematically rigorous, estimates. This table can serve as a first basis for investigations of the influence of nuclear

data uncertainties on integral reactor parameters. Furthermore the final chapter contains some general remarks on uncertainties with which one has generally to do for reaction types important in reactor design also for those nuclei not treated in part I.

2. The second table contains unresolved discrepancies between different experiments and nuclear data evaluations. It is primarily adressed to the authors between whose results the discrepancy exists, but also to other experimental and evaluation nuclear physicists.

3. The third table contains a request list for further important experimental, theoretical and evaluation work with specifications of energy range, desired accuracy and priority.

Documentation and argumentation in part I were done so extensively for the particular purpose that the reader gets a complete picture and understanding of each individual evaluation and can build his own judgement with occasionally other conclusions. In view of the frequent lack of an adequate documentation of frequently used data sets like e.g. the ABN set, this completeness of documentation was felt particularly necessary, in order to contribute to the solution of discrepancies between different microscopic and multigroup cross section sets.

## 3. Physical high lights

In addition to these more formal remarks concerning the organisation and content of part I we mention some physical topics which have been investigated particularly extensively. This concerns mostly those data types, which have a decisive influence on important reactor parameters like critical mass, breeding ratio , neutron spectrum etc. We mention

1. Na, critical discussion of the resonance experiments, particularly of the controversial measurements and resonance analyses due to Hibdon from Argonne. A small section is devoted to the many experimental investigations and the clarification of the properties of the important 3 keV resonance. The criticism against Hibdon consists in the following

   a. Frequently statistical scattering in the measured cross sections was interpreted in terms of resonances.

b. For l>1 the (l,J) assignments to the individual resonances are dubious, since the strength functions become by far too large compared to optical model expectations.

c. Hibdon did not consider, that at higher energies several parity allowed l values can contribute to a resonance, and assigns the whole neutron widths to one l value. This might explain point b. Unfortunately we had not yet available the measured data for Na, thus we could not make our own parameter evaluation. Therefore for the moment we took over Hibdon's parameters with the above reservations.

2. Cr, Fe, Ni, Mo: capture experiments in the keV range.

The discrepancies between different differential experiments and between the directly measured infinitely dilute resonance integrals and those calculated from the differential data are extensively discussed. They could be resolved only in the case of Mo, for the other nuclides differences by a factor two and larger remain still unsolved.

3. Na, Fe: inelastic excitation cross sections. Particularly for Fe very many but discrepant informations are available, which are discussed and evaluated in favour of the measurements of Montague et al. from Harwell.

4. U 235, U 238, Pu 239: resonance parameters and cross sections in the ranges of resolved and statistical resonances.

More than one quarter of part I is concerned with this topic. On the one side this is the consequence of the large amount of available experimental and theoretical investigations, on the other side this reflects the importance of these resonance cross sections in the framework of reactor physics. We mention only some points:

U 235: this is one of the most frequently and most extensively investigated nuclei. A comprehensive presentation and critical comparison of all measurements of resolved and unresolved resonance cross sections, mainly of $\sigma_T$, $\sigma_f$, $\eta$ and $\alpha$ is given. Different more recent cross section measurements and evaluations are compared groupwise. Particularly fission and capture resonance integrals and their discrepancies with the epithermal KAPL α measurements are discussed and numerous corrections to the existing measurement interpretations proposed, which could contribute to a reduction of these discrepancies. Resolved resonance parameters are recommended for more than 200 resonances up to 150 eV. Also, as for U 238 and Pu 239, a "best" set of statistical resonance parameters for s and p wave neutrons is given.

U 238: from the existing experimental resonance analyses with a weighted least squares fit "best" sets of resonances parameters were determined for more than 200 resonances up to about 4 keV. It is shown, that the level spacings and reduced neutron widths of clear s wave resonances follow very well the theoretically requested Wigner and Porter-Thomas distributions. The determination of statistical parameters for p wave neutrons like $S_1$ by fits to measured average total cross sections yields results in good agreement with the expectation of different optical models.

Pu 239: only very recently the true features of the s wave resonances have become apparent by combination of results of the fission channel theory, saddle point experiments and very well resolved linear accelerator resonance cross section measurements. This development is extensively described. Resolved resonance parameters are given for resonances up to 300 eV.

5. Pu 239: $\sigma_f$ in the keV range. The numerous discrepancies between different measurements are extensively discussed. At present the most careful and reliable measurements appear to be those of White et al. from Aldermaston. As is well known, these are rather low compared to all former measurements. Meanwhile they have been three times experimentally confirmed: by recent measurements of James/Harwell, Gilboy, Knoll/Karlsruhe (measurement of the ratio $\sigma_f^{49}/\sigma_f^{25}$ up to 200 keV, if these are converted to $\sigma_f^{49}$ with our recommended $\sigma_f^{25}$) and Hemmendinger et al. (nuclear explosion measurements form Los Alamos). Furthermore the White data can be theoretically reproduced and are compatible with statistical resonance parameters deduced from the resonance experiments and saddle point schemes as e.g. proposed by Lynn/Harwell.

6. Pu 239: $\alpha$ in the keV range. The energy dependence of $\alpha$ in the keV range is essentially determined by earlier KAPL measurements below 100 keV and the well known measurements of Diven et al./Los Alamos above 30 keV up to 1 MeV. The rapid decrease of $\alpha$ between 20 and 60 keV can be explained by a fission threshold, probably for 1+ fission, and the corresponding increase of $\bar{\Gamma}_f$. This decrease of $\alpha$ has been confirmed by more recent measurements of de Saussure et al. /Oak Ridge reported at the Paris conference on "Nuclear Data for Reactors" in October 1966.

7. U 235: $\alpha$ and $\sigma_f$ in the keV range. Also here the White $\sigma_f$ data are recommended which are on the average about 7 % lower than the former (n,p) normalized best Harwell and Los Alamos measurements. Below 1 MeV $\alpha$ is established to an accuracy of about ± 20 % by Los Alamos and Oak Ridge measurements which agree in the range of experimental error.

8. U 235, U 238, Pu 239: $\bar{\nu}$ (E). The energy dependence of the average number of fission neutrons is particularly extensively discussed; all measured values have been renormalized to $\bar{\nu}_{25}$ (2200 m/sec) and the average number of spontaneous fission neutrons of Cf 252 as basic standards. The energy dependence appears to be somewhat more complicated than linear; particularly for U 235 unregularities appear to exist below 1 MeV. For all three nuclei simple energy polynomials were minimized in order to fit the data best.

9. U 238: $\sigma_\gamma$ in the keV and MeV regions. Below 100 keV strongly divergent measurements are available. However, from average resonance parameters known from resonance measurements and from statistical theory fits to measured average total cross sections for s and p wave neutrons $\sigma_\gamma$ can be predicted to an accuracy of about ± 20 % without consideration of the statistical fluctuations. Between 100 keV and 15 MeV at present $\sigma_\gamma$ appears to be ascertained to about ± 10 % by more recent reliably normalized and carefully corrected Harwell measurements.

10. U 238: inelastic excitation cross sections. The level scheme of U 238 and all available measurements and Hauser-Feshbach calculations for $\sigma_{n'}^{E_j}$ are extensively discussed and compared, with the following result: at present the levels are known up to about 1.5 MeV. For each of these levels the energy dependence of the inelastic excitation cross section has been determined on the basis of experimental results and of inter- and extrapolations. In spite of this progress the results still remain somewhat unsatisfactory. The cross section uncertainties are still mostly of the order of ± 20 %. Furthermore the cross section values themselves are uncertain: mostly the measurements have only been performed at 90°, they had to be converted to total cross sections by assuming scattering isotropy; particularly in the neighbourhood of the threshold this assumption is not assured.