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NUCLEAR ENERGY AGENCY STEERING COMMITTEE FOR NUCLEAR ENERGY

Data Bank Management Committee

Statistical Verification and Validation of the EXFOR Database: (n,γ), (n,n'), (n,2n), (n,p), (n,α) and Other Neutron-Induced Reaction Cross-Sections

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Statistical Verification and Validation of the EXFOR Database: (n,y), (n

and Other Neutron-Induced Reaction Cross-Sections

For Official User Neutron-Induced Reaction Cross-Sections
 FOR

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Foreword

The OECD Nuclear Energy Agency (NEA) Data Bank operates as an international centre of reference for its member countries with respect to basic tools, such as computer codes and nuclear data, used for the analysis and prediction of phenomena in the nuclear field. It provides a direct service to its users by acquiring, developing, improving and validating these tools and making them available as requested.

In the continuity of NEA Working Party on Evaluation Co-operation (WPEC) Subgroup-30 on improving the accessibility and quality of the EXFOR database, the NEA Data Bank initiated a number of activities to further improve and validate its nuclear databases. In particular, it was proposed to perform a comprehensive review of cross-section data in the EXFOR database. This report describes the development of an efficient review system and its application to more than 15 000 cross-section data sets on neutron-induced threshold, activation and capture reactions.

Acknowledgements

This work was initiated by the NEA Data Bank in close collaboration with the IAEA Nuclear Data Section. Many thanks to V. Zerking and N. Otsuka (IAEA) for providing efficient access to the EXFOR database in extended computational format and to all original articles. Special thanks go to E. Dupont and O. Cabellos for helpful feedback and for handling all administrative aspects.

Contents

List of abbreviations and acronyms

Chapter 1

Introduction

Among the existing databases with experimental nuclear reaction data, EXFOR [1] is by far the most important and most complete. Maintained by the Nuclear Reaction Data Centres (NRDC) network, the library now contains numerical data of more than 160 000 data sets from more than 22 000 experiments performed since 1935, see [2] for complete statistical information. The database mainly contains numerical data and experimental/bibliographic information on experiments for incident neutron, charged particle $(A \leq 12)$ and photon-induced reactions on a wide range of isotopes, natural elements and compounds, for incident energies up to about 1 GeV. One could make a rough estimate of the investment value (salaries, equipment, working hours etc.) of a typical experiment, which is not attempted here, and probably would be astounded by the value that the EXFOR database represents, both in terms of money and historical knowledge.

The importance of the database was also recognised by the NEA Working Party on International Nuclear Data Evaluation Co-operation (WPEC), which started WPEC Subgroup-30 on "Quality improvement of the EXFOR database" in 2007 [3]. With help from NRDC, Subgroup-30 has significantly contributed to the long-term objective to establish EXFOR as an easy accessible and correct database, with as most important deliverables:

- A computational database that contains the entire EXFOR in tabular ("x-y-dy") format, from which *all* nuclear data that exist in EXFOR can be retrieved in an unambiguous manner, if available accompanied by covariance data.
- An EXFOR master database from which many data and format errors have been removed.

The conclusions of the final report of Subgroup-30 mention various activities that should be continued to increase the quality of EXFOR, which includes among others more complete covariance information, online updating of measurement values with new monitor/standards information, extension of the XC4 format, etc. For this report, two important conclusions of Subgroup-30 are highlighted:

- *"Automatic test of the XC4 database by translation into a directory-structured database categorised by projectile/nuclide/reaction and automatic comparison of the data with the world's nuclear data libraries."*
- *"A wealth of statistical info on EXFOR problems is available, but this has not yet been translated into a plan of attack for large-scale EXFOR correction. This will be taken up by the NRDC. Arguably the best way to proceed is to perform these corrections reaction class by reaction class. For example, many activation cross-sections may need to be revisited. The checking procedures outlined in this (Subgroup-30) report have revealed many cases*

where isomeric and total cross-sections were interchanged, and the only way to correct that is to revisit the EXFOR entries one by one. Other classes of data should be visited in the same way."

In this report these two Subgroup-30 recommendations are combined: cross-sections from all available EXFOR subentries should eventually be compared with the corresponding values in nuclear data libraries. Table 1.1 gives a summary of the number of cross-section measurements, per reaction class, that have been identified in the current version of EXFOR. On the basis of that comparison, scores have been assigned. For this report, all (n,*γ*), (n,n'), (n,2n), (n,p), (n,*α*) crosssections, plus other less measured (n,x) cross-sections like (n,d), (n,t), (n,h), (n,np) and (n,n*α*) etc, i.e. about 15 000 subentries out of a total of about 25 000, have been covered in more detail than just automatic comparison. Put differently, the only reaction classes *not* reviewed are (n,tot), (n,el), (n,non), and (n,f). These are reaction classes with a large number of measured data sets, including specific challenges such as a resonance range, which we also had to face for the (n,*γ*) reactions of this report. They may be visited later. A more detailed explanation of Table 1.1 follows later in this report. When the values were suspicious, the publication was reviewed and either a "review" flag was given to the data set or, in case of an error, a recommendation for a corrective action was sent to NRDC. Since reviewing papers is a time consuming process, it is essential to define goodnessof-fit estimators for EXFOR data that optimise this reviewing process. The applied method will be outlined in thisreport.

The current report is set up as follows. Chapter 2 outlines how the original EXFOR data collection is transformed into a database that can be subjected to a statistical analysis. In Chapter 3, a classification for scoring of EXFOR data sets is proposed. Next, in Chapter 4 the goodness-of-fit estimators that lead to the scoring are defined. Finally a graphical comparison is presented of all experimental data, together with the available major nuclear data libraries, covered in this paper.

Table 1.1: Total number of neutron-induced *cross-section* subentries available in XC4 format, compared in this work, and scoring in reviewing classes

Chapter 2

Preparation of database

A Fortran computer program, with preliminary name NEWBASE, has been made which performs the comparison between experimental data and data libraries. For this, the code reads in three large databases:

- The entire "mother" EXFOR database in the original exchange format, here used as one file *x4all.x4.*
- The entire EXFOR database in extended computational XC4 format, produced by Zerkin at the IAEA, here used as one file *x4all.xc4.*
- The major nuclear data libraries.

The Newbase code processes all these data, after which the NEWBASE database is produced in directories n/ $g/d/d/d/d$ h/ a/ and i/ (heavy ions), for the various projectiles.

When the translation from the XC4 computational database to the directory-structured database is made, the comparison with existing nuclear data libraries is performed simultaneously, as well as checks and statistical analyses. After a few hours on a single PC processor, the conversion is done and all checking and statistical results are available.

The whole suite of databases used to produce the experimental nuclear reaction database is presented in Figure 2.1 as a flowchart. The central message is that an experimental nuclear data library is provided which is much easier to access, plot and use in nuclear data evaluation. In the process, its quality is tested by large-scale comparison with nuclear data libraries, and statistical results on basically everything of interest become available. For example, suspicious data are ordered in several outputfiles.

Figure 2.1: Databases produced out of EXFOR

Chapter 3 Scoring of EXFOR data sets

To efficiently verify the EXFOR database, a score should be given to each subentry (data set). Initially these scores will be given automatically, by comparing the experimental values of the subentry with nuclear data libraries. Next, paper reviews and possible corrections may be performed, and subentries may be placed in a scoring class which is different from the initial one. In this section, a classification is proposed which puts this into effect. Next, the order of steps to come to an improved, verified EXFOR library is outlined. The classification will first be defined in a qualitative way. In a later section, the numerical criteria for the classes are defined.

For each subentry, a data block has been created including the basic information of the subentry review and the score. This database with all the scores is kept separately from EXFOR. If appropriate, it can be used in combination with EXFOR for evaluation work.

3.1 Scoring classes

As an initial classification, the data are categorised in three numerical classes: (1) close to, (2) reasonably close to or (3) far away from other data sources (usually evaluated data libraries). In addition, a symbol (T, R, N or E) is assigned to a dataset to assign the review status.

3.1.1 Subentries which are not reviewed or not automatically compared (blank)

blank **Neither reviewed nor compared with evaluations.**

The subentry is not (yet) cross-checked with information from other measurements, libraries and/or calculations. This is the default score.

3.1.2 Subentries which are automatically compared with data libraries (T)

T1 **Automatically compared with libraries: small deviations.**

The subentry contains (very) probably the reaction and data measured by the author, and although the associated publication has not been checked by the reviewer, the quantities have central values and uncertainties which are close to other measurements, libraries and/or calculations.

T2 **Automatically compared with libraries: questionable deviations**.

The subentry contains maybe the reaction and data measured by the author, and the

associated publication has not (yet) been checked by the reviewer. The quantities have central values and uncertainties which deviate to some extent from other measurements, libraries and/or calculations.

T3 **Automatically compared with libraries: strong deviations**.

The subentry contains probably not the reaction and data measured by the author, and the associated publication has not (yet) been checked by the reviewer. The quantities have central values and uncertainties which strongly deviate from other measurements, libraries and/or calculations.

3.1.3 Subentries which are reviewed by checking the publication (R or N)

R1 **Paper reviewed: small deviations.**

The subentry contains certainly the reaction and data measured by the author, since the associated publication has been checked by the reviewer. The quantities have central values and uncertainties, which are close to other measurements, libraries and/or calculations.

R2 **Paper reviewed: questionable deviations.**

The subentry contains certainly the reaction and data measured by the author, since the associated publication has been checked by the reviewer. The quantities have central values and uncertainties which deviate to some extent from other measurements, libraries and/or calculations.

R3 **Paper reviewed: strong deviations.**

The subentry contains certainly the reaction and data measured by the author, since the associated publication has been checked by the reviewer. The quantities have central values and uncertainties which are strongly deviating from other measurements, libraries and/or calculations.

- N1 **Automatic score T1, but pdf of paper not available for checking**
- N2 **Automatic score T2, but pdf of paper not available for checking**
- N3 **Automatic score T3, but pdf of paper not available for checking**

3.1.4 Subentries which contain errors and require specified action (E)

E1 **Error: subentry contains other quantity or wrong values – small deviations.**

Although the quantities have central values and uncertainties which are close to other measurements, libraries and/or calculations, the subentry does not contain the reaction or data measured by the author, but either another quantity or a slightly different numerical value. Obviously, these errors are hardest to find, since these subentries initially get a 'T1' score. Action: confirmation and correction by Data Centres.

E2 **Error: subentry contains other quantity or wrong values – questionable deviations.** The subentry does not contain the reaction or data values measured by the author, while

the quantities have central values and uncertainties which deviate to some extent from other measurements, libraries and/or calculations. These are errors in subentries which initially received a 'T2' score. The associated publication has been checked by the reviewer, and the values found are wrong. Action: confirmation and correction by Data Centres.

E3 **Error: subentry contains other quantity or wrong values – strong deviations.**

The subentry contains reaction and data that do not agree at all with other measurements, libraries and/or calculations. The associated publication has been checked by the reviewer, and often the values found are wrong. Sometimes, no origin of the value or alternative meaning for the value could be found. Action: further analysis, confirmation and correction by DataCentres.

3.2 Various stages of quality assignment

Stage 1

All EXFOR entries that can be automatically compared with nuclear data libraries get a score T1, T2 or T3. A score T1 will probably not be changed anymore. Only if unexpected new information comes to surface, from either the experimental or modelling side, this may change. Hence, the result of this stage is:

- T1: Definite assignment in database
- T2+T3: Could or should be reviewed

Stage 2

The papers of subentries with score T2 and T3 are reviewed. In the course of time, the boundary between T1, T2 and T3 may be altered. This depends on the number of false alarms in the T2 class, which determines whether the decision for a paper review should be more or less strict. After paper review, a subentry with an initial score of T2 will end up in R2, N2 or E2, while a subentry with an initial score of T3 will end up in R3, N3 or E3. Hence, the result of this stage is:

- R2+R3: Definite assignment in database
- \bullet E1+E2+E3: Should be corrected
- N3 (and maybe N2): should have priority for acquiring the pdf file of the paper, so that it can be reviewed

Stage 3

Cases with score E1, E2, E3 result in a message to the Data Centres with a recommended correction. After this correction, these subentries will be reviewed again after which they may be upgraded to R1, R2 or R3 in the next EXFOR update. Hence, the result of this stage is:

• R1+R2+R3: Definite assignment in database

Stage 4

The final scores, i.e. after all corrections, will be either blank, T1, N1, N2, N3, R1, R2 or R3.

It is noted that the scoring classes may be subject to change in the future. One could for example decide to use other numerical indicators, for example real numbers instead of just the integer 1, 2 and 3. What is most important now is the assignment of an 'R', specifying confirmation that the paper contains indeed the compiled quantity and value, even if there is a (large) discrepancy from other measured values or values from nuclear data libraries.

Chapter 4

Goodness-of-fit estimators for EXFOR

To judge a single experimental data point, one may compare it with various other estimates for that point:

- Other measurements for the same reaction and energy range.
- CENDL-3.1: Chinese Evaluated Nuclear Data Library (China), a general purpose library for neutrons.
- EAF-2010: European Activation File (UKAEA Culham/NRG Petten), a special purpose library for activation reactions.
- ENDF/B-VII.1: Evaluated Nuclear Data File (USA), a general purpose library for neutrons.
- IRDFF-1.0: International Reactor Dosimetry and Fusion File (IAEA), a special purpose library for a limited number of reaction channels.
- JEFF-3.2 : Joint Evaluated Fission and Fusion file (NEA Data Bank), a general purpose library for neutrons.
- JENDL-4.0: Japanese Evaluated Nuclear Data Library (Japan), a general purpose library for neutrons.
- TENDL-2015: TALYS Evaluated Nuclear Data Library (NRG Petten), a general purpose library for neutrons and all other incident particles.
- If necessary, alternative nuclear model codes, or the same (TALYS) but run in an entirely different mode, e.g. with only microscopic (non-phenomenological) inputs.

The existing nuclear data libraries should be able to give a reasonably good prediction of many reaction data. It should of course be realised that contents of these data libraries are already heavily dependent on the experimental data which are checked. Usually, they consist of nuclear model calculations tuned to EXFOR data, but often the experimental data are included, often through some least-squares fit, themselves as well. At first sight, the problem is simple: If it is known that libraries are usually reasonably close to the experimental data for a certain reaction channel, alarm bells should start ringing if the deviation of an experimental data set for such a channel is suddenly much larger. However, large deviations may also come from bad performance of the library, and may even occur if the visual agreement on linear scale is good. For example, for reactions close to threshold the difference between evaluation and experiment may easily be a factor of 10. In general the rule holds that the smaller the cross-section, the larger the relative error. It is therefore important to judge not only the calculation/experiment (C/E) values and the reported experimental uncertainty, but also the absolute deviation. In several cases, it turns out that there are problems in EXFOR, and many of them can not so easily be detected with ways other than by comparison with automated model calculations, which is why these EXFOR problems have remained undetected for decades. Therefore, this first global attempt to classify EXFOR problems in a consistent manner is timely. The EXFOR mistakes which are easiest to detect concern C/E values around 0.001 or 1000, suggesting the well-known error of mistaking barn for millibarn. Unfortunately, the majority of cases is more difficult to judge. The current comparison should also help to solve a particular category of mistakes in EXFOR: reaction identifiers which are assigned in wrong, inconsistent or even multiple ways, which can be regarded as an "injustice" for otherwise good-quality experimental data, since they are wrongly coded or sometimes even untraceable. In other words, if the data libraries are expected to give a reasonably good prediction for a reaction and a large deviation for a data set is obtained, it may be that the EXFOR compiler made a mistake and that the evaluated result is not compared with the correct experimental quantity. In that case, the EXFOR reaction identifier should be corrected.

4.1 Estimators used for this work

To discover and classify problems, first three goodness-of-fit estimators are defined, which represent an average deviation between data libraries and an experimental data set that runs over N data points. If they are all three very large, something is wrong somewhere. They are the F-factor

$$
F = 10^{\sqrt{\frac{1}{N} \sum_{i}^{N} f_i}}
$$
\n(4.1)

where the term for each individual data point is

$$
f_i = \left(\log \frac{\sigma_T^i}{\sigma_E^i}\right)^2,\tag{4.2}
$$

the χ^2 estimator,

$$
\chi^2 = \frac{1}{N} \sum_{i}^{N} \chi_i^2,
$$
\n(4.3)

where the term for each individual data point is

$$
\chi_i^2 = \left(\frac{\sigma_T^i - \sigma_E^i}{\Delta \sigma_E^i}\right)^2,\tag{4.4}
$$

and the absolute deviation

$$
D = \frac{1}{N} \sum_{i}^{N} d_i,
$$
\n(4.5)

where the term for each individual data point is

$$
d_i = |\sigma_T^i - \sigma_E^i|.\tag{4.6}
$$

In these equations, the subscript T of the cross-section σ stands for theory (representing data libraries) and E for experimental, while $\Delta \sigma_E^i$ is the experimental cross-section uncertainty. Hence, each subentry (data set) that contains a cross-section excitation function, or only 1 point, is described by three average numbers: F , χ^2 and D , while also all individual components $10^{\sqrt{f_i}}$, χ_i^2 and d_i are kept track of in the analysis. Another factor we will use below indicates the relative magnitude of the cross-section itself, namely

$$
Q_i = \frac{\sigma_T^i}{\sigma_{non}^i} \tag{4.7}
$$

with σ_{non}^{i} the theoretical nonelastic cross-section, and σ_{T}^{i} the theoretical partial reaction crosssection.

The F-factor is a kind of twisted C/E= σ_T/σ_E value. In fact, each f_i component of the sum inside F contributes to C/E if it is larger than 1, and E/C if it is smaller than 1. This is a more appropriate quantity than the average C/E, since averaging C/E values over many points may not be very meaningful if the individual values cross unity at some point. Equation (4.1) remedies this. A value of F=1.2 means that the entire data set is on average about 20% off. F is used as the leading indicator in this statistical study, i.e. for each reaction channel the results are sorted in order of increasing *F* to identify the worst cases. Figures 4.1-4.7 show the distribution of all subentries over the various F values. Note that the term "data set", i.e. the sum over *N*, can apply to one EXFOR subentry, e.g. one excitation function, all subentries for the same (Z,A) nuclide and type of reaction (MT number), all subentries for the same (Z,A) nuclide, all subentries for the same reaction channel (MT number), all subentries for the same projectile, and finally to the entire EXFOR database, or at least the part that could be compared. For all this, average F values are recorded. In addition, all these averages can be taken for each nuclear data library (i.e. ENDF/B-VII, JEFF, etc.) separately, or averaged over all of them. For the purpose of checking EXFOR, the goodness-of-fit for one subentry, i.e. one experimental data set for one energy or a range of energies, averaged over all libraries, is used as the leading indicator.

Figure 4.1: Distribution of F values for the (n, γ) reaction

Figure 4.2: Distribution of F values for the (n,2n) reaction

Figure 4.3: Distribution of F values for the (n,p) reaction

Figure 4.4: Distribution of F values for the (n,*α*) reaction

Figure 4.5: Distribution of F values for the (n,n') reaction

Figure 4.6: Distribution of F values for the (n,n') reaction to discrete levels

Figure 4.7: Distribution of F values for the $(n,3n)$, (n,np) and $(n,n\alpha)$ reactions

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Table 4.1: $F_{1\sigma}$ and $F_{2\sigma}$ values per reaction channel. A fraction of 68.27 and 95.45 %, respectively, of all F values fall inside the given boundaries. To indicate the statistical significance, also the number of included experimental data sets to come to these values is listed. Only channels with at least 20 experimental data sets have been assigned such boundaries.

Reaction	$F_{1\sigma}$	$F_{2\sigma}$	#Sets
(n,n')	1.40	5.8	213
(n,n) m	1.52	3.5	251
(n, 2n)	1.25	2.50	1675
$(n,2n)$ g	1.41	2.45	397
(n,2n)m	1.28	3.6	719
(n,3n)	2.27	23.6	84
(n, n ₁)	2.6	20.	491
$(n, n2 - 40)$	3.3	80.	312
(n,y)	1.47	6.55	5188
(n,y) g	2.11	10.5	143
(n,y)m	2.10	11.3	211
(n,p)	1.31	3.55	1846
(n,p) g	1.82	8.0	188
(n,p)m	1.70	7.0	426
(n,d)	3.0	15.0	45
(n,t)	2.1	27.0	137
(n,a)	2.0	12.0	1068
(n,a)g	2.4	13.0	78
(n,a)m	2.75	13.0	196
(n, np)	7.5	121.7	148
(n,na)	7.2	6.75	54
(n, xp)	1.43	2.99	87
(n,xt)	2.00	159.	23
(n, xa)	2.07	9.07	164

It is noted here that the average goodness-of-fit estimators are necessarily biased, due to data in the various data libraries that stem from the same source. For example, ENDF/B-VII adopts data from JENDL and, to a lesser extent, JEFF, while JEFF adopts data from ENDF/B-VII and JENDL. Many reaction channels of EAF come from TENDL, but also from other libraries. Hence, there is always some "double counting" in the statistical averages, but as long as this does not affect the quality assignment and the required corrections too much, this is acceptable.

Another standard indicator is of course χ^2 , and then the extra aspect for testing is that apart from the central values the uncertainties given in EXFOR can be checked as well. If χ^2 does not have the same rank as *F* in the sorted list of estimators, there may be something wrong with the reported

uncertainty.

Finally, large F or χ^2 values may actually be acceptable, if the underlying quantities have a small absolute value. This occurs often for measurements close to threshold. To identify those cases, the absolute deviation in mb, *D* is an additional helpful quantity.

In sum, for testing of EXFOR it is best to monitor all three indicators simultaneously.

Now that the goodness-of-fit estimators have been defined, the reviewing classification can be defined. The F values for all experimental data sets in a reaction channel have been ranked from small (close to 1) to large. For certain reaction channels the F values are relatively smaller than for others, see Figures 4.1-4.7. This can have several reasons:

- The measurements are easier to perform, so that extreme outliers are generally not expected.
- The reaction channel is easier to model.
- There are more measurements per reaction channels, so that experimentalists are more influenced by previous work.
- etc.

This also means that so called "suspicious" F values are lower for some reaction channels than for others. For each reaction channel, the F value is determined for which "1-sigma", i.e. 68.27% of all F values fall inside this particular F value. The similar F value for "2-sigma", i.e. 95.45%, is determined. This leads to the values given in Table 4.1. The reviewing classes are now as follows

Class 1 : (T1, N1, R1 and E1): $1 \le F \le F_{1\sigma}$, Class 2 : (T2, N2, R2 and E2): $F_{1\sigma} < F \le F_{2\sigma}$, $\chi^2 < 30$, $Q_i < 0.10$ $F > F_{1\sigma}$, χ^2 < 30, Q_i < 0.05, Class 3 : (T3, N3, R3 and E3): $F_{1\sigma} < F \le F_{2\sigma}$, $\chi^2 > 30$, $Q_i > 0.10$ $F > F_{2\sigma}$, $\chi^2 > 30$, $Q_i > 0.05$.

At the moment of this writing, it is felt that class '3' should always be reviewed by checking the associated documentation (publication), while class '2' should be reviewed if, despite the more favourable numerical criterion, the visual fit is bad, also compared to other experiments. Table 1.1 shows the results of the current comparison. Column *All* gives all subentries available in XC4 format. Column *Compared* gives the subentries that have been compared with nuclear data libraries. We have left out comparisons with cross-section values of less than 0.001 mb, so a few XC4 sets have not been compared. Also, in a few cases, no library contains the reaction channel for which a measurement was made. Column $F < 5$ gives the subentries for which $F < 5$, i.e. comparison with the previous column gives the number of (extreme) outliers which are, of course, reviewed but not taken into account for the calculation of statistical estimators. Next the number of subentries for the reviewing classes are given. The final column *Reviewed* is a reminder that not all reaction classes have been reviewed yet.

All papers with an 'R' classification have been reviewed, while those with an 'E' classification have been sent to NRDC for correction. When these corrections have been applied, the 'E' category for these reactions should be turned into an 'R'. Similarly, the 'N3' category should disappear for these reactions, since after retrieval of the pdf papers from other sources, the papers have been reviewed and the code should change into 'R3'. Note that there are only a few 'E's,

especially when compared with the 'R's. This can have severalmeanings:

- By far the majority of experiments in these reaction classes have been correctly compiled.
- A more efficient reviewing criterion is needed, only a few % ofthe suspicious values turn out to be compilation errors.
- A remarkable large amount of experimental data has been published which deviate considerably from the norm.

Note also that at the moment of this writing, there are a few T3 entries left. The reason is that one of the publication databases that is input to this system claims that a pdf file of the paper is available, while this appears to be not the case in the paper repository. Hence, these T3 scores could be changed into N3. The T3 score is retained however as a reminder. In a next version, when the databases are synchronised, these scores should be converted.

A few more specific comments about Table 1.1 are in order. For inelastic scattering to discrete levels, XC4 only gives MT=51 as reaction identifier. The excitation energy is in the data table itself. The RIPL discrete level database is included here to guess which discrete level it concerns. Hence, the 726 discrete inelastic cross-section data sets are distributed over various MT numbers between MT51 and MT90. Above the $6th$ discrete level (MT56), the assignment becomes dubious, but we have nevertheless kept it. Sometimes the automatic quality assignment simply does not work, because there is too much resonance structure as compared to the nuclear data libraries. An example is the ${}^{52}Cr(n,n')$ reaction by Mihailescu. The data fall in category 3, but visually look very reasonable. This is a problem which needs to be solved when reactions with many resonance measurements (e.g. total, capture) arestudied.

To obtain information on the effect of the experimental error, we have correlated F with χ^2 for three reaction classes in Figure 4.8. A large χ^2 value can have two causes: a large deviation of the library value from the central experimental value and/or a small experimental uncertainty. If all experimental uncertainties would be of similar magnitude, one would expect all symbols in Figure 4.8 to be placed around the curve $y = (F-1)^2/r^2$, where *r* would be the average relative measurement error (10% or $r=0.1$ in the case of $(n,2n)$). Symbols lying far above the average curve represent subentries that deserve closer inspection, because either the measurement error is unrealistically small or the distance *D* is so large that one may suspect a wrong compilation action.

4.1.1 Special case: Reactions with resonances

A goodness-of-fit estimator like χ^2 or *F* is only appropriate when the underlying values are not too much fluctuating. For example, a point wise description of the resonance range of a low-energy cross-section may produce huge values for such estimators, while they are simply only a bit out of phase when compared with other evaluations (a similar problem with using χ^2 as a goodness-of-fit estimator for oscillating elastic angular distributions was extensively discussed for the KD03 optical model[4]).

To detect the real outliers for e.g. (*n, γ*) reactions, it is more appropriate to first collect the experimental point wise data into pre-specified energy groups, and obviously to do the same for the nuclear data libraries with which the experimental data are compared. For this we have taken the 69 group WIMS structure as available option in PREPRO [5]. Hence, all nuclear data libraries have been processed with RECENT (to make the data point wise) and GROUPIE (to group the data in the same structure as applied for the EXFOR database) and next all estimators can be calculated where one point now represents one energy group. Simple averages for both the central value and the standard deviation for the EXFOR points have been taken, which for the present purpose suffices.

4.2 Additional estimators

Clearly, when testing EXFOR automatically one needs to be clever in order to avoid unnecessary subsequent (manual) testing. Efficiency is maximal when minimising:

- False negatives: the goodness-of-fit estimators suggest there is no problem, while in reality there is. The problem remains in EXFOR.
- False positives: the goodness-of-fit estimators suggest there is a problem, but checking the publication reveals that the correct data is entered into EXFOR. This means a waste of time.

As in real life, one may be more worried about false negatives than false positives, so it may be wise, time permitting, to take a conservative approach towards a quality classification scheme. Actually, a false positive at least gives the possibility to assign a 'suspicious' label to the corresponding data set, since the compiler made no mistake, but the goodness-of-fit estimators are well away from the average. In an attempt to use all three goodness-of-fit estimators at once, a new set of estimators is currently investigated, the K-factors, which should be more full-proof to identify whether a data point or set is "wrong". A K-factor for a data set of N data points is defined as:

$$
K^{(k)} = 10^{\sqrt{\frac{1}{N} \sum_{i}^{N} k_i^{(k)}}},
$$
\n(4.8)

where $k_i^{(k)}$ is the goodness-of-fit estimator per point. The "0-th order" K-factor is just the Ffactor, i.e.

$$
k_i^{(0)} = f_i = \left(\log \frac{\sigma_T^i}{\sigma_E^i}\right)^2 \longrightarrow K^{(0)} = F \tag{4.9}
$$

To minimise the false alarms for a wrong data set, one may introduce various "penalties" into the definition of K , so that the K-distribution becomes more stretched than the F-distribution, and "true" outliers deviate even further from unity.

First, the weight of the absolute distance D can be taken into account by comparing the theoretical, or evaluated, partial cross-section with the theoretical nonelastic cross-section σ_{non}^{i} . Threshold problems or (very) weak channels are then inhibited, which for the current testing is justified since it is rather common to have a large relative deviation between theory and experiment, without one of the two being clearly wrong. For each data point a penalty factor is defined,

$$
r_i = (1 + Q_i)^{p_r} \tag{4.10}
$$

where Q_i was defined in Equation (4.7) and p_r is a power to scale the importance of this case. Currently, $p_r = 2$. The goodness-of-fit estimator $K^{(1)}$ is then given by Equation (4.8) with

$$
k_i^{(1)} = f_i \cdot r_i \tag{4.11}
$$

Next, the weight of the experimental error is taken into account by comparing it with the deviation of the evaluation from the central value, i.e.

$$
e_i = \left(1 + \frac{f_i - 1}{d\sigma_E^i / \sigma_E^i}\right)^{p_e}
$$
\n(4.12)

where p_e is a power to scale the importance of this case. Currently, $p_e = 2$ seems to be a reasonable value. With this factor, one may hope to catch cases where possibly the reported precision of the measurement was too optimistic, or a wrong compilation of the experimental error. In any case, it will amplify the deviation from the norm. Taking this into account, the goodness-of-fit estimator $K^{(2)}$ is then given by Equation (4.8) with

 $\overline{1}$

$$
k_i^{(2)} = f_i \cdot r_i \cdot e_i \tag{4.13}
$$

These K-factors are written to the final statistical files, but more research is needed to find out if this is a better indicator than the current one based on F .

4.3 Future estimators

Actually, a third penalty can be introduced, namely the deviation of an experimental data point from the other experimental points for the same reaction. So far, all deviations can be seen as "theoretical outlier" or "evaluated outlier", while comparing with similar measurements would lead to purely "experimental outliers". For example, it could happen that there are many experimental data sets for the same reaction with an F between 1 and 1.10, while one measurement has F=1.50. This value itself would possibly not give rise to alarm, but the fact that it deviates from so many other sets does. For this extra test a second loop over the whole database is needed, i.e. after it has been created, so that a statistical factor for each data point is available before this next step. This is not yet implemented.

Ultimately, the best would be to use a test completely based on a sound probabilistic (Bayesian) inference scheme. For each experimental data point in EXFOR, one would then construct a probability density function from all *other* information available for that data point. This other information would consist of other measurements, the collection of data libraries and possibly additional nuclear model codes. The only piece of information which would *not* be used is the experimental data point under consideration. Using the constructed probability density function, obtained by multiplying the probability density functions of all sources, one can then calculate a confidence interval for the data point. It is planned to implement this in a next version of the testing system.

4.4 Comparison with nuclear data libraries

The comparison outlined in the previous section was based on the *average* deviation from the nuclear data libraries. It is of course also possible to differentiate per nuclear data library to discover additional trends. Table 4.2 shows, for the major reaction channels covered here, the average F values and the number of experimental data sets considered. TENDL-2015 is the most complete nuclear data library, in terms of nuclides, reactions and energies and therefore can be compared with most EXFOR data sets. The minimal average F value per reaction channel varies from library to library. Note that for isomeric reactions, it is only meaningful to consider F values for libraries with a special emphasis on, or a lot of, reactions to isomeric states.

The F values can also be binned per incident energy, averaged over all nuclides. This is displayed in Figures 4.9-4.12, for all libraries. For isomeric reactions, only libraries with a significant amount of, or effort in, isomeric reactions have been included in the plots. The energy scale for these figures has been shifted. If we would simply plot the F values as a function of incident energy, an insignificant scatter plot would show up, since the threshold is different for each reaction, and the deviation from nuclear models is largest around the threshold. To take Q-values and Coulomb barriers into account in an empirical way, we have determined for 30 each reaction the incident energy *E*1mb where the excitation function crosses the value of 1 mb. This corresponds to the cross-section value around which several measurements have been attempted. Plotting F values as a function of *E − E*1mb then reveals some trends which are to be expected. First, around threshold, i.e. $E = E_{1m}$ the deviation is relatively large, near the peak it is smaller, and in the tail of the excitation function, i.e. *E* −*E*1mb is around 15 MeV, the deviation from models or libraries increases again.

Figure 4.9: F values, averaged over all nuclides, for $(n,2n)$ reactions as a function of incident energy, for the various nuclear data libraries $(E_{1mb}$ is an estimate for the threshold energy and is the incident energy where the cross-section crosses the 1 mb value)

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Figure 4.10: F values, averaged over all nuclides, for (n,p) reactions as a function of incident energy, for the various nuclear data libraries (E_{1mb} is an estimate for the threshold energy and is the incident energy where the cross-section crosses the 1 mb value)

Figure 4.11: F values, averaged over all nuclides, for (n,*α*) reactions as a function of incident energy, for the various nuclear data libraries $(E_{1mb}$ is an estimate for the threshold energy and is the incident energy where the cross-section crosses the 1 mb value)

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averaged over all nuclides, for (n,n') reactions as a function of incident energy, for the various nuclear data libraries $(E_{1mb}$ is an estimate for the threshold energy and is the incident energy where the cross-section crosses the 1 mb value)

It is important to note that the number of experimental data sets included in the average differs from library to library, see Table 4.2. The good performance of the, experiment based, IRDFF-1.0 F values is a non-surprising result of this. Other observed trends are the good (n,*α*) of CENDL-3.1, the good (n,n') of JEFF-3.2 in the 10-15 MeV range and the overall performance of EAF-2010 for isomeric reactions. For the rest, the libraries perform roughly equally well.

4.5 Graphical comparison

For each combination projectile – target nucleus – reaction channel, an automatic plot is produced in which all experimental data sets are compared with the most important nuclear data libraries. This allows testing whether the numerical outliers are also graphical outliers. Obviously, this can only be done in a strongly automated manner, yielding some plots which are completely overloaded with experimental data sets. This may be improved in a future version of the system.

In the various plots, the nuclear data libraries consistently have the same colour. Experimental data sets are sorted by age, not only in the legend, but also by colour: the oldest data sets are represented by black symbols, and the colour of the various data sets is gradually changed until "red hot" for the most recent data sets. The score of each data set is also given in each legend. For some plots, the scale may seem too wide, but that is because the choice was made to include every experimental data point, including outliers.

Note that the comparison also contains plots for natural elements, for which quite some experimental data are present in EXFOR. For these cases, the nuclear data library curves are reconstructed from the isotopic evaluations, each weighted by their natural abundance.

Some experimental data sets have (almost) no counterpart in nuclear data libraries. This is especially the case for total particle production cross-sections like (n,xn), (n,xp) etc. Therefore, we have used TALYS calculations for those reactions to detect outliers and to assign scores.

Table 4.2: EXFOR data sets compared with nuclear data libraries per reaction channel: Number of data sets and average F values (including reaction classes which have not yet been reviewed)

Chapter 5

Conclusions

All (*n, γ*), (*n, n*′), (*n,* 2*n*), (*n, p*), (*n, α*) and other (n,x) cross-sections like (n,d), (n,t), (n,np) and (n,n*α*) etc. currently present in the EXFOR database have been systematically compared with the corresponding values in the major nuclear data libraries. The resulting statistical information gives rise to various interesting trends in the data, including a list of data sets which can be coined "suspicious" as the cross-section values deviate a lot from the current nuclear data libraries and/or other measurements. For all data sets of category 3, but also many sets of category 2, the associated publications have been reviewed. In most cases, it turned out that the reported quantity was indeed correctly compiled into EXFOR. However, for about 30 cases, the EXFOR compilation was wrong, for either the numerical value or the reported quantity, and appropriate actions have in the meantime been taken by NRDC to correct this. More important than these errors is the confirmation that many experiments for the various reactions have indeed been correctly compiled. A deviation from the mean, especially conspicuous in the case of many experiments of the same reaction, may have to do with the intrinsic quality of the experiment. Such more detailed studies are left to evaluators who focus on one or a few isotopes only.

The experience of the current comparison leads to the statement that within 2 remaining similar batches, one for (n,f), and one for (n,tot), (n,el) and (n,non), *all* cross-sections of the EXFOR database, see Table 1.1, can be reviewed. After that, other quantities such as angular distributions, spectra, gamma production, fission neutron quantities etc., and data for projectiles other than neutrons could bereviewed.

Finally, the term *quality* has been avoided as much as possible in this report. There is never any real proof, on the basis of numerical comparisons only, that an outlier is representing a bad measurement, whether the numerical values have been checked or not. The fact that such data deviate strongly from other data of the same nuclear reaction, may however be helpful to data evaluators who wish to discard such data sets. It is recommended that at least the status symbol of each data set, i.e. T, R, N or E, should be recorded in EXFOR or in a relateddatabase.

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