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Summary Report of the Third Research Co-ordination Meeting on Improvement of the Standard Cross Sections

International Atomic Energy Agency
Vienna, Austria

18 - 22 October 2004

Prepared by
A.D. Carlson, G.M. Hale and V.G. Pronyaev

November 2004

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

Produced by the IAEA in Austria
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Abstract

Results were discussed that have been obtained during two and a half years of work under the Coordinated Research Project (CRP) on Improvement of the Standard Cross Sections. Major attention was focused on reducing the ambiguity between different R-matrix fits; seeking consensus between participants about what approach should be used to minimize the effect of Peelle's Pertinent Puzzle; procedures for combining the results of the R-matrix model with non-model fits; and determining the reactions and energies where smoothing should be used. The proposed timetable includes the release of the standard cross section tables by 18 November 2004 and preparing a draft report with a detailed description of the evaluation procedure by 30 April 2005.

November 2004

CONTENTS

1. Summary of the Meeting

Alan Nichols, Head of the IAEA Nuclear Data Section, opened the meeting. He welcomed all participants and observers of the IAEA Co-ordinated Research Project (CRP) on “Improvement of Standard Cross Sections”, and stressed the importance of the extension of the CRP objectives to heavy elements and release of the preliminary version of the standards by the end of 2004. Although the CRP will finish in 2005, the International Nuclear Data Committee, as advisory body to the IAEA, endorsed the continuation of this activity as an NDS Data Development Project to begin in 2006. This re-affirmation presents an opportunity to undertake regular updates of these standards, which will be needed in the future.

Allan Carlson was elected as Chairman, and **Gerry Hale** as Rapporteur of the meeting. The Agenda was adopted with some changes of the order of presentations by participants due to the delay in the arrival of one participant (**Annex 1)**. A list of participants is given in **Annex 2**.

Session 1 was devoted to the participants’ presentations of their work over the previous year. **Sergei Badikov** presented a paper on the measure of uncertainty for correlated data, in which the square root of the determinant of the covariance matrix of the uncertainty can be considered as such a measure. Comparisons of variances or traces of matrices can only lead to misunderstandings of the evaluated uncertainties.

Evgeniy Gai demonstrated analytically that another global measure of uncertainties, such as the sum of all elements of the covariance matrix of uncertainties, is an approximately conserved quantity and does not depend on any model (or non-model) approaches used in the least square fit. This important property of the covariance matrix of the uncertainty can be applied to check the general implementation of the error propagation law in the fitting codes.

Soo-Youl Oh presented his use of the Monte Carlo method to provide estimates of model-calculated quantities and their probability density functions (PDF). The method can be used for the assessment of error propagation in an arbitrary model calculation and it was shown that the method is useful for the case of a non-linear model with large uncertainties of the model parameters. Random sampling methods from a multivariate normal distribution or certain given PDFs were presented. One big open question is how to determine the PDFs of correlated model parameters as the starting point of the MC simulation.

Allan Carlson provided an overview of new experimental results included in the standards database. Most experimental activities have been completed and the latest low-uncertainty results are included in the GMA database. Though a number of measurements and or analyses were not completed in time to be used in this evaluation, most of them would have had only a small impact on the evaluation. It is important to maintain an experimental effort to provide very high accuracy data needed for improvement of the standards database.

Franz-Josef Hambsch reported on a new analysis of the ^{10}B(n,α_0) and ^{10}B(n,α_1) measurements with a Frisch multi-gridded ionization chamber. The analysis is based on a Legendre polynomial fit of the alpha-particle angular distributions in the kinematic regions where no alpha particle counts are lost. These angular distributions have been used in a RAC fit and the absolute branching ratios between the two channels - in a GMA combined fit. The study suggests that the branching ratios obtained by L.W. Weston and J.H. Todd (Nucl. Sci. Eng., **109**, 113, 1991) are too low.

Toshihiko Kawano reported the results of studies of Peelle’s Pertinent Puzzle, and its resolution through a probabilistic approach. When complete information does not exist about how the uncertainties contribute in the measurements (i.e., the model for data reduction starting with the measured number of counts is unknown), the best approach is to average the posterior evaluations obtained with different models, thus increasing the final uncertainties.

Vladimir Pronyaev reviewed the status of the Standards (as of October 2004). The latest developments include: updating of the thermal constants by including new data such as a high-precision thermal scattering result for ^{235}U – which leads to better consistency with an accepted K1 integral value; updating of the GMA database with accurate data; adjustment of an additional component of the uncertainty (the medium energy range correlation uncertainty) introduced for handling outlying data; renormalization of all cross sections measured relative to hydrogen to the new hydrogen standard; partial resolution of the ambiguity in the R-matrix fits for the ^{6}Li(n,t) cross section; implementation of the option to reduce the PPP problem; selection and testing of the R-matrix+GMA combining procedure; selection and testing of the data smoothing procedure; testing some preliminary results in simple benchmarks.

Hartmut Hofmann presented the results of calculations of the cross sections and partial channel expansions for the Refined Resonating Group Model for the ^{3}He(n,t) cross section, these results can be directly compared with R-matrix fits of experimental data. Results were also shown for calculations using NN potentials for the ^{6}Li(n,t) cross section. Calculations for the ^{6}Li(n,t) cross section using the RRGM would require prohibitively long time.

Gerald Hale reported results of ^{1}H(n,n) and ^{6}Li(n,t) evaluations obtained with the EDA R-matrix code. The fitting of the experimental data, especially the high precision charged particle experimental data appeared very good. But the resulting evaluated covariance matrices have low variances, and even lower off-diagonal covariances than those obtained with the RAC R-matrix code. These covariance matrices are needed for testing and justification. The chi-squared expression used in the EDA R-matrix fit, which differs from that using the full error propagation law, is equivalent to the latter if absolute uncertainties of the experimental data obtained from their percent uncertainties relative to a posterior evaluation are used in the fit.

Nancy Larson presented a detailed proposal for R-matrix code inter-comparison to understand and possibly resolve ambiguities in the data fits observed with different codes (EDA, RAC, SAMMY). The R-matrix code SAMMY, has options for different implementations of the error propagation law, and could help to resolve ambiguities.

Chen Zhenpeng presented papers in which the latest results of evaluations for the ^{6}Li(n,t), ^{10}B(n,α_0) and ^{10}B(n,α_1) reactions with the R-matrix code RAC were shown. The energy ranges for the fits were substantially expanded (up to 20 MeV in neutron energy), allowing a better understanding of the partial channel contribution in the energy range of interest for standards, although making a search for the minimum in the chi-squared multi-dimensional surface more complex due to a large increase of parameters. The RAC code with the full error propagation law produces very realistic uncertainties, even when they are small. The uncertainties are small because many experimental data are used in the fits and high-precision pre-evaluated values (with uncertainties of ~ 0.2%) are used at thermal energy points.

Session 2 and **Session 3** were devoted to discussions of remaining problems, and looking for ways to achieve their resolution through consensus.

Recommendations:

1. Resolution of ambiguity observed in the R-matrix fits with the different codes: first the uncertainties of the experimental data used in all codes should be approximately the same (due to different procedures used in different codes they may not be identical) and as much as possible they should be realistic and based on the conditions of the experiments; the reasons for discrepancies associated with (J^{π}) partial channel expansions should be resolved. Any remaining small differences between R-matrix fits can be treated as a "model" uncertainty. The evaluated central values can be obtained as the non-weighted average between the R-matrix fits. An additional component of uncertainty, the model uncertainty, calculated as half the difference between fits, can be added to the covariance matrix of uncertainty. This result can be used in the combining of heavy element standards (using a programme such as GMA) with light element standards as the result of the coupling due to cross section ratios.

2. The GMA code can be used to combine R-matrix evaluations with the standards for the heavy elements. Non-redundant sets of data produced in the R-matrix evaluation can be used as pseudo-experimental data sets in the GMA combined fit to obtain the results for all the cross sections. Those experimental data sets used in the R-matrix analysis should be eliminated from the database used in the combined fit to avoid double counting. The ^{6}Li(n,n), ^{6}Li(n,t), ^{10}B(n,n), ^{10}B(n,α_0), and ^{10}B(n,α_1) reaction cross sections and full covariance matrices (containing cross-reaction correlation blocks) for the lithium (first two) and for the boron (last three reactions) should be used.

3. Smoothing should be used in the regions where the structure in the cross sections is not physically reasonable. Attention should be paid to the points near thresholds of reaction channels, where smoothing may distort the observed cross-section behavior. Some wiggles due to differences in the energy calibration in different experiments (e.g. ^{6}Li(n,t) cross section and ^{6}Li(n,t)/^{235}U(n,f) cross section ratio measurements near the resonance in the ^{6}Li(n,t) at 0.24 MeV) can appear in the evaluated ^{235}U(n,f) cross section that should behave smoothly. Shifting of the position of the 0.24 MeV resonance in the ^{6}Li(n,t) cross section by 1.5 keV causes a 2% variation in the ^{6}Li(n,t) cross section, that propagates as variation in the ^{235}U(n,f) cross section.

4. Smoothing was recommended for the ^{197}Au(n,γ) cross section in the energy regions from 0.21 to 0.25 MeV and from 0.98 to 1.6 MeV; for the ^{238}U(n,γ) cross section from 0.17 to 0.27 MeV and from 0.45 to 0.96 MeV; and for the fission cross section of ^{235}U, ^{239}Pu and ^{238}U above 25 MeV. The use of a model shape patch was also recommended near 54 MeV for the ^{235}U(n,f) cross section because a significant sharp dip is observed in the shape of the cross section based on a single set of available experimental data.

5. Clear recommendations should be given concerning the use of the covariance matrices of the evaluated standards when estimating uncertainties of cross sections measured relative to the standards or in calculations of integral quantities. A full covariance matrix of the evaluated standards should be generally used in all cases. Removal of any parts of the full covariance matrix of the evaluated standards may lead to significant underestimation of the uncertainties of derived quantities.

The participants also considered the actions and assigned responsibilities for the preparation of a final version of the standards and the associated documentation.

2. List of actions

No.	Action	Participant(s)	Terms
1.	Prepare and distribute to all participants: CD-ROM with data, codes and results for standards as they were on 18 November 2004.	Pronyaev	18 Nov 2004
2.	Run TEST2 prepared by G. Hale, and compare evaluated central values and covariance matrices. Codes used in the intercomparison – EDA, RAC, SAMMY, PADE2, GLUCS, SOK, GMA.	Hale, Chen Zhenpeng, Larson, Badikov, Tagesen, Kawano Pronyaev	31 Dec 2004
3.	Prepare H(n,n) angular distribution standards in the center of mass system as Legendre polynomial expansion for neutrons with incident energies below 20 MeV.	Hale	4 Nov 2004
4.	Prepare H(n,n) high energy standards and covariance matrices of uncertainties for En < 200 MeV.	Hale	Feb 2005
5.	Fit ^{11}B system data using the EDA R-matrix code and the updated database.	Hale	Dec 2004
6.	Obtain standards using: the GMA combining procedure and additional data from the ^{10}B R-matrix result obtained with the new EDA fit; high-energy fission cross sections renormalized to the new hydrogen standard; and corrections and proposals obtained after release of the preliminary standards.	Pronyaev	Apr 2005
7.	Prepare draft versions of chapters for the IAEA-TECDOC, with detailed descriptions of the procedures and results of the evaluations of the standards.	CRP participants and contributors	Apr 2005
8.	Prepare files of standard cross sections and covariance matrices of uncertainties in ENDF-6 format.	Pronyaev, Tagesen, Soo-Youl Oh	Oct 2005

3. Responsibilities for preparation of the final report of the CRP (IAEA TECDOC)

The title of the report describing the final results obtained by the CRP will be “An International Evaluation of Neutron Cross Section Standards”. Responsibilities for the preparation of the chapters are as follows (the underlined name indicates the participant responsible for the preparation of the specified draft chapter):

1. Introduction - brief review of the approach used for the previous standards evaluation (called “old standards” below); unresolved problems in the old standards evaluation; main objectives in the new standards evaluation (A. Carlson, V.G. Pronyaev).

2. Methodology of the evaluation and codes - justification for the old Poenitz methodology for the new standards; improvement of the methodology (brief summary); work with uncertainties of discrepant data; physical and technical fixes to reduce PPP; combining the low- and high-energy standards in one fit and the procedure for combining the light and

heavy element standards; brief description of the codes used in the evaluation: EDA, RAC, SAMMY, GLUCS, GMA, and their intercomparisons and tests (V.G. Pronyaev, all participants).

3. Experimental database improvement - W. Poenitz (1987) experimental database with 1997 updates; discrepancies between experimental data; 2003-2004 update; extending the database to high energies ($E_n > 20$ MeV); corrections for particle leaking to the results obtained with Frisch-gridded ionization chambers; and recommended revision of the uncertainties of some of the data (A.Carlson, F.-J. Hambsch, H. Vonach, D.L. Smith, V.G. Pronyaev).

4. Microscopic nuclear models and light element standard cross sections - ambiguities in R-matrix parameterization of wide and distant poles; RGM, RRGM, NN potential results for ^{3}He+n and ^{6}Li+n systems (H.M. Hofmann, G. Hale).

5. R-matrix theory and evaluation of light element standards - experimental database; EDA and RAC results for ^{7}Li and ^{11}B systems; consistency, uncertainties of the evaluated data in the R-matrix model fits; problems with positive definiteness of the covariance matrix of the uncertainties of the evaluated data derived from the covariance matrix of the parameters (G. Hale, Chen Zhenpeng, N.M. Larson, S.A. Badikov).

6. PPP and its minimization - PPP history and reasons for PPP; PPP manifestation in fits of realistic multi-point data sets including subsets of data from the GMA database and the full GMA database; physical and technical fixes for PPP; updating of the codes used for standards evaluation to minimize PPP; demonstration that different technical fixes produce consistent results (D.L. Smith, Soo-Youl Oh, T. Kawano, E.V. Gai, S.A. Badikov).

7. Evaluation of the standards for heavy and light elements and the combining procedure - GMA fit of heavy and light element standards, with a combining procedure using the R-matrix light element standards evaluations treated as data sets in the GMA fit along with all data for heavy element standards and ratios between light and heavy element standards; results of the evaluation, including central values, uncertainties, cross-energy and cross-reaction correlations; additional components of the uncertainties that were added – as R-matrix numerical solution uncertainty and uncertainty of the technical fix used to minimize PPP (V.G. Pronyaev, all participants).

8. Data presentation for standards - original results produced by GMA; smoothed point-wise evaluated data with increased uncertainties (if needed due to smoothing) and deleted cross-reaction correlation blocks of the total covariance matrix with levels of correlations below a few percent as tables (human-readable) and as evaluated data files, plots for evaluated standards and for differences with old standards (V.G. Pronyaev, S. Tagesen, Soo-Youl Oh).

9. Justification for the recommended uncertainties (V.G. Pronyaev, all participants).

4. Annexes

Annex 1

Agenda and time schedule

Third Research Co-ordination Meeting on
Improvement of the Standard Cross Sections for Light Elements
Room A-2643
International Atomic Energy Agency
Vienna, Austria
18 – 22 October 2004

Monday, 18 October

08:00 - 08:40 **Registration** (Check Point 1)

09:00 – 9:10 **Opening Session:**

- Welcome Address from IAEA
- Election of Chairman and Rapporteur
- Adoption of Agenda (Chairman)

9:10 - 12:30 **Session 1: Presentations by Participants**

[Coffee break when appropriate]
(max. 40 minutes for each presentation and discussion)

1. ***Sergei A. Badikov,*** Institute of Physics and Power Engineering, Obninsk, Russia.
2. ***Evgeniy V. Gai,*** Institute of Physics and Power Engineering, Obninsk, Russia.
3. ***Soo Youl Oh***, KAERI, Republic of Korea.
4. ***Allan D. Carlson***, National Institute of Standards and Technology, Gaithersburg, USA.

12:30 - 14:00 **Lunch and Administrative/Financial Matters**

14:00 - 17:30

Session 1: Presentations by Participants (cont.)

5. ***Franz-Josef Hambsch***, Institute for Reference Materials and Measurements, Geel, Belgium.
6. ***Toshihiko Kawano***, Los Alamos National Laboratory, Los Alamos, USA.

7. ***Vladimir G. Pronyaev,*** International Atomic Energy Agency, Vienna, Austria.

Tuesday, 19 October

9:00 - 12:30 Session 1: Presentations by Participants (contd.)

8. ***Hartmut M. Hofmann***, Universität Erlangen-Nürnberg, Erlangen, Germany.
9. ***Gerry M. Hale***, Los Alamos National Laboratory, USA.
10. ***Nancy M. Larson***, Oak Ridge National Laboratory, USA.
11. ***Chen Zhenpeng,*** Tsinghua University, Beijing, China.

12:30 - 14:00 Lunch

14:00 - 17:30 Session 2: Discussions on key topics

[Coffee break when appropriate]

- Microscopic nuclear models and resolving ambiguity in R-matrix partial channel contributions
- Intercomparison of the R-matrix fits for ^{7}Li system test case
- EDA-RAC ambiguity in ^{7}Li system R-matrix fit for complete data base and convergence of the results
- EDA-RAC differences in the off-diagonal covariances for reconstructed cross sections
- Procedure to exclude PPP
- Combining of R-matrix and non-model fits
- Data smoothing
- Presentation of data for different users (full coupled data files for standards, data for separate reactions)

Wednesday, 20 October

9:00 - 12:30 Session 2: Discussions on key topics (continued)

12:30 - 14:00 Lunch

14:00 - 17:30 Session 2: Discussions on key topics (continued)

18:30 - 21:30 Dinner

Thursday, 21 October

9:00 - 12:30 **Session 3: Decisions and conclusions**

- Final status of GMA database
- Fixing of R-matrix evaluation (central values and covariances) for ^{7}Li and ^{11}B systems
- Fixing of combining procedure for light and heavy standards evaluation
- Fixing of the time-table for release of Standards to 18 November 2004
- Responsibilities and time-table for preparing of the documentation on Standards
- Preparing of the meeting summary and conclusions

12:30 - 14:00 **Lunch**

14:00 - 17:30 **Session 3: Decisions and conclusions (continued)**

Friday, 22 October

9:00 - 12:30 **Session 3: Decisions and conclusions (continued)**

12:30 - 14:00 **Lunch**

14:00 - 16:00 **Session 3: Decisions and conclusions (continued)**

Annex 2

INTERNATIONAL ATOMIC ENERGY AGENCY

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IAEA 3rd Research Co-ordination Meeting on “Improvement of the Standard Cross Sections for Light Elements”

IAEA Headquarters in Vienna, Austria
18 to 22 October 2004
Scientific Secretary: Vladimir G. PRONYAEV

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Annex 3

Short reports submitted by participants

Short report on the results for 2004

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Results of nuclear data evaluation carried out with statistical methods are usually presented as a vector of estimated values and corresponding covariance matrix. As a rule for the same object (cross-section, angular distribution) there is a set of evaluations performed within the framework of various physical models. Covariance matrices from different evaluations – quadratic tables of numbers – can be compared on the basis of integral measure of uncertainty. Besides, a check of validity of the estimated data is of prime interest. Exceeding estimated integral uncertainty over experimental one indicates error in statistical processing.

Square root of determinant of a covariance matrix was considered as an integral measure of uncertainty for a random vector. It was emphasized that small uncertainties of the components of a random vector can be “compensated” by large correlations between components of other one at keeping approximately the same value for the determinants of the covariance matrices. An algorithm for comparison of experimental and estimated (after model and “non-model” fits) covariance matrices was proposed. The algorithm is consisted in 1) separation of all the energy range of interest by intervals number of which is less or equal to the number of parameters in the model fit, 2) folding experimental and estimated covariance information in covariance matrices for uncertainties of averaged (over intervals) experimental and estimated cross-sections, 3) comparison of the determinants of the covariance matrices. The algorithm was applied for comparison of the results of ^{6}Li(n,t) reaction cross-section evaluation carried out on the basis of five sets of measurements. As shown, difference between integral uncertainties of cross-sections estimated in model and “non-model” fits is essentially smaller the one between pointwise (differential) cross-section uncertainties. So, consideration of alone uncertainties of estimated data leads to misunderstanding evaluation results.

Progress Report: Oct. 2003 to Sept. 2004

22 Oct. 2004

Soo Youl Oh

Activities So Far

- Implementation of the Box-Cox transformation method into GMA code (under progress),
- Study on the error propagation by utilizing the Monte Carlo method,
- Derivation of smoothing formula, and
- Presentation of a paper (on resolution for PPP by Box-Cox transformation) at PHYSOR 2004 (April 2004, Chicago)

1. Implementation of the Box-Cox transformation method into GMA code (under progress)

At this moment, a logarithmic transformation is being tested for a single kind of reaction. A difficulty in implementing the transformation into GMA was met in case of the ratio or shape data.

2. Assessment of error propagation by Monte Carlo method

During the period, studied is the Monte Carlo (MC) method for the evaluation of a quantity that is a function of known parameters. Recently the MC method is under discussion in nuclear data community as an alternative to the conventional law of error propagation. It is pointed out that the MC method shall be used not only for the assessment of error propagation but also for the estimation of mean value. For several given functions, the MC mean values and uncertainties were obtained using a short computer program written for this study. Comparing the MC-evaluated values with those from the conventional law of error propagation shows, as it was expected, significant differences in cases of highly non-linear functions with parameters of large uncertainties. In addition, a preliminary study on the convergence of the estimate shows its strong dependence on the covariance of model parameters.

3. Derivation of smoothing formula

A formula was derived for the smoothing the results of GMA. By using the formula, some unphysical fluctuations can be reduced.

4. Paper presentation at PHYSOR 2004

The paper deals with the Box-Cox transformation for resolving the anomaly known as PPP. The results for test cases on not only the PPP itself but also rather realistic evaluation of the Li-6(n,t) reaction cross section showed good performance of such a transformation.

Summary of work done last fiscal year

A.Carlson

Interacted with experimenters to encourage release of data for use in the evaluation.

Completed analysis of NIST ^{10}B total cross section data and made it available for the standards evaluation.

Worked on estimation of Medium Energy Range Correlations for fission data.

Determined which experiments in the standards database used hydrogen as a standard. Then determined whether the measurements were relative to the total cross section or the differential cross section. For those relative to the differential cross section, the angle that used was determined. In all cases, the version of the hydrogen cross section was deduced and calculations were made to obtain the correction factors needed for conversion to the new hydrogen standard.

Wrote with collaborating authors, papers for the ND2004 conference on measurements of the hydrogen scattering cross section, a status report on the database being used for the standards evaluation, and a progress report on the evaluation of the standards.

Organized a side meeting after the ND2004 conference to discuss the status of and the problems with the evaluation.

Worked as the contact person between the WPEC and the CRP. Also worked as the contact person between the CSEWG and the CRP.

Chaired the second RCM. Worked with the IAEA Scientific Secretary to help maintain the level of research necessary for the CRP.

Assisted in writing a summary report of the second RCM. Hosted the RCM through NIST.

Progress on the ^{10}B(n,α) branching ratios and angular distributions

F.-J. Hambsch
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The analysis of the ^{10}B(n,α_0)/ ^{10}B(n,α_1) branching ratios and the corresponding angular distributions was finalized and the data submitted for inclusion into the GMA database. The measured energy range was extended to 2 MeV incident neutron energy for the branching ratios. The quality of the new data resolved the old puzzle of inconsistent data during the former standards evaluation for ENDF/B-VI.

Legendre Polynomial fits to the angular distributions were performed both for ^{10}B(n,α_0) and ^{10}B(n,α_1). The experimental data were treated in several different ways to understand the influence of systematic uncertainties. For the first time a close to $2x2\pi$ angular range has been covered by this experiment based on a Frisch gridded double ionization chamber.

The data have been used in the RAC evaluation for the light elements by Chen Zhenpeng. A considerable improvement of the fit for the ^{11}B system was observed. Also the angular distributions were fitted very well in RAC.

Preparation of a poster for the presentation of the status of the experimental database at the ND2004 conference. Also the corresponding paper was written.

Microscopic Calculation and Data Analysis in Light Nuclei

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The initial aim was to calculate directly *R*-matrix poles. Since it is well known, that for a scattering calculation the relative thresholds have to be reproduced well by wave functions determined from a chosen effective NN-interaction, we decided to take only those width parameters into account, which lead to appreciably varying functions within the channel radius.

First calculations in the ^{7}Li-compound system, using only ^{4}He - ^{3}H and ^{6}Li - n channels yielded low-lying poles in good agreement with known results. Adding more channels, resulted in *R*-matrix poles accumulating just above all thresholds. The same turned out for the ^{11}B-compound system. Changing parameters of the calculations slightly, like channel radii or width parameters, yielded small changes for the low-lying poles, which are known anyhow, but huge changes for the poles above thresholds. We found no reliable way to combine these many poles to a few resonances of the analysis. Therefore, we considered this approach not useful for the analysis further on.

When the cross section for the ^{6}Li(n,t)^{4}He reaction became available, broken down individual partial waves, we did calculations for various effective NN-potentials. These calculations showed qualitative agreement for the ^{7}Li-system and allowed to explain interference patterns found in an *R*-matrix analysis. For the ^{11}B-system at energies above the standards region, new structures were proposed.

For the ^{4}He-system microscopic calculations were done from first principles using realistic NN- and NNN-potentials. These calculations were compared to the *R*-matrix analysis of G.M. Hale. The agreement for some partial waves was perfect. For others slight differencies showed up, and only for very few partial waves qualitative differences occurred, but the effects of these partial waves onto cross sections were minor.

The calculated result for the coherent n-^{3}He scattering length agrees within the small errors of a recent measurement of the real part of this quantity. Since the calculation is done for J = 0 and J = 1 separately and the calculated incoherent scattering length does not agree with the recent datum, we consider the agreement for the coherent scattering length fortuitous.

The calculated ^{3}He(n,p) cross sections in the standards region are just above the ENDF values for the NN-interaction alone and just below these values for NN- and NNN-interaction together. We consider these results well suited for further determination of the structure of the NNN-force.

Conclusion: For systems A $\leq$ 4 microscopic calculations using realistic forces are of the same quality as *R*-matrix analyses. This, hopefully, can be extended to A = 5, eventually for modified NNN-forces. For heavier systems, only effective forces are feasible, hence, only qualitative agreement seems possible.

Progress on Light-element Standards at Los Alamos using EDA

G. Hale

Over the past year, good progress was made on the R-matrix analyses of the A=2,4, and 7 systems in order to provide the standard cross sections for n+p scattering, and for the ^{3}He(n,p) and ^{6}Li(n,t) reactions. Lately, the N-N analysis, which also includes data for n+p capture and γ+d photodisintegration, has concentrated on including all the reasonable measurements of the n+p total cross section at energies up to 30 or 40 MeV. A final fit was obtained to more than 5000 data points having a chi-square per degree of freedom of 0.83. The new total cross sections deviate by no more than 0.5 % from the previous evaluation, but the differential cross section for small-angle proton scattering is about 2.5 % lower than before at 10 MeV. These differences will have some impact on the actinide fission cross section standards measured relative to hydrogen.

New data were added to the ^{4}He analysis that affected the n+^{3}He cross sections, including that for the ^{3}He(n,p) standard reaction. These additions led to highly constrained predictions of the spin-dependent neutron scattering lengths [1] that were consistent with the existing experimental values. Quite recently, however, high-precision measurements [2] of the scattering lengths have been reported that are inconsistent (within uncertainties) with the R-matrix predictions (but in very good agreement, incidentally, with the microscopic RRGM value for the coherent scattering length). We are reviewing the situation with respect to adding these new data to the analysis, and the possible conflicts with the other measurements recently included.

The analysis of reactions in the ^{7}Li system continues to represent all the data included reasonably well, especially the high-precision measurements of cross sections and analyzing powers for t+α elastic scattering. Recently a solution was obtained with the original uncertainties of the t+α data doubled, as well as those of a shape measurement by Macklin of the ^{6}Li(n,t) cross section relative to ^{235}U(n,f) over a wide energy range. Outlying data points (χ^2>10) were also eliminated in this analysis, giving an overall χ^2 per degree of freedom of 1.16, comparable to the value obtained by RAC. Differences persist with the ^{6}Li(n,t) cross section calculated by RAC, especially at energies above 1 MeV, reflecting differences in the ^{7}Li level structure obtained by the two analyses at energies above the $5/2^-$ resonance. In the standards, region, however, the RAC calculation was adjusted to agree closely enough with the EDA result that the CRP members felt the two could be averaged to obtain the standard cross section for this reaction.

Another persistent difference between the two codes is in the output covariances (correlations). These are being explored further in a test of the performance of the three R-matrix codes EDA, RAC, and SAMMY, using a simplified (but realistic) data base from the ^{7}Li system. The covariances from EDA were tested extensively against pseudo-data generated with known statistical properties, and they matched exactly with expectations. EDA’s chi-square expression, when “marginalized” over normalizations, was shown to be essentially the same near a solution as that used by RAC, SAMMY, and the generalized least-square codes.

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Synopsis of presentation for RCM # 3

N. M. Larson, October 25, 2004

1. New capability for treatment of uncertainties in SAMMY

A significant capability has been added to the SAMMY R-matrix code as a direct result of studies undertaken for this CRP: Matrix algebra manipulation was used to determine what changes would be needed in the conventional definition of off-diagonal data covariance matrix (DCM) in order to produce agreement between results from two supposedly identical procedures. The first procedure, fitting to raw (uncorrelated) data, is assumed to give correct results; the second procedure, fitting to reduced (correlated) data, was shown to give the same results when reformulated slightly (using true values rather than experimental values in the DCM). Details were presented in a conference paper ["Treatment of Data Uncertainties," N. M. Larson, ND2004 (*International Conference on Nuclear Data for Science and Technology*, Sept. 26-Oct. 1, 2004)].

Within the SAMMY code, this new definition of DCM has been implemented for use with any parameter for which partial derivatives can be calculated. Thus it is now possible to treat resolution function parameters, for example, in one of three ways: the value can be held fixed and assumed to be perfectly well known (zero uncertainty), the value can be varied (so that the parameter is treated as a search parameter during the fitting procedure), or the value may be held fixed and the uncertainty included in the DCM. The designation for parameters treated in this third fashion is PUP (propagated-uncertainty- parameter). Implementation of the PUP option is a major step towards satisfying the long-standing desire to take all possible experimental uncertainties into account during an evaluation.

2. Test2: ^{6}Li(n,t), ^{6}Li(n,n), and total cross section comparisons

Upon receipt of the EDA output for Test2 from Gerry Hale on October 11, 2004, attempts were made to compare various methods of treating the normalizations (as contributors to DCM or as fitting parameters). Unfortunately there was insufficient time to fully understand the input or to perform detailed comparisons between the three codes (EDA, SAMMY, and RAC); under this time constraint, only simple comparisons within SAMMY were possible. Preliminary results gave no surprises: with large uncertainties on the input normalizations, large differences in calculated cross sections (as high as 20%) could be found when comparing various treatments of the normalizations. In the near future, these comparison studies will be explored further using realistic input values corresponding more closely to those used in the EDA runs.

3. *Possible agenda for systematic code-comparison to resolve RAC/EDA differences*

The underlying causes for differences between the output of the R-matrix codes EDA and RAC will not be fully understood until relevant features of these codes are compared individually. (The SAMMY code, which does not contain all features needed for the light-element evaluations, is included in these comparisons because it has greater flexibility for treatment of correlations than do EDA or RAC.)

A beginning was made two years ago, when comparison tests confirmed that equivalent values of R-matrix parameters led to equivalent values for theoretical cross sections, provided EDA used non-relativistic kinematics. A logical next step would be to compare partial derivatives of the theoretical cross sections with respect to R-matrix parameters. Once differences in partial derivatives are resolved, comparisons should be made of results from fitting one data set with no off-diagonal components of the DCM, varying only one R-matrix parameter, with no iterations for non-linearities. This step should be repeated for other types of R-matrix parameters, and then with more than one parameter. Next, iterations should be permitted, again with only one parameter initially. Further tests would continue to add refinements one at a time: (a) off-diagonal data covariance matrix corresponding to normalization only, with one data set, one parameter, and no iteration; (b) more than one parameter; (c) with iteration; (d) more than one data set; (e) including other types of correlations. At every stage, the three codes must use exactly equivalent input.

Carrying out detailed comparison tests of this nature will give us better insight into some of the reasons for differences between RAC and EDA results.

The New Evaluation for Standards Cross Sections ^{6}Li(n,t)^{4}He, ^{10}B(n,α1)^{7}Li*, and ^{10}B(n,α) ^{7}Li*

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(Oct. 28, 2004)

In order to improve the standards cross sections ^{6}Li(n, t)^{4}He, ^{10}B(n,α1)^{7}Li*, and ^{10}B(n,α0+α1) ^{7}Li*, the ^{7}Li and ^{11}B system have been analyzed with R-matrix code RAC. The characteristics of analysis include:

1. Full error propagation law used in RAC

The formula about error propagation in R-matrix code RAC is as follows [1, 2, 3]:

$$\vec{y} - \vec{y}_0 = D(\vec{P} - \vec{P}_0) , \qquad (1)$$

$$D_{ki} = (\partial y_k / \partial P_i)_0 . \qquad (2)$$

$\vec{y}$ refers to vector of calculated values, D to sensitivity matrix, $\vec{P}$ to vector of R-matrix parameters. Subscript 0 means optimized original value, *k* and *i* are for fitted data and R-matrix parameter subscript, respectively. The covariance matrix of parameter $\vec{P}$ is

$$V_{\vec{p}} = (D^{+} V^{-1} D)^{-1} , \qquad (3)$$

V refers to covariance matrix of the data to be fitted. The covariance matrix of $\vec{y}$ is

$$V_{\vec{y}} = D V_{\vec{p}} D^{+} \quad . \qquad (4)$$

The sensitive matrix elements D_{ij} were calculated with 7 points finite difference methods

$$D_{ij} = \{T(p+3\Delta)-T(p-3\Delta)+ 9[T(p-2\Delta)-T(p+2\Delta)]+45[T(p+\Delta)-T(p-\Delta)]\}/(60\Delta) \qquad (5)$$

Formula adopted for optimizing with R-matrix fitting is

$$\chi^2 = (\vec{\eta} - \vec{y})^{+} V^{-1} (\vec{\eta} - \vec{y}) \Rightarrow \text{minimum} , \qquad (6)$$

$\vec{\eta}$ refers to the vector of experimental data

2. Reduced R-matrix formula used in RAC

RAC is written according to the R-matrix formula given by Lane[1]. The kernel formula are

$$R_{cc'} = \sum_{\lambda\mu}^{N_1} \gamma_{\lambda c} \times \gamma_{\mu c'} A_{\lambda\mu} + \sum_{\lambda}^{N_2} \frac{\gamma_{\lambda c'} \times \gamma_{\lambda c}}{E_{\lambda} - E} + R_{cc'}^{\infty} , \qquad (7)$$

$$\left[A^{-1}\right]_{\lambda\mu} = \left[E_{\lambda}^{res} - E + \sum_{c} (S_c(E) - B_c) \gamma_{\lambda c} \gamma_{\mu c} - \frac{i}{2} \Gamma_{\lambda\mu}^{e}\right] \delta_{\lambda\mu} \quad . \qquad (8)$$

Parameters of R-matrix include reduced width amplitude γ, position of energy level E_{γ}, boundary condition B_c, constant background of distant levels $R_{cc'}^{\infty}$, channel radius a_c width of reduced channel $\Gamma_{\lambda\mu}^{e}$.

Use of the reduced R-matrix formula permits the code to be used to analyze the data in the higher energy region.

3. Neutron energy of data extended to 25 MeV

The neutron energy is extended to 25 MeV, and the reasons for this approach include:

1. GMA database: some data at higher energies (larger than 4 MeV) are included; in order to use the whole GMA database and to make convenient for final combine procedure, the reduced R-matrix formula has to be used.
2. General speaking, able to obtain more reasonable background parameters for standard cross section at lower energies.
3. To make united analysis for whole ^{7}Li or ^{11}B system - able to produce the evaluated values for many kinds of cross sections in one procedure (do not need to use optical model fitting, nor mathematic fitting), this will increase the consistency of evaluated cross sections.

4. Any kind of correlation matrix can be calculated in RAC

The correlation of evaluated results comes from the model parameters and the correlation of experimental data. Any two evaluated cross sections theoretically have correlations and the evaluated correlation matrix can only be calculated in RAC if a suitable set of non-informative data is incorporated in the database.

5. No PPP occured in RAC fitting

6. A large amount of new experimental data is included in the analysis for ^{11}B system

The new total cross section of **Wasson-94** with very small errors**,** the new differential cross sections $^{10}B(n,\alpha_0)^{7}Li$, $^{10}B(n,\alpha_1)^{7}Li^*$ with large number of data from Dr. Hambsch, and (n,α0) /(n,α1) branch with smaller errors of **Dr**. **Hambsch** have played very important role. The new integral $^{10}B(n,\alpha)\,^{7}Li$ cross sections by **Dr. Giorginis** with smaller errors have played very important role in background determination.

The reaction channels and data information for ^{11}B system is as follows:

Reaction	E_n or E_t (MeV)	Number of Data Integrated	Different	Polarization
$^{10}B(n, tot)$	1e-11 to 25.	1409	0	0
$^{10}B(n, n)\,^{10}B$		225	1453	40
$^{10}B(n,\alpha 0)^{7}Li$		185	1959	0
$^{10}B(n,\alpha 1)\,^{7}Li^*$		529	1953	0
$^{10}B(n,\alpha 0+\alpha 1)\,^{7}Li^*$		259	0	0
$(n,\alpha 0)\ /\ (n,\alpha 1)$		217	0	0
$^{10}B(n, n1)^{10}B^*$		46	348	0
$^{10}B(n, t)^{8}B_{e}$		20	0	0
$^{7}Li(\alpha, \alpha 0)\,^{7}Li$	1.8 to 21.	0	754	0
$^{7}Li(\alpha, \alpha 1)\,^{7}Li^*$		243	364	0
$^{7}Li(\alpha, n)^{10}B$		74	672	0

7. Evaluation of ^{6}Li(n, t)^{4}He has passes meticulous comparison

Evaluation of ^{6}Li(n, t)^{4}He reaction with RAC and EDA has passed the test of meticulous comparison. The agreement of the final results of two codes is excellent.

The reaction channels and data information for the ^{7}Li system is as follows:

Reaction	E_n or E_t(MeV)	Number of Data (sum 7727)		
		Integrated	Different	Polarization
^{6}Li(n, tot)	1e-11 to 30	1908	0	0
^{6}Li(n, n) ^{6}Li	1e-4 to 18	219	863	181
^{6}Li(n, t)^{4}He		1143	701	0
^{6}Li(n, n1) ^{6}Li*		27	0	0
^{6}Li (n, p)^{6}He		41	25	0
^{6}Li(n, d)^{5}He		23	33	0
^{6}Li(n, n2) ^{6}Li*		10	0	0
^{6}Li n, 2n)^{5}Li		4	0	0
^{4}He(t, t)^{4}He	2.0 to 17.0	0	1132	657
^{4}He(t, n1)^{6}Li*		0	19	0
4He(t, n2)6Li*		0	2	0
^{4}He(t, n)^{6}Li		0	53	0

In the final fitting procedure, the neutron energy in the database is reduced to 4 MeV as used in EDA (total data number is 6097), the background parameters obtained from the above database are fixed, the full error propagation law is adopted. So the agreement of the final results of RAC and EDA is extremely good.

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