Brief Summary of the Consultants' Meeting on "Improvement of the Standards Cross Sections for Light Elements", held on 2 to 4 April 2001

IAEA Headquarters, Vienna, Austria
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5 April 2001

The main task of the Consultants' Meeting was to discuss the programme of the planned IAEA Co-ordinated Research Project (CRP) on "Improved Standards Cross Sections for Light Elements". The first Research Co-ordination Meeting of this CRP is planned for 2002. The CRP will concentrate on improving and documenting the methodology (primarily R-matrix analysis) used in the evaluation of light element neutron cross section standards and the "combination procedures" used to perform a simultaneous evaluation of all neutron standards data at the final stages of the standards evaluation process. A particular goal is to better understand the origins of the reduction of uncertainties often seen in the R-matrix analyses of the cross sections of the H(n,total), ^{3}He(n,p), ^{6}Li(n,t), ^{10}B(n,α) and ^{10}B(n,$\alpha_1\gamma$) reactions. More generally, the project will attempt to examine all sources of bias or uncertainty associated with the use of practical R-matrix codes for data evaluation (physical approximations in the model, missed levels, simplified treatment of measurement correlations, fitting ambiguities, numerical instabilities, etc.). The CRP will also assess the effect, if any, on the output uncertainties of using a χ^2 search rather than competing statistical techniques, such as generalized least squares. At the end of the CRP, the developed improved evaluation methodology will be applied to the analysis the critically reviewed database of experimental information being prepared by the complementary WPEC activity on neutron standards.

The Agenda and Time Schedule of the meeting are given in the Attachment. After presentation of the R-matrix and least square analysis codes (EDA, SAMMY, RAC, KALMAN, GMA, GLUCS and ZOTT), basic approximations and limitations of the various approaches to data evaluation were considered through round-table discussions.

All participants agree that constraints on the range of parameters and cross sections due to use of the strict physical models (e.g. R-matrix) for data fitting can improve the quality of data evaluations. The inclusion in the fitting all channels leading to the same compound system is especially important. There are many cases when data for inverse partial reactions with a charged particle in the entrance channel have much higher precision than the neutron induced reaction selected as a standard. The use of data on polarization helps to avoid some ambiguities in a search of parameters. However, due to truncation of the R-matrix expansion and admixture of the direct reactions, the largest approximation in the model behavior may bring the replacement of these truncated states and contributions of other reaction mechanisms with a background R-matrix. Thus we can not expect that the cross section shape obtained in the model fit in some energy range with a limited number of parameters is a strict physical model shape (e.g. some well-known classical or quantum-mechanical distributions).

The other considered sources of strong uncertainty reduction are rather common for all least-square fits and include: neglecting by the correlations existing between different experimental data and fitting of the discrepant data with the resulting low uncertainties but high χ^2 per degree of freedom.

The participants came to the conclusion that CRP should start with the consideration of simple test cases, specially designed for demonstration of the error propagation in the R-matrix fits. All steps of error propagation, from covariance matrix of uncertainty of experimental data to the covariance matrix of the parameter uncertainty and conversion of the uncertainty of the parameters in the uncertainty of the evaluated cross sections should be checked and inter-compared between different codes. These checks and inter-comparisons should be done step by step moving from simple to more and more elaborated cases. First tests should be done for numerically simulated pseudo-experimental one-channel cross section curve and randomly distributed statistical component of error. Tests should be done for data having different ratios between statistical and systematical components of errors. Then the case with a few simulated non-correlated experimental data sets should be studied. At this stage, comparisons should include also non-model Bayesian treatment where one experimental data set is taken as a prior. This will be fully equivalent to the search of standard least square solution for a set of experimental data, and codes based on this approach will be also included into comparison. These tests should demonstrate the existing difference between codes using model and non-model data treatment.

The tests, which will be done for more realistic multi-channel cases should demonstrate the effect of inclusion of different channels and respective uncertainty reduction for the reaction channel of the standard cross section. The effect of inclusion of realistic correlations, which may exist between different measurements should be also shown. The danger of treatment of the discrepant data, data which may not only cause the numerical instabilities in the solutions but also lead to the small uncertainties at high χ^2 per degree of freedom will be demonstrated. In this case the reduction of the uncertainties as it is well known is the order of square root from χ^2.

In parallel with the test cases, the improvement of existing R-matrix codes will be done. It may include rewriting of EDA for modern computer platforms, which do not require programming of the management of the data stored in fast memory, generalization of SAMMY for treatment of coupled set of direct and inverse channels, extension of the RAC program to include a treatment of full covariance matrix of uncertainties of experimental data, parameters and evaluated data and extension of KALMAN in the direction of more complete R-matrix calculations.

It is planned that four groups from developing countries may receive IAEA research contracts (grants) and six to eight groups from developed countries may receive research agreements (which provide IAEA financial support for participation in each of the three planned Research Coordination Meetings). The CRP may start in January 2002 and continue for three to four years.