WPEC subgroup proposal

Title: Assessment of the unresolved resonance treatment for cross section and covariance representation

Justification for a Subgroup:

In the resolved resonance range, the experimental resolution is smaller than the width of the resonances; consequently resonances can be "seen" and resonance parameters can be extracted via cross section fitting using methodology such as the R-matrix formalism and generalized-least-squares techniques. In the unresolved resonance region, however, the fluctuations in the measured cross sections are smaller than those in the resolved range but are still important for correct calculation of the energy self-shielding of the cross sections. These fluctuations are due to unresolved multiplets of resonances for which it is not possible to determine parameters of individual resonances as in the resolved region. The mechanism utilized for cross section treatment in the unresolved region is based on average values of physics quantities obtained in the resolved range. Average values for level spacing, strength-functions, widths and other relevant parameters are used as input for calculations in the unresolved energy region.

The formalism most used in the evaluated nuclear data library in the resolved resonance region is the reduced R-matrix Reich-Moore formalism. Effects such as the interference in the fission channels for fissile isotopes like ²³⁵U are well described with the Reich-Moore formalism. While the formalism used in the resolved region is adequate to describe the cross sections, in the unresolved resonance region the cross sections are represented by the less rigorous Single-Level Breit-Wigner formalism. Statistical model codes use Hauser-Feshbach theory for the calculation of average total and partial cross sections. The energy dependence of the parameters is obtained using various formulations and parameterization of the level densities, fission barrier penetrations, and capture widths. The parameters based on a statistical model analysis of the experimental average cross sections must then be converted into 'equivalent' Single-Level Breit-Wigner parameters is to reproduce the fluctuations in the cross sections for the purposes of energy self-shielding calculations. The present proposal aims at assessing the use of the Single-Level Breit Wigner formalism and suggesting improvements.

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Project Definition:

The project will be divided in three parts, namely, I) assessing the existing methodology based on the Single-Level Breit-Wigner Formalisms; II) evaluating other existing formalisms for treating the unresolved resonance region; III) implementing new formalism and testing them;

I. In the first part, the strategy consists of using the 235 U and 238 U resonances as the prototype for testing as follows:

- a) The resonance region for ²³⁵U extends up to 2.25 keV. An unresolved resonance representation will be generated in the energy region from 100 eV to 2.25 keV;
- b) Cross section processing codes such as NJOY and AMPX will be used to process the unresolved resonances for several dilutions and temperatures;
- c) The self-shielding factor calculated with the resolved formalism will be compared to that calculating with unresolved formalism for ²³⁵U in the energy range from 100 eV to 2.25 keV;
- d) Similar calculations for ²³⁸U will be performed in the energy region from 1 keV to 20 keV.

The 235 U and 238 U are fissile and fertile isotopes for which the energy level spacing of swave resonances is 0.5 eV and 20 eV, respectively. They will provide the grounds for testing the unresolved resonance formalism.

II. In the second part, other existing resonance formalisms will be investigated. The characteristic functions methodology of the Wigner's R-matrix introduced Lukyanov at the Sofia University will be studied. New developments done by R. N. Hwang of Argonne National Laboratory will be also investigated.

III. In the last part of the proposal, an attempt will be made to implement these alternative formalisms in processing codes.

Project Justification

It appears that the existing unresolved resonance formalism based on the Single-Level Breit-Wigner cross section representation can not describe correctly the interference effect in the fission channels. In addition, energy dependence of the unresolved resonance parameters is not taken into account for the covariance information. These matters will be investigated.

Deliverables:

• Part I

Generate unresolved resonance parameters for ²³⁵U from 100 eV to 2.25 keV.

Generate unresolved resonance parameters for ²³⁸U from 1 k to 20 keV.

Process ²³⁵U and ²³⁸U with NJOY and AMPX and generate self-shielding factors for several temperatures and dilutions; compare results with calculations using the resolved resonance formalisms.

• Part II

Review existing unresolved resonance formalisms.

• Part III

Recommendations: make recommendation for ENDF format using more rigorous treatment for the unresolved resonance region.

Milestones:

2008-2009

Perform unresolved resonance analysis for ²³⁵U and ²³⁸U. Process the Single-Level Breit-Wigner unresolved resonance evaluations and perform comparison. (Part I)

2009-2010

Use intermediate-energy benchmarks to test the adequacy for the unresolved-resonance cross sections. Study the existing unresolved formalisms indicating what are the advantages and disadvantages. Make recommendations. (Part II and Part III)

2010-2011

Prepare final report.