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LUCAS HEIGHTS

DATA PREPARATION AND BIBLIOGRAPHY FOR THE GYMEA LIBRARY NDXC

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ABSTRACT

A summary of data preparation methods and codes is given together with a compilation of references which were the sources for data contained in the GYMEA library NDXC.

CONTENTS

1. INTRODUCTION

The preparation of microscopic cross section data is invariably the first step in providing information for neutronics codes. The more highly automated this process can be made, the more flexible and extensive is the range of survey and design calculations that can be carried out. At the A.A.E.C. Research Establishment, a number of data preparation programmes are available which can construct libraries of group cross sections for the burnup code GYMEA (Pollard and Robinson 1966).

This report documents the sources of data for each nuclide employed in the current GYMEA cross section library NDXC, and summarizes the methods of preparation. The basic master library consists of a binary tape, although cards used in the preparation of this tape are available. Details of cards which form the library when loaded with the EDITOR programme (Ford 1966) are discussed.

The library is somewhat project-oriented, particularly towards thermal systems. Not all resonance parameters for the fertile nuclides are included, nor is there an adequate representation of inelastic scattering for these nuclides. These omissions remove the possibility of performing fast reactor calculations with the present library.

2. LIBRARY CROSS SECTIONS

2.1 Resonance Reactions

The cross section representation currently used is that adopted by Doherty (1964). The principle behind this particular type of "resonance-removed" representation is that the data library should contain the corrections necessary to allow for approximations made in the GYMEA resonance theory calculations. It was decided that the most straightforward representation would be a combination of resonance parameters and a temperature-independent background cross section which does not possess the rapid fluctuations of the resonance contours.

The code itself can then employ resonance parameters in a symmetric single-level approximation to take account of Doppler broadening and resonance self-shielding, with all of the resonance absorption so calculated placed in one energy group. With this procedure, only the temperature dependence of the background cross section is neglected.

2.2 Resonance-Removed and Resonance-Adjusted Cross Sections

For nuclides which have total widths of resonances much smaller than the level separation, the Breit-Wigner (1936) single-level approximation was used to compute the resonance-removed correction. This correction has the form, at 0°K:

$$\sigma_{n,\gamma}(E) = 6.502 \times 10^5 \sum_{\substack{\text{resonance}\\\text{region}}} \left(\sqrt{\frac{E_r}{E}} - 1\right) \frac{\Gamma_n \Gamma_\gamma}{E_r} \frac{g_J}{(E_r - E)^2 + \Gamma^2/4} \quad , \ldots(1)$$

where Γ_n,Γ_γ and Γ are the elastic scattering, capture, and total widths respectively of a resonance centred at E_r, and g_J is the spin weight factor. For a single level, the shape is as shown in Figure 1. The symmetric part of the resonance cross section is removed in this way and replaced by the correct asymmetric form, because GYMEA assumes that the resonance is symmetric, and that all of the resonance area is in one group.

A difficulty arises with the resonance-removed correction when dealing with integral data. The resonance-removed correction is spread over the neutron energy spectrum, including the thermal region. Low energy resonances which lie near the cadmium cutoff at 0.4 eV have an appreciable proportion of the correction extending into the thermal region, as illustrated in Figure 1. For this reason, current library thermal cross sections for fissile isotopes will be lower than the experimental data, while the asymmetry correction and the correction for the symmetric part of the tails can lead to underestimates or overestimates respectively of resonance integrals, depending on which effect dominates. New methods which remove these discrepancies, known as "resonance-adjustment", have been evolved (Cook 1966) and will be utilized in the preparation of future libraries.

2.3 Inelastic Scattering and Other Reactions

Inelastic scattering cross sections are included within the total scattering cross section, although they are not dealt with by means of emission spectra. The error caused by the omission of the contribution from degraded secondary neutrons is of minor significance except for very fast systems.

The (n,2n) reaction in beryllium has been dealt with as negative absorption which produces an additional neutron per collision. A standardized (n,2n) emission spectrum derived by Axford et al. (1964) was used to describe group-to-group neutron transfer. Variations in the high energy flux spectra were assumed to have a negligible effect upon the averaged emission spectrum, hence the spectrum of Axford et al. was taken to be a characteristic one.

3. LIBRARY FORMAT

The arrangement of the library provides six reactions per nuclide, with cross sections distributed over 120 energy groups according to the scheme outlined by Pollard and Robinson (1966). The reactions are:

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	REACTION	DESIGNATION
1.	(n,γ) or (n,p), (n,α)	NG, or NG1, NP, NAL
2.	Fission	NF
3.	Absorption	NAB
4.	$\bar{\nu}$ × Fission or Scattering	NUF, NNE
5.	Transport	NTR
6.	(n,2n) or spare reaction	N2N, NG2

The microscopic cross sections loaded onto tape by EDITOR can be in free format but must be arranged in increasing order of lethargy per reaction.

For resonance reactions, if experimentally derived resonance parameters are available in the GYMEA resonance region, extending from 454 eV down to 1 eV, these can be included in the library preparation of resonance-removed cross sections and are listed in the library after the above six reactions in the standard A.A.E.C. resonance card format:

$$(\text{F7.3, 1PE11.3, 1P4E10.2}) \quad \text{for} \quad (U, E_r, \Gamma_n, \Gamma_\gamma, \Gamma_f, g_J) \quad .$$

The loading sequence allots resonances to the appropriate energy groups.

4. PROGRAMMES AVAILABLE FOR DATA PROCESSING

GUNYA 1 computes resonance parameters from the empirical adaptation of the free gas model. It prepares yield and statistical resonance data for fission products.
Reference: Cook (1966) AAEC/E-163

GUNYA 2 prepares data libraries from resonance parameters, suitable for direct input to GYMEA. It treats fissile and non-fissile nuclides, with the exception of light nuclides.
Reference: Cook (1966) AAEC/E-163

GUNYA 3 calculates the energy of the lowest resonance in such a way that the experimentally observed thermal cross section and resonance integral are obtained.
Reference: Cook (1966) AAEC/E-162

GUNYA 4 determines the parameters of negative energy resonances in such a way that the correct thermal cross section is obtained.
Reference: Cook (1966) AAEC/E-163

LUBRA 0 is used to generate point cross section data from resonance parameters, including Doppler broadening.
Reference: Kletzmayr (1966) AAEC/E-165

LUBRA 1 calculates infinitely dilute resonance integrals, estimates average parameters in the unresolved region, and includes higher ℓ states.
Reference: Kletzmayr (1966)

LUBRA 2 checks the GYMEA resonance theory against various other approximations.
Reference: Kletzmayr (1966)

LUBRA 3 computes temperature coefficients of reactivity due to the Doppler effect.
Reference: Kletzmayr (1966)

LUBRA 4 essentially constructs group cross section data from the output of LUBRA 0.
Reference: Kletzmayr (1966)

PLOT sets out graphical representations of GYMEA libraries.
Reference: Rodwell (1965 Unpublished)

PEAS is a programme which carries out an exact integration of the slowing down equation for a Breit-Wigner resonance absorber and one moderator.
Reference: Pollard (1964)

EDITOR is a loading programme which also permits general editing of a library tape.
Reference: Ford (1966)

5. CROSS SECTION DATA SOURCES

NUCLIDE	REACTION	DATA SOURCE	COMMENTS
Be9	1. NAL	BNL325B	
	3. NAB	AWRE	
	4. NNE	AWRE	
	5. NTR	GAM AND PIXSE	GAM at high energies PIXSE at low energies
	6. N2N	BNL325B	
O16	3. NAB	AWRE and BNL325B	Consists chiefly of (n,p)
	4 NNE	AWRE	
	5. NTR	GAM AND PIXSE	GAM at high energies PIXSE at low energies
C12	1. NG	AWRE	
	3. NAB	AWRE	Entirely (n,γ)
	4. NNE	AWRE	
	5. NTR	GAM and PIXSE	GAM at high energies PIXSE at low energies
H1 (in H_2O)	1. NG	AWRE	
	3. NAB	AWRE	Entirely (n,γ)
	4. NNE	AWRE	
	5. NTR	MOMUS, PIXSE, and WINDATA	WINDATA, MOMUS at high energy Thermal data from PIXSE (effective width model)
D2 (in D_2O)	1. NG	AWRE	
	3. NAB	AWRE	
	5. NTR	MOMUS	
Li6	1-6	AWRE	
T3	1-6	AWRE	
He3	1-6	AWRE	
Th232	1-6	AWRE	Resonance parameters from Garg et al. (1964)
Pa233	1-6	BNL325A	
U232	1,3,5	1/v from KAPL	
U233	1-6	Pattenden and Harvey (1963) Yeater et al. (1962)	
U234	1-6	BNL325A and GUNYA	
U235	1-6	AWRE + BNL325A res. par.	
U236	1-6	AWRE + BNL325A res. par.	
U238	1-6	AWRE + BNL325A res. par.	
Pu239	1-6	AWRE + BNL325A res. par.	

NUCLIDE	REACTION	DATA SOURCE	COMMENTS
Pu240	1-6	BNL325A + GUNYA	From Diven and Hopkins (1961)
Pu242	1-6	BNL325A + GUNYA	
72 Fission Products	1-6	BNL325A	Thermal $\sigma(n,\gamma)$ and resonance integrals are from Garrison and Roos (1962) and England (1965)
Zr Isotopes 90,91,92,93, 94,96.	1-6	ORNL-3425	
10 test nuclides are also available:			
B10	1-6	All from BNL325A and B	
Al27			
Cr52			
Mn55			
Fe56			
Ni58			
Co59			
Cu63			
W186			
Au197			

The 72 fission products used are:

Br81,Se82,Kr83,Kr84,Kr85,Kr86,Rb85,Rb87,Rb88,Sr88,Sr89,Sr90,Y89,Y90,Y91,Mo95, Mo97,Mo98,Mo100,Tc99,Ru101,Ru102,Rh103,Ru104,Rh105,Pd105,Pd106,Pd107,Pd108, Ag109,Cd113,In115,Sb125,Tc128,I127,I129,Tc130,I131,Xe131,Xe132,Xe133,Cs133, Xe134,Xe135,I135,Cs134,Cs135,Xe136,Cs137,Ba138,La139,Ce140,Pr141,Ce142,Nd143, Nd144,Nd145,Nd146,Pm147,Pm148,Pm148m,Nd148,Sm149,Nd150,Sm150,Sm151,Sm152, Eu153,Eu154,Sm154,Eu155,Gd155,Gd156,Gd157.

The yields from fission for these isotopes were obtained from Walker (1965).

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GAM : Joanou, G.D., and Dudek, J.S. (1961). - GAM-1-A consistent P_1 multigroup code for the calculation of fast neutron spectra and multigroup constants, GA 1850.

KAPL : Knolls Atomic Power Laboratory (1961). - Chart of the Nuclides.

MOMUS : Blaine, R.A. (1963). - MOMUS - A program to construct, up-date, and modify the neutron microscope cross section master tape. NAA-SR-MEMO 8823 (Atomics International).

PIXSE : Macdougall, J.D. (1963). - PIXSE. AEEW-M318.

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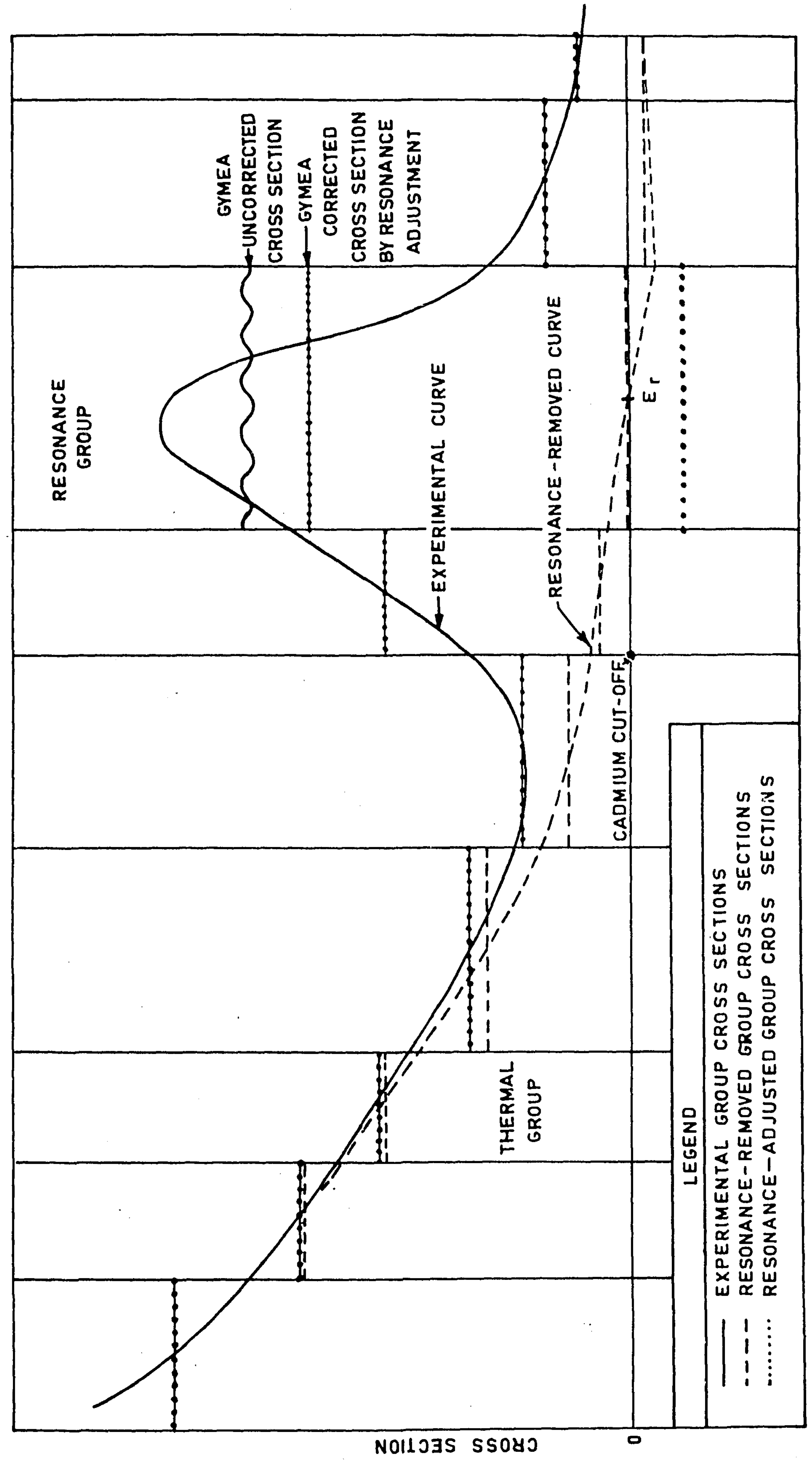

FIGURE 1. RESONANCE REMOVED AND RESONANCE ADJUSTED CROSS SECTIONS