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FAST BREEDER REACTOR
STATIC PHYSICS METHODS DEVELOPMENT
AND ANALYSIS PROJECT

— Quarterly Technical Report —

January - March 1968

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Babcock & Wilcox

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1. INTRODUCTION

In March 1967 The Babcock & Wilcox Company (B&W) initiated a program of analytical methods development applicable to the physics design of fast breeder reactors. One phase of this effort has as its goal the development and utilization of a design-oriented, one-dimensional criticality and depletion code applicable to the physics analysis of fast reactors. This phase of the methods development effort is under full sponsorship of the U.S. Atomic Energy Commission (AEC). Utilization of the code will consist of an investigation in which the design code FARED will be used to relate the sensitivity of certain fast reactor design parameters to the complexity of the physics model used to evaluate them. Finally, several fast reactor critical experiments will be analyzed to verify the applicability of the code and its cross-section libraries. Future topics of study under the FARED project include (1) extension of the criticality and depletion segments to two dimensions with provision for complex fuel management studies, and (2) study of the importance of generating multigroup cross sections using space-dependent spectrum weighting.

An additional task has been added to the FARED project: it involves the utilization of an existing criticality and depletion code (ZEUS) in a fast reactor burnup study. This task is described in detail in section 4.

This third quarterly progress report covers the work done on the FARED project during the period January - March 1968. The major accomplishments during this period are as follows:

1. Completion of the tape generating routine RETAP (excluding EDIT).
2. Completion of STRIP modifications except for isotope lumping to speed source calculation.

3. Continuation of the attempts to execute ultra-fine and 68-broad-group versions of MC².
4. Substantial coding of the unresolved segment in REGA.
5. Initiation of library preparation for the FARED Task 4.

2. ENDF/B IMPLEMENTATION

2.1. The MC² Code

Three separate MC² implementation efforts are in progress at this time:

1. Implementation of a 68-broad-group version of MC². This version of MC² is nearly complete and will be operational in early April. It is anticipated that cross sections from this version will be available for use in the Task 4 studies. The primary objective of this work, however, is to provide cross sections for preparation of the REGA library tape.

2. Successful execution of an ultrafine group problem. In our first attempt to execute a practical ultrafine group case, failure occurred in the OGARLA subroutine due to system hardware failure. Several attempts to overcome the problem have been unsuccessful, and system personnel from NYU are examining the problem.

3. Implementation of a modified MC², which uses the unresolved treatment of reference 1 and fission spectrum weighting in evaluating the inelastic scattering matrix.

ENDF/B work has been hampered by serious software (compiler) and hardware (disc malfunction) troubles which resulted in extended periods of downtime (one period lasted three weeks) during January and February. The 68-broad-group version of MC² is working properly except for the transfer matrix edit, which should be corrected in the next few runs. The ultrafine group problem was executed successfully up to the AVER subroutine in Chain 6; that is, the flux calculation is complete and the problem is failing before the final edit.

2.2. Library Preparation for Criticality Checks

We are preparing a more complete MC² library for use in an analysis of ZPR III-Assembly 48 criticals and for future use in Task 4 studies. The library will contain the following:

¹⁰ B	Fe
C (corrected for inelastic scattering)	Ni
¹⁶ O	Mo
Na	¹⁸¹ Ta
²⁷ Al	²³³ U
Cr	²³⁴ U
⁵⁵ Mn	²³⁵ U
²³⁶ U	²³⁸ U
²³⁹ Pu	²⁴⁰ Pu
²⁴¹ Pu	²⁴² Pu

In support of the CSEWG ENDF/B evaluation effort, a portion of the critical analysis will be performed as soon as the appropriate MC² runs are complete.

3. FARED CODE DEVELOPMENT

3.1. RETAP — The REGA Library Code

The REGA library preparation and maintenance code RETAP has successfully executed a library generation test case. The EDIT routine is partially complete and is being held in this state until all foreseeable additions and deletions to RETAP are completed. A description of the code is given in the Appendix.

3.2. The REGA Routine

Programming of the unresolved resonance routine is well underway,¹ and the merging of this routine with the STRIP code² is expected to be completed by May 15. The following modifications to the STRIP code have been completed:

1. Calculations now proceed in the direction of decreasing energy.
2. Dancoff factor calculations have been added.
3. Mesh parameters for fast reactor calculations have been specified. The new values of β_0 , β_∞ , d_0 , d_∞ , h , and S have been determined as the optimum for fast reactor calculations and are no longer supplied as user input.
4. Two different temperatures may be used for the coolant and pin regions (the coolant may contain resonance absorbers).
5. Resonance escape probability calculations and asymptotic moderator flux options have been eliminated.
6. Material specification is now given by element only, since peak data now contain the necessary isotopic data.

Provisions for the same resonance absorber in both fuel and moderator and for element lumping capability are being added to the STRIP code. The unresolved model has been modified to correspond with that

contained in the MC² code,³ i.e., flux depression in the energy interval ΔE due to resonance absorption is accounted for in the preparation of the effective cross section.

Work is continuing on the preparation of MACH1 for inclusion in the RAIM segment and specification of the distributed Doppler coefficient calculation.

4. FAST REACTOR DEPLETION STUDY

4.1. Objectives

The basic objectives of the Task 4 effort are to derive burnup reactivity balances and to give a preliminary indication of the contribution of fission products to the change in reactor characteristics with burnup for selected fast reactor cases. The effects of uncertainties in the nuclear data for fission products and one other important isotope (^{239}Pu) will be compared; all calculations will be made with the ZEUS criticality and depletion package (DRIP + DHRG3 + GAMMIX + SIZZLE).

The basic ground rules for the calculation are as follows:

1. Two-zone spherical cores with volumes of about 2000 and 8000 liters will be assumed. The two core zones will be represented by a material mixture of 37% oxide fuel, 20% steel structure, and 43% sodium. The presence of any controlling B_4C will diminish the sodium fraction. The blanket will be 45 centimeters thick and will be represented by two fractions, the average composition of which will be 45% oxide fuel, 20% steel, and 35% sodium. The fraction representing the end blanket will duplicate the core mixture but will have no control material. Surrounding the blanket will be a reflector 20 centimeters thick, composed of equal parts of steel and sodium.

2. The fuel and fertile material will be 90% dense oxide. The initial plutonium isotope fractions are 0.76 ^{239}Pu , 0.19 ^{240}Pu , 0.035 ^{241}Pu , and 0.015 ^{242}Pu .

3. ENDF/B reaction cross sections and resonance parameters for sodium, oxygen, ^{238}U , ^{239}Pu , ^{240}Pu , ^{241}Pu , and the fission products will be used to construct the basic 68-group cross-section library used by the DHRG3 segment of the ZEUS package. Data for the remaining materials will be taken from libraries currently used by the contractor.

4. The two core zones will simulate a nominal degree of power flattening, which can be achieved by differences in feed enrichment. Fuel exposure at discharge will not exceed 10 at. % localized burnup. Fuel of at least two levels of exposure will occupy each zone during operation; that is, at least two refueling cycles are necessary to burn each element to its discharge exposure.

5. The incremental plutonium buildup in the blanket fraction will be accounted for closely. The blanket fraction representing the axial blanket will be cycled with the core. The contractor will select suitable methods of radial blanket management consistent with flux level and plutonium concentration.

6. B_4C control material will be used to maintain an effective criticality of 1.00 ± 0.005 . The control material volume will be interchanged uniformly with core sodium. No control material will be present at the end of life for cases with decreasing reactivity.

7. Other factors required for the analysis will be those normally used by the contractor for calculations of this kind.

Not more than six cases will be analyzed. Each of the two core sizes will be calculated with three combinations of cross-section data. The reference combination will be based on the ground rules. The second set will use reference data except that fission product capture cross sections at all neutron energies will be increased 50%. The third set will use reference data except for a 50% increase in the ^{239}Pu capture cross sections at all neutron energies.

Except where noted otherwise, the following information will be obtained at equilibrium fuel cycle conditions for each case calculated.

1. Total fission product reactivity worth at the beginning and the end of the cycle, and the contribution to fission product worth resulting from capture.

2. (for the two reference cases only) Comparison, at the beginning and the end of the cycle, of the fission product scattering contribution to worth and the worth of the scattering contribution of fissioned heavy atoms.

3. The worth, separately, of ^{238}U , ^{239}Pu , ^{240}Pu , and ^{241}Pu inventory changes between the beginning and the end of the cycle.

4. The worth of the blanket plutonium inventory buildup from the beginning to the end of the cycle.

5. A representative sodium void decrement at cycle beginning and end. In addition, the effect of substituting the start of the cycle fission product inventory and also the start of the cycle blanket plutonium inventory on the end-of-cycle sodium void decrement will be determined.

6. Isothermal Doppler coefficients at cycle beginning and end.

7. Incore and total coefficients at cycle beginning and end.

8. Power peak-to-average values at cycle beginning and end.

ZEUS is a one-dimensional criticality and depletion package for use in the physics analysis of fast breeder reactors. It is composed of the following codes:

1. DRIP — generates effective resolved and unresolved resonance cross sections using the IR approximation in the resolved resonance range and statistical theory (as in MC^2) in the unresolved resonance range. Rapid and accurate calculation of the Doppler-broadening function $J(\theta, \beta)$ is performed by the JFIT routine, which uses a compact table and second-order asymptotic expressions. DRIP is called by DHRG3.

2. DHRG3 — prepares group constants for use in the spatial flux and eigenvalue segment. DHRG3 is a revised version of the GAM code.

3. GAMMIX — couples the DHRG3 code to the diffusion theory and depletion segments. It allows the user to make any number of DHRG3 runs (corresponding to different reactor compositions) and merge the microscopic data from these runs to form a single 18-group cross-section library. The user may obtain one or more cross-section sets for a single isotope, labeling each set with a different ID, to account for different spectral weighting between regions, e.g., between core and blanket regions. The DHRG3 runs, merging, labeling, and library tape preparation are performed automatically.

4. SIZZLE — comprises the AIM-6 code coupled to a 6-group point depletion routine. AIM-6 performs an 18-group (five downscatter groups) diffusion theory calculation for the space-dependent flux and reactor eigenvalue; the 18-group cross-section set is collapsed by regions to six groups for use by the depletion routine. PERT input fluxes (six groups) are provided on punched cards and macroscopic data for use in PDQ6 and PDQ7 may also be edited.

Several other codes have been prepared as part of the overall ZEUS project, although they are not components of the ZEUS package. The major codes in this category are as follows:

1. TRANS — prepares P_0 and P_1 (up to P_3 is permissible) elastic transfer matrices for the DHRG3 68-group library. The code accepts tabulated scattering cross sections (1500 points) and Legendre coefficients ($l = 30$) and performs the required double integrals using an efficient and accurate integration algorithm that allows user control of integration accuracy.

2. DIMIS — prepares inelastic scattering matrices from discrete level and/or statistical data as supplied, for example, by ENDF/B. The ENDF/B model is assumed in the statistical region, i.e., the level data are not extrapolated into the statistical region.

3. STRIP — is an external resonance integral program that may be used to supply effective resolved resonance cross sections to the DHRG3 code. It performs a numerical solution of the integral slowing-down equations for a two-region cell using an internally generated energy mesh (varying mesh width with energy). The program accounts for overlap and interference effects involving up to 15 resonance absorbers.

4.2. Cross-Section Preparation

Cross-section preparation for this Task 4 study is nearly complete. Elastic and inelastic scattering matrices have been prepared for sodium, oxygen, iron, ^{238}U , ^{239}Pu , ^{240}Pu , and ^{241}Pu . Preparation of smooth cross-section data is complete, and an analysis of the data used in the resolved and unresolved resonance region is in progress.

APPENDIX
The RETAP Code

1. General

RETAP is a program for generating or updating a REGA library tape. The program uses free-format input subroutines as well as directives to label data and to issue commands. As a part of the code, an editing routine is called by an EDIT command to edit the tape by files of nuclides.

Directives	Description
TAPES	Tape assignments to follow.
NIN, i	The existing REGA library tape is "i" $2 \leq i \leq 9$.
NOUT, j	The generated tape is to be "j" $2 \leq j \leq 9$ $i \neq j$.
FILE ONE (data for FILE ONE)	File 1 data to be given.
FILE TWO	File 2 is given.
DCDATA (depletion chain data)	Depletion chain data next.
DELETE (chain ID number for chains to be deleted)	Delete the following chains.
FILE THREE	File 3 data next.
DELETE (nuclide ID's)	Delete the following nuclides from file 3.
RRDATA (resolved resonance data)	
FILE FOUR	File 4 data next.
URDATA (data for unresolved region)	Unresolved data to follow.
DELETE (nuclide ID's)	Delete the following nuclides.

Directives	Description
FILE FIVE	File 5 to follow.
XSDATA (microgroup xsection data)	xsection data to follow.
DELETE (nuclide ID's)	Delete the following nuclides.
FILE SIX	File 6 data to follow.
DELETE (nuclide ID's)	Delete the following nuclides from file 6.
TMDATA (transfer matrix data)	Transfer matrix data to follow.
FINIS	Stops the program.

Note that the xxDATA and the DELETE directives may be in any order within a FILE directive section. Any FILE directive may be omitted with its DELETE and xxDATA, but if any FILE is included, it must contain at least a DELETE or an xxDATA directive (not necessarily both). The FILE directives must be in increasing order. If a nuclide ID is contained in an xxDATA section, it is automatically deleted from the existing tape (if an update). If TAPES is omitted, then NIN = 0 and NOUT = 2; if TAPES is included, then NIN should not be assigned as 2 unless NOUT is assigned $\neq$ 2.

2. Data Description

The data input to RETAP should follow the general format outlined in reference 1. For simplicity, the same symbol-names will be used except as noted.

FILE ONE — This file will contain the general tape information and will give the microgroup energy bounds. The data are as follows:

IDT(I), $I \leq 10$ Parameters describing the tape.

Column 72

\$ [alphanumeric tape description] Each card must contain a \$ sign in Column 1; there can be as many as 100 cards.

\$

EGRP(I) Microgroup energy bounds.

FILE TWO — This file contains depletion chain data in the following manner:

LCHAIN(1)

NCID₁, LFG, NSOR₁, IDS(1), MSR(1), . . . , IDS(NSOR₁), MSR(NSOR₁)

.

.

.

NCID_n, LEG, NSOR_n, IDS(1), MSR(1), . . . , IDS(NSOR_n), MSR(NSOR_n)

where LFG indicates if NCID is fissionable (1 = yes, 0 = no)
 n = number of nuclides in this chain

LCHAIN(2)

(etc.)

FILE THREE — This file contains data for resolved resonances as follows:

IDR	Nuclide ID.
NPKS	Number of peaks.
NECOR	Number of capture xsection corrections.
NECORF	Number of fission xsection corrections.
AM	Mass.
SPIN	Spin.

R		Scattering length.
EZERO(I)	} Repeat for NPKS	Peak energy.
AJ(I)		Spin state.
GAMN(I)		Neutron width.
GANG(I)		Capture width.
GAMF(I)		Fission width.
ABN(I)		Abundance.
ECORA(J)	} Repeat for NECOB	Energy point.
RCAP(J)		Capture xsection for this energy.
ECORB(K)	} Repeat for NECORF	Energy point.
RFIS(K)		Fission xsection for this energy.

Repeat the list above for each nuclide.

FILE FOUR — This file, containing data for the unresolved region, is as follows:

IDU		Nuclide ID.
NJSO		Number of states for $\ell = 0$.
NJS1		Number of states for $\ell = 1$.
ECUR		Upper bound for this region.
ECK		Lower bound for $\ell = 1$.
M		Number of points at which $\ell = 0$ calculation is to be performed.
N		Number of points at which $\ell = 1$ calculation is to be performed.
NRN(I)	}	Number of energy points for reduced neutron width.
NEF(I)		Number of energy points for fission width.
MU(I)		Number of exit channels for this state.
BJ(I)		} NJSO + NJS1
GG(I)	Mean capture width.	
D(I)		Mean level spacing.
EFN(J)	} NRN	Energy point.
GNZ(J)		Reduced neutron width.
EFF(K)	} NEF	Energy point.
GF(K)		Fission width.

Repeat the list above for each nuclide.

FILE FIVE — This file contains microgroup cross-sections as follows:

IDM		Nuclide ID.
IFIS	$\left. \begin{array}{l} 1 = \text{yes} \\ 0 = \text{no} \end{array} \right\}$	Fission and NU data given.
IN2N		N_{12N} xsection given.
IEP		$\sigma_{n,p}^l + \sigma_{n,a}^l$ data given.
IFP		$\sigma_{n,p}^l + \sigma_{n,a}^l$ data given.
XCAP(I)	$\left. \begin{array}{l} \\ \\ \\ \\ \\ \\ \end{array} \right\}$ NGRP	Capture xsection.
XFIS(I)		Fission xsection.
FNU(I)		No. of neutrons/fission.
XN2N(I)		n, 2n xsection.
XEP(I)		$\sigma_{n,p}^l + \sigma_{n,a}^l$ xsection.
XCAPP(I)		
XFISP(I)		

Repeat the list above for each nuclide.

FILE SIX — File 6 consists of transfer matrix data as follows:

<u>IDMX</u>	Nuclide ID.
NDS	No. of downscatters for matrix 1.
NDT	No. of downscatters for matrix 2.
XTRO(I, J)	Matrix 1.
[(I=1, NGRP, J=I, MIN (I+NDS, NRP))]	
XTR1(I, J)	Matrix 2.
[(I=1, NGRP, J=I, MIN (I+NDT, NGRP))]	

Repeat the list above for each nuclide.

Note: The input above may be modified later to meet the needs of the following segments of FARED: RAIM and REDEP.

The main program of RETAP is illustrated in the flow chart on the following page.

Figure A-1. Flow Chart for the RETAP Program

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