Computer Code Abstracts

3DB

A Three-Dimensional Diffusion Theory Burnup Code

- 1. Name of Code: 3DB.¹
- 2. Computer for Which Code is Designed: UNIVAC 1108. Programming Language: FORTRAN-IV.
- 3. Nature of Code: 3DB is a three-dimensional (X-Y-Z, R- θ -Z, triangular-Z) multigroup diffusion code for use in detailed fast-reactor criticality and burnup analysis. The code can be used to:
 - a. compute k_{eff} and perform criticality searches on time absorption, reactor composition, and reactor dimensions by means of either a flux or an adjoint model
 - b. compute material burnup using a flexible material shuffling scheme
 - c. compute flux distributions for an arbitrary extraneous source.
- 4. Method of Solution: Eigenvalues are computed by standard source-iteration techniques. Group rebalancing and successive over-relaxation with line inversion are used to accelerate convergence. Adjoint solutions are obtained by inverting the input data and redefining the source terms. Material burnup is by reactor zone. The burnup rate is determined by the zone and energy-averaged cross sections which are recomputed after each time-step. The isotopic chains, which can contain any number of isotopes, are formed by the user. The code does not contain built-in or internal chains.
- 5. Restrictions on Complexity: Since variable dimensioning is employed, no simple bounds can be stated.
- 6. Running Time: A k_{eff} calculation with a $20 \times 20 \times 20$ mesh using 2 energy groups requires ~30 min on a UNIVAC 1108. Each successive burnup time-step takes $\sim \frac{1}{4}$ of the above time.
- 7. Unusual Features: The input data are arranged so the code can be used easily for k_{eff} and search calculations without burdening the user with burnup parameters.
- 8. Related and Auxiliary Programs: The format of the input data (e.g., cross sections, geometry and composition specifications) is compatible with the oneand two-dimensional transport codes DTF-IV² and 2DF,³ the perturbation code PERT-V,⁴ the one-dimensional cross-section generating code 1DX,⁵ and the two-dimensional diffusion-burnup code 2DB.⁶ All six codes use the same input module.
- 9. Status: In use.

- 10. Machine Requirements: A 65k memory and 11 peripheral storage devices.
- 11. Material Available: A source deck, sample problem, and operation instructions including a copy of Ref. 1, are available from the authors.
- 12. Acknowledgment: This paper is based on work performed under U.S. Atomic Energy Commission Contract AT(45-1)-1830.
- 13. References:

¹R. W. HARDIE and W. W. LITTLE, Jr., "3DB, A Three-Dimensional Diffusion Theory Burnup Code," BNWL-1264, Battelle Northwest Laboratory (1970).

²K. D. LÁTHROP, 'DTF-IV, A FORTRAN-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering," LA-3373, Los Alamos Scientific Laboratory (1965).

³ "2DF, A Two-Dimensional Transport Code," developed at the Los Alamos Scientific Laboratory, (unpublished).

⁴R. W. HÁRDIE and W. W. LITTLE, Jr., "PERT-V, A Two-Dimensional Perturbation Code for Fast Reactor Analysis," BNWL-1162, Battelle Northwest Laboratory (1969).

⁵R. W. HARDIE and W. W. LITTLE, Jr. "1DX, A One-Dimensional Diffusion Code for Generating Effective Nuclear Cross Sections," BNWL-954, Battelle Northwest Laboratory (1969).

⁶W. W. LITTLE, Jr. and R. W. HARDIE, "2DB User's Manual-Revision 1," BNWL-831 REV1 Battelle Northwest Laboratory (1969)

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FARED

- 1. Name of Code: FARED-A One-Dimensional Fast Reactor Physics Design and Analysis Code.
- 2. Computer for Which Code is Designed: CDC-6600
- 3. Nature of Physical Problem Solved: The FARED code was designed to permit a wide variety of one-dimensional fast reactor physics design calculations. Realistic physics models and free-format directive input allows the user to perform criticality, depletion,

and fuel management studies economically and accurately. The entire code, including the microgroup data library preparation, is an integrated package requiring little or no user intervention during wideranging design studies.

FARED contains an internal cross-section-averaging routine which is responsible for preparing broad group cross-section sets for various material regions of the reactor. The cross-section averaging is performed in program REGA, which computes a B_1 flux and current in up to 20 reactor block compositions for use as weighting functions in the cross-section collapsing calculation. REGA will collapse the RETAP group structure (100 or less) to no more than 30 polygroups with up to 15 groups of downscatter. A microscopic cross-section set will be generated for each reactor block. A reactor block may be a single zone or a combination of zones of similar material content (e.g., core, blanket, reflector), and each block may contain up to 30 different nuclides. A homogeneous or heterogeneous resolved and unresolved resonance treatment is provided to compute effective microgroup resonance cross sections for the block mixture or up to two cell types per block.

Real and adjoint flux distributions are calculated for one-dimensional slab, cylindrical, or spherical geometries. The real fluxes are normalized to yield the desired total reactor power. Criticality searches may be performed on the reactor dimension, transverse buckling or zone compositions. Enrichment searches may be performed to yield desired ratios of maximum (or average) power densities in several zones. Zonewise depletion is calculated either for a given time period or until specified criticality, burnup, or nuclide concentrations are satisfied. Flexible fuel management is available permitting specified material units to be moved into, out of or shuffled within the reactor. A wide variety of edits may be performed. including perturbation and kinetic parameters calculations.

4. Method of Solution: The procedure for computing broad-group microscopic cross sections is similar to that used in the GAM code. For each homogeneous block composition, REGA performs a B_1 computation for the flux and current in each microgroup and uses these as weighting functions to form microscopic cross-section sets for the broad-group structure specified by the user. For resonance nuclides, effective resonance capture and fission cross-section contributions are computed in the unresolved resonance range in a manner similar to that used in the GANDY code. A statistical averaging over chi-squared distribution is used but interference scattering is ignored. Averaging over the distribution is performed using the quadrature scheme introduced by Greebler and Hutchins. The STRIP routine in FARED is responsible for the calculation of effective resonance cross sections in the resolved resonance range. A multigroup collision probability procedure is used to compute the average flux in the lump or mixture for each group in an ultrafine-group mesh which spans the entire resolved resonance range; the boundary for each ultrafine group is computed by STRIP as the calculation proceeds down the energy range. The, calculation begins at the highest energy peak, all resonance nuclides considered. Note that this procedure accounts for overlap and interference effects.

The real and adjoint diffusion equations are solved by a standard fission-source iteration procedure. A starting fission-source distribution is provided by the user. After each iteration the new fission-source distribution is normalized to unity. The depletion equations are solved by a second-order approximation for each of a series of specified minor time steps. The power distribution is assumed constant during each minor time step and the fluxes are renormalized at the end of each of these intervals. The flux distributions are then recalculated at the end of the series of minor time steps. All criticality searches employ the same general algorithm for uniformity in the iterative procedure.

Restrictions on the Complexity of the Problem:

Number of microgroups	$2 \leq N \leq 100$
Number of multigroups	$2 \leq N \leq 30$
Number of downscattering groups	$1 \leq N \leq 15$
Number of mesh points	$3 \leq N \leq 150$
Number of unique nuclides	$1 \leq N \leq 50$
Number of zones	$1 \leq N \leq 20$
Number of blocks	$1 \leq N \leq 20$
Number of zone materials	$1 \leq N \leq 100$
Number of nuclides per block	$1 \leq N \leq 30$
Number of zones per block	$1 \leq N \leq 20$
Number of resonance cells per block	$0 \leq N \leq 2$
Number of nuclides per cell composition	$1 \leq N \leq 15$
Number of nuclides per block composition	$1 \leq N \leq 30$
Number of resonance nuclides per block	$0 \leq N \leq 7$.

In addition to the specific restrictions listed above, dynamic storage allocation may restrict the size of combinations of other parameters.

Typical Machine Time: The execution time for the sample problem given in Vol. 3 of the references was ~18 min on the CDC-6600. This problem includes the calculation of three sets of 17-group microscopic cross sections (core, blanket, and reflector), composition searches, depletion for several time periods, fuel management and extensive edit calculations.

Unusual Features of the Program: The FARED code is a totally integrated fast-reactor design package. It is designed for fast and accurate one-dimensional physics design and survey studies with a strong emphasis on input simplicity. The following are some of the special features of the program:

a. The user is permitted two resonance cells per block to treat, for example, a resonance control material as well as a fuel lump containing resonance nuclides.

b. The microscopic cross sections may be recalculated at any time to account for composition changes during depletion.

c. Depletion chains are constructed by the user and nuclide lists are expanded to include all nuclides in the chain which are produced during depletion. d. The breeding and conversion ratios are automatically defined by specifying certain nuclides as fissile in the depletion chain.

e. Power-density searches are available which adjust material compositions to achieve the desired system eigenvalue and specified ratios of maximum (or average) power densities in given search zones.

f. Nuclide depletion includes destruction by (n,α) and (n,p) reactions and production by (n,2n).

g. The length of a depletion sequence may be determined by the maximum allowable burnup of certain material units, a minimum allowable concentration of certain nuclides or a minimum eigenvalue.

h. A wide variety of edits are available including extensive perturbation edits and the calculation of beta-effective, prompt-neutron lifetime, and promptand delayed-neutron worths.

i. The use of free format input directives allows the user great flexibility in specifying data and constructing sequences of calculations and edits.

- 8. Related and Auxiliary Programs: RETAP-A code for preparing a microgroup library for use by the FARED Code. The library tape generated by this program contains seven data files as follows:
 - (1) Microgroup energies
 - (2) Depletion chain descriptions
 - (3) Resolved resonance data
 - (4) Unresolved resonance data
 - (5) Smooth cross sections and matrices
 - (6) Fission spectra
 - (7) Depletion, fission-product and delayed-neutron data.

An update may be performed on an existing library to add or change nuclide data for any file.

9. Status: The program is currently in production use at Babcock & Wilcox. The following material is available from the Argonne Code Center:

Magnetic Tape Transmittal:

FARED Source Deck	(15387 cards)
RETAP Source Deck	(3916 cards)
RETAP Sample Input	(16471 cards)
RETAP Sample Output	
FARED Sample Input	(79 cards)
FARED Sample Output	

Reference Reports:

Volume 1 - User's Manual

- Volume 2 Listing of RETAP and FARED Codes
- Volume 3 Listing of RETAP and FARED Sample Problem Output
- Volume 4 Production Tests and Sensitivity Studies Using the FARED Code
- 10. Machine Requirements: CDC-6600 or equivalent machine with 1423008 core storage. Sixteen tape drives

or distinct disk files are needed in addition to the usual input and output devices and system requirements.

- 11. Programming Language: Standard CDC FORTRAN IV language is used with the exception of two short COMPASS machine language routines. The program is in overlay structure with three primary overlays and thirteen secondary overlays.
- 12. Operating System: CDC SCOPE 3.
- 13. Any Other Programming or Operating Information: The two COMPASS machine language routines are described in the Reference and are easily convertible to another machine language. Provision is made for varying the number of characters per word in the program.
- Acknowledgment: This research was sponsored by the U.S. Atomic Energy Commission under contract number AT(30-1)-3867.
- 15. References:

¹D. H. ROY, J. M. TILFORD, A. Z. LIVOLSI, P. N. COLPO, C. D. CARMICHAEL, and J. A. JACOBSEN, "Fast Breeder Static Physics Methods Development and Analysis Project," Vol. 1-FARED: One-Dimensional Fast Reactor Physics Design and Analysis Code; Vol. 2-Listing of FARED and RETAP Programs; Vol. 3-Listing of Sample Problem Output from RETAP and FARED Programs, BAW-3867-9 (October 1969).

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REPCDC

- 1. Name or Designation of Program: REPCDC.
- Computer for Which Program is Designed and Others Upon Which it is Operable: CDC-6600.
 Programming Languages: FORTRAN IV, except for random number generators of CDC-6600 at BNL.
- 3. Nature of Physical Problem Solved: Monte Carlo calculation of Resonance Reaction Rates and Resonance Integrals in Reactor Lattices using ENDF/B data. Square or hexagonal lattices of cylindrical rods can be treated. The rods can be subdivided into annular regions at different temperatures. The library contains ²³⁸U and ²³⁵U as well as four isotopes of plutonium. The effect of temperature changes on the Monte Carlo estimates can be studied.
- 4. Method of Solution: Neutron trajectories are traced in the lattice over an energy interval specified in the input. Reaction rates are obtained from the neutron weight which is appropriately modified at each collision. The Breit-Wigner single level formula with interference scattering and Doppler broadening is used to calculate resonance cross sections, as specified in the ENDF/B manual.