

Computer Code Abstracts

CCA - 94

1. Name of Program: ISOCRUNCH.
2. Computer for Which Program is Designed and Others upon Which it is Operable: IBM 7090, CDC 1604-A.
3. Nature of Problem Solved: ISOCRUNCH can be used to compute the amount of each isotope in a reaction and decay chain for any specified neutron flux and time, to sum the contributions of various chains to the same isotope, to graph on an associated electroplotter the yield of an isotope vs time for a given flux and to find the optimum time for maximum yield of an isotope in a chain.
4. Method of Solution: The amount of each isotope in a given reaction and decay chain is computed from the exact analytical solution of the Bateman equations, which describe such processes. The graphical option of this program uses a plotting subroutine written for the Benson-Lehner Model J Electroplotter. Optimization of the time for maximum yield of an isotope is accomplished by a gradient search subroutine.
5. Basic Physics Approximations in the Problem Formulation: This program does not take into account the self-shielding of a target in a reactor or the dependence of reaction cross sections on neutron energy which could be handled by adjusting the input data.
6. Restrictions on the Complexity of the Problems: This program will handle up to 50 isotopes in a chain and sum selected isotopes up to 10 chains.
7. Typical Running Time (IBM-7090): The running time on the computer only can be estimated as about three seconds per isotope times the number of nonzero initial concentrations.
8. Related Program: This program is an extension with modifications on the program CRUNCH (ORNL-2958), which was developed to compute the amount of each isotope in a single reaction or decay chain.
9. Status: Presently in use.

10. Reference:

- ¹Charles W. Friend and J. R. Knight, "ISOCRUNCH—Modifications to the CRUNCH Program for the IBM 7090," USAEC Report ORNL-3689, Oak Ridge National Laboratory.
11. Programming Language Used: This program was written in FORTRAN II language for the IBM 7090, and in FORTRAN 63 language for the CDC 1604-A.
12. Material Available: Program decks and referenced document available from authors.

Charles W. Friend

Oak Ridge National Laboratory
Oak Ridge, Tennessee

J. R. Knight

CDPF, Oak Ridge National Gaseous Diffusion Plant
Oak Ridge, Tennessee

Received September 18, 1964

Revised January 8, 1965

CCA - 96

1. Name of Program: HOT-1
2. Computer for Which Program is Designed: Philco-2000
Programming Language: FORTRAN
3. Nature of Problem Solved: HOT-1 is a digital computer program to solve two-dimensional plane and axially symmetric steady-state heat-conduction problems with diagonal boundaries and interfaces. Mesh spacing (at most 5000 points) is completely variable. As many as 99 regions are permitted in order to describe spatial variations in material properties, heat-generation rates, and boundary conditions. Material properties are assumed to be region-wise constant and independent of temperature.
4. Method of Solution: A nonuniform mesh is imposed on the region of solution, with mesh intervals chosen so that all region interfaces pass through and connect mesh points in either a horizontal, vertical, or diagonal manner. The differential equations are approximated by

five-point difference equations at the mesh points, and the resulting matrix equation is solved by Peaceman-Rachford iteration technique.

5. Restrictions on the Complexity of the Problem: Contact resistances are not specifically included in the program computations, but must be approximated by use of thin regions of a low-conductivity material. Heat-generation rates, boundary film coefficients, and boundary sink temperatures are assumed to be known. The program is intended to handle up to 99 regions, 5000 mesh points, 250 mesh points in each coordinate direction. This program is intended to operate within the BKS System.
6. Typical Running Time: 5 min, Philco-2000-212.
7. Present Status: In production.
8. Reference:

R. B. Smith and J. Spanier, "HOT-1: A Two-Dimensional Steady-State Heat Conduction Program for the Philco-2000," WAPD-TM-465, (July 1964).

9. Authors of Program:

W. D. Peterson

R. B. Smith

J. Spanier

A. E. Sumner, Jr.

Westinghouse Electric Corporation
Bettis Atomic Power Laboratory
P. O. Box 79
West Mifflin, Pennsylvania 15122

Received October 16, 1964

CCA - 97

1. Names of Programs: RECAP-1, RECAP-2, RECAP-3
2. Computer for which Programs are Designed: Philco-2000
Programming System: TAC and FORTRAN
3. Nature of Problem Solved: Monte Carlo estimation of epithermal-resonance capture rates and interference effects in systems containing several spatially distinct regions composed of several resonance absorbers. The geometries available are: 1) a repeating array of slabs (RECAP-1); 2) a hexagonal or square array of circular cylinders (RECAP-2); and 3) rectangular and 60° parallelogram geometry (RECAP-3).
4. Method of Solution:

The energy range of interest may be arbitrarily subdivided into a maximum of 100 groups. To permit a detailed cross-section description, each group, for example g , may be further subdivided into a maximum of 1000 energy intervals. Doppler-broadened cross sections are calculated at each energy point

and retained on magnetic tape. In the resolved energy range, resonance parameters obtained experimentally are used; and in the unresolved energy range, Porter-Thomas statistical distributions are used for the required resonance parameters. The number of groups to be treated statistically is isotope-dependent.

All neutron histories are processed for each group as follows: For group g , the cross sections are obtained from magnetic tape and stored in rapid memory. All events (scattering, absorption, and lengths of free flight) are determined through the use of pseudo-random number sequences until the energy of each neutron falls below the lower cutoff of that group. This condition terminates the history for group g and the emergent parameters for all neutrons are retained on magnetic tape. For the $g+1$ group, cross sections are obtained from tape and stored in rapid memory. The calculation of this group is then performed by reading the emergent parameters from tape and continuing the tracking process until all neutrons degrade in energy below the lower cutoff of the $g+1$ group. The calculations of subsequent groups are similar.

To calculate the absorption rates, the Σ_a/Σ_T estimator is used. Smooth and resonance absorption edits are performed for each isotope per region per energy group. The probable error is computed at the end of each history for each quantity tallied.

5. Unusual Features:

- 1) Smooth and resonance absorptions are edited separately. These edits are convenient in arriving at L-factors (self-shielding factors) for slowing-down programs such as MUFT. To calculate L-factors, the 'heterogeneous resonance integral' is obtained from the resonance capture rates.
- 2) To start a neutron in the energy range under consideration, the slowing-in-source is computed analytically, i.e. it is not necessary to extend the energy range of interest in order to achieve an asymptotic slowing-in-source.
- 3) An approximate sampling method was formulated so as to put the unresolved-resonance cross sections in the same form as those for the resolved resonances; i.e. a fixed tabulation of cross sections stored on magnetic tape for a given temperature.
- 4) A 'two-isotope' method is used either for editing fissions and captures separately or for treating elements with their natural isotopic abundances.
- 5) In addition to elastic scattering, the program permits a 'delta scatterer.' The use