CINDER'90 CODE FOR TRANSMUTATION CALCULATIONS

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ABSTRACT

The CINDER'90 code and library continue to be developed for the description of nuclide inventories produced in a wide range of radiation environments. Although generally applicable, CINDER'90 is typically applied with ancillary codes and the LAHET Code System to describe a variety of accelerator transmutation problems. The first release version of the CINDER'90 code and library LibC90a permit the calculation of inventories of 3400 nuclides of Z $\leq$ 103, using evaluated neutron reaction data below 20 MeV. Data extension efforts are now progressing to extend reaction data to 150 MeV for neutrons and protons, limited to targets of Z $\leq$ 84, in LibC90b. Public release of the code and libraries is now planned for the Fall of 1997.

1 Introduction

CINDER'90 is a neutron transmutation code evolved from earlier versions of CINDER [1] and REAC, [2] using the algorithm of CINDER with modifications to accommodate the input of additional constant destruction and production rates associated with reactions outside of the code's particle or energy domain. In conjunction with other codes simulating the radiation environment, CINDER'90 has been used to describe nuclide inventories in a variety of applications. The library of nuclear data, constantly growing in breadth and quality with international cooperation, now describes 3400 nuclides in the range $1 \leq Z \leq 103$. The CINDER code began its evolution in 1960 at the Bettis laboratory in support of thermal reactor simulation calculations [1]. Its evolution to CINDER'90 is traced in detail in Ref.[3] through 1992, at which time it was limited to activation problems in the range $Z \leq 84$. The impetus for the code's development to that point was the solution of activation problems of medium- and high-energy accelerator facilities (SSC, LHC, LAMPF, LANSCE, MLNSC, etc.) typically associated with beam spills, beamstops, and air activation. With the addition of coding and data to describe transmutation of higher-Z nuclides, including the spontaneous fission (SF) and neutron-induced fission (n,f) of actinides, the range of applications is greatly extended.

2 Code Description

All CINDER versions use Markovian chains to determine temporal densities of nuclides in a neutron environment, solving for independent contributions to atom densities in each of a number of linear nuclide chains. Earlier CINDER versions required the *a priori* formation of a consistent set of linear chains to describe all significant nuclides and transmutation paths for a family of problems (e.g., thermal reactors). This chain formation reflects the comparison of competing transmutation paths (e.g., decay constant λ_i vs reaction probability $\phi\sigma_j$ for each decay path i and reaction path j); choices made in the necessary limiting of the length and number of chains reflect the magnitude of each $\phi\sigma_j$ as determined by the energy-dependence and magnitude of each cross section σ_j and of the neutron flux ϕ typifying the family of problems.

In CINDER'90, rather than using a preexisting chain structure, each path from each nuclide defined by available nuclear data is followed until all tests of significance are failed. A key quantity resulting from the analytic solution for the density of the i^{th} nuclide in a chain is the time-integrated transmutation of that nuclide. This quantity, called the *passby,* indicates the sum of densities of all subsequent nuclides produced in all paths emanating from the i^{th} nuclide; an insignificant *passby* is an important test for path termination.

A significant, recent change in CINDER'90 code philosophy relates to the formation of outlying nuclides far from stability as products of reactions input from other codes but absent from the CINDER'90 library. Previously, a β^+ or β^- path of decay toward stability was established by defining the half-live and decay energy of each nuclide missing from the library, using default data. This exercise required the automated but timely creation of a new library for each problem. The new procedure simply redirects the production probability of each outlying nuclide to the closest present isobar, expediting the calculation.

CINDER'90 calculates only the atom density, activity density, and cumulative SF and (n,f) events for each nuclide in each time step. The code calculates fissions both analytically and numerically with trapezoidal integration (averaging beginning and ending fission rates over the step). These calculated results, a concentrated file of problem-specific library data, and a file of data specifying table selections, titles, and column headings are passed to TABCODE. This is an ancillary program that reads the calculated density, activity, and fission-rate results and produces as many as forty-three selected tables by combining the CINDER'90 results with basic nuclear data and regulatory limits for each of the nuclides.

CINDER'90 typically begins a problem with the atom densities of the homogenized materials of a region, for which the flux spectrum has been calculated in another program simulating the radiation environment; the flux spectrum is retained throughout the problem, but the flux magnitude may be varied from step to step in modeling the irradiation history as desired. Alternatively, a CINDER'90 calculation can begin with a nuclide inventory produced in a previous CINDER'90 calculation tracing the material's irradiation history in a different radiation environment. In problems modeling radiation environments with significant fluxes of particles other than neutrons within the energy extent of the library, a file of the net production of reaction products in these additional fluxes must be calculated independently in a simulation code (e.g., LAHET) and supplied to CINDER'90: reactions on these product nuclides in the additional fluxes are typically not included in the simulation, but reactions on the products in the neutron flux are followed in CINDER'90.

In the analysis of complex, multi-region geometries having unique neutron fluxes, the inventory properties produced in TABCODE calculations for the separate regions are retained and passed to ALLCODE. This is an ancillary code that accumulates significant quantities from all regions and provides convenient tables describing the complete geometry.

3 DATA DEVELOPMENT

The CINDER'90 development effort has been at least as much a data development and evaluation effort as a code development effort. CINDER'90 has built on the library structure of the REAC code [2], which solved for reaction products and a few generations of product daughters. Both codes suffered initially from data limited in scope and quality, and both have evolved independently in quality and breadth. The continuing collection, evaluation, and adjustment of data for CINDER'90 has been successful largely because of the cooperation of data evaluators throughout the international data community.

Much of the cross-section data of the CINDER'90 library for $Z \leq 84$ has come from Version 3 of the European Activation File (EAF-3) [4] produced at the Netherlands Energy Research Foundation (ECN). The cooperation between that laboratory and our effort has been exemplary. We have participated with them in the validation [5],[6] and improvement[7] of the data and look forward to the application of the evolved ECN Activation File (ECNAF) data in the library of CINDER'90.

Features of some projects in the Accelerator Driven Transmutation Technology Program at Los Alamos require the accurate treatment of neutron-induced fission of actinides — a familiar domain of well established earlier CINDER versions[1]. The extension of the library to higher Z elements has depended greatly upon ENDF/B-VI data [8][9] for cross-section and decay data. The fifty fission yields of Preliminary ENDF/B-VI [10] have been used to describe fission-product production in problems containing actinide materials.[11] Also, data of JEF-2.2 [12] have contributed as entries in the Master Decay Library maintained by F. M. Mann et al. [13] used, in part, in the library. A recent Japanese chart of the nuclides, showing theoretical half-lives of many outlying nuclides far from stability, has been used to extend the library.

4 FUTURE PLANS

The development of the CINDER'90 code and data have followed the paths demanded by the involvement of Los Alamos in accelerator-driven facilities[3] . The future development of the code depends upon the laboratory's expected continued participation in such projects.

These calculations have typically coupled simulation results from the LAHET Code System (LCS) of Monte Carlo codes.[14] In LCS, the LAHET code [15] uses on-line reaction models for data describing neutrons above some energy ELON and ions at all energies; neutrons born at or transported to an energy below ELON are passed to a version of the MCNP Monte Carlo code[16], which uses evaluated cross-section data extending at least to ELON in transporting the neutrons in the lower energy regime. MCNP transport data libraries, in the past limited to a maximum neutron energy of 20 MeV, have fixed ELON at this energy or lower. The validity of the LAHET modeled cross sections has been observed to be questionable at lower energies, perhaps below about 150 MeV.

Transport data libraries have been produced for limited nuclides using evaluated data for coupled, continuous-energy n-γ transport and for coupled, multigroup n-p-γ transport, permitting the neutron interface at ELON between LAHET and MCNP to be raised to 150 MeV in many problems. The cross-section data of CINDER'90 must therefore be extended to 150 MeV. This data extension effort has resulted in the postponement of the release of the operational code and 20-MeV library until the Fall of '97. At that time it is anticipated that the code will be released with the present 20-MeV library LibC90a for $1 \leq Z \leq 103$ and a preliminary library LibC90b extending to 150 MeV for both proton– and neutron–induced activation limited to $1 \leq Z \leq 84$

5 CONCLUSIONS

CINDER'90 is a unique transmutation code having a library of 63-group cross sections and requiring no library preparation prior to execution. The code requires a multigroup neutron flux for $E_n \leq 20$ MeV and nuclide production rates for reactions at higher neutron energies or for additional particles. The code has been developed for accelerator-driven problems, but is applicable to any transmutation problem for which simulation calculations of particle reactions are available. Data work is continuing and a library describing neutron and proton reactions to 150 MeV is under development.

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