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TITLE: RECENT DEVELOPMENT OF THE CINDER'90 TRANSMUTATION CODE AND DATA LIBRARY FOR ACTINIDE TRANSMUTATION STUDIES

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RECENT DEVELOPMENT OF THE CINDER'90 TRANSMUTATION CODE AND DATA LIBRARY FOR ACTINIDE TRANSMUTATION STUDIES

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ABSTRACT

CINDER'90 is a neutron transmutation code evolved from earlier versions of CINDER and REAC, 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 $1 \leq Z \leq 103$.

INTRODUCTION

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. (2) 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, 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.

CODE DESCRIPTION

CINDER is used to track, for each nuclide (Z, A and state), all transmutation paths (decays and neutron reactions) producing product nuclides differing from the original. It uses 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 pre-existing chain structure, each path from each nuclide 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,* equals the sum of densities of all subsequent nuclides produced in all paths emanating from the i^{th} nuclide.

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. 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 isobar, expediting the calculation.

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(2).

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 both analytic fission rates and trapezoidal fission rates (averaging beginning and ending values over the step). These calculated results, a 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. These tables are described in Table I.

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 below the 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 as outlined in Table II. Note that the second set of four tables produced by ALLCODE contain the same information as the first set of four, except that the later data are ranked at some selected time.

Table I: The 43 Tables Produced by TABCODE for Each Region

Order	Content
Quantities by Nuclide:	
1	Atom Density by Nuclide (atoms/barn-cm)
2	Total Mass (kg) by Nuclide
3	Activity Density (curies/cc)
4	Total Activity (curies) by Nuclide
5	Decay Power Density (watts/cc) by Nuclide
6	Total Decay Power (watts) by Nuclide
7	Macroscopic Neutron Absorption (/cm) by Nuclide
8	Radionuclide Hazard Air Dilution Factor by Nuclide
9	Radionuclide Hazard Water Dilution Factor by Nuclide
10	Spontaneous Fission Density (#/cc-s) by Nuclide
11	Spontaneous Fission Power Density (w/cc) by Nuclide
12	Spontaneous Fission Power (w) by Nuclide
13	Neutron-Induced Fission Density (#/cc-s) by Nuclide
14	Neutron-Induced Fission Power Density (w/cc) by Nuclide
15	Neutron-Induced Fission Power (w) by Nuclide
16	Total Fission Density (#/cc-s) by Nuclide
17	Total Fission Power Density (w/cc) by Nuclide
18	Total Fission Power (w) by Nuclide
19	Major (>.1%) Nuclide Contributors to Mass
20	Major (>.1%) Nuclide Contributors to Activity
21	Major (>.1%) Nuclide Contributors to Decay Power
22	Major (>.1%) Nuclide Contributors to Absorption
23	Major (>.1%) Nuclide Contributors to Air Dilution
24	Major (>.1%) Nuclide Contributors to Water Dilution
25	Major (>.1%) Nuclide Contributors to SF Power
26	Major (>.1%) Nuclide Contributors to (n,f) Power
27	Major (>.1%) Nuclide Contributors to Total Fission Power
Quantities by Element Z:	
28	Total Mass (kg) by Element
29	Total Activity (curies) by Element
30	Total Decay Power (watts) by Element
31	Total Macroscopic Neutron Abs. (/cm) by Element
32	Total Air Dilution Factor by Element
33	Total Water Dilution Factor by Element
34	Total Fission Power (watts) by Element
Quantities by Nuclide Mass A:	
35	Total Mass (kg) by Nuclide Mass A
36	Total Activity (curies) by Nuclide Mass A
37	Total Decay Power (watts) by Nuclide Mass A
38	Total Macroscopic Neutron Abs. (/cm) by Mass A
39	Total Air Dilution by Nuclide Mass A
40	Total Water Dilution by Nuclide Mass A
41	Total Fission Power (watts) by Nuclide Mass A
Quantities by Energy:	
42	Macroscopic Neutron Absorption (/cm) by Energy Gp.
43	Multigroup Gamma Spectra (#/bin-s-cc)

Table II: Summary Tables Produced by ALLCODE

Order	Content
Quantities by Nuclide:	
1	Total Mass by Nuclide, kg --- All Regions
2	Total Activity by Nuclide, ci --- All Regions
3	Total Decay Power by Nuclide, w --- All Regions
4	Total Fission Power by Nuclide, w --- All Regions
Quantities by Nuclide -- Ranked at a Selected Time:	
5	Total Mass by Nuclide, kg - All Regions - Ranked
6	Total Activity by Nuclide, ci - All Regions - Ranked
7	Total Decay Power by Nuclide, w - All Regions - Ranked
8	Total Fission Power by Nuclide, w - All Regions - Ranked
Quantities by Region:	
9	Total Mass by Region, kg --- All Regions
10	Total Activity by Region, ci --- All Regions
11	Total Decay Power by Region, w --- All Regions
12	Total Air Dilution Factor by Region --- All Regions
13	Total Water Dilution Factor by Region --- All Regions
14	Total Fission Power by Region, w --- All Regions

DATA DEVELOPMENT

CINDER'90 has built on the library structure of the REAC code (3), 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.

The CINDER'90 development effort has been at least as much a data development and evaluation effort as a code development effort. Some characteristics of the content of the present CINDER'90 library are described in Table III.

Much of the data of the CINDER'90 library has come from the EAF-3 library (4) produced at ECN. The cooperation between that laboratory and our effort has been exemplary. We have participated with them in the validation of EAF-4 and look forward to the application of EAF-4.1 data in our 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.

The extension of the library to higher Z elements has depended greatly upon ENDF/B-VI data (5,6) for cross-section and decay data. The fifty fission yields of Preliminary ENDF/B-VI have been used to describe fission-product production because of the preponderance of benchmark calculations made with these data in comparisons with measurements and available now for CINDER'90 validation. Also, data of JEF-2.2 have contributed as entries in the Master Decay Library maintained by F. M. Mann and others (7).

Data validation efforts to date have concentrated on comparisons of calculated activities

with data measured for non-actinide problems (8). A comprehensive comparison with all measured neutron reaction data of the CSISRS data file is underway (9).

Table III: Content of Present CINDER'90 Data Library

Value	Quantity
25	Maximum Neutron Energy, MeV
63	Neutron-Group Cross Sections
25	Photon-Group Spectra
3400	Total Nuclides
259	Stable Nuclides
3141	Unstable Nuclides
2762	Ground State Nuclides
583	1st. Isomeric State Nuclides
55	2nd. Isomeric State Nuclides
55	Nuclides Decaying by Spontaneous Fission
736	Nuclides Having Reaction Paths
66	Nuclides Having (n,f) Paths
15269	Total Non-fission Reaction Paths
4041	Total Non-fission Decay Paths

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. The future development and eventual release of the code depend on the laboratory's expected continued participation in such projects

These calculations have typically coupled simulation results from the LAHET Monte Carlo code, which uses on-line reaction models for data describing neutrons above 20 MeV and ions at all energies. In the LAHET Code System (LCS), neutrons born or transported below 20 MeV are passed to the MCNP Monte Carlo code that uses evaluated data libraries in transporting the neutrons in the lower energy regime. The validity of the LAHET modeled cross sections has been observed to be questionable at lower energies, perhaps below about 100 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 between LAHET and MCNP to be raised to 100 MeV in many problems. The use of this data eliminates the production of reaction products above 20 MeV for use in CINDER'90. The cross-section data of CINDER'90 must therefore be extended to 100 MeV. We are fortunate in that two Russian compilations have recently been completed to 100 MeV. These are:

- MENDL-2, a library of 57835 threshold reactions on 505 long-lived ($T_{\frac{1}{2}} \leq 1$ day)

and stable nuclides in the range $13 \leq Z \leq 84$ (10); and,

- WIND, a library of 576 reactions on $^{232-238}U, ^{237,239}Np, and ^{236-244}Pu$ (11).

It is anticipated that these data, along with GNASH code results retained from the 100-MeV transport data development effort, will contribute greatly to the extension of the CINDER'90 library to 100 MeV. However, the melding of these data with the existing library will require a considerable evaluation effort.

The second release of ENDF/B-VI fission yields, described in Ref. (12), and now available and will be incorporated into the CINDER'90 library as time permits.

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.

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