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Computer Code Abstract

DANDE—A Linked General Code System for Core Neutronics/Depletion Analysis

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Abstract—*DANDE—a modular neutronics, depletion code system for reactor analysis—is described. It consists of nuclear data processing, core physics, and fuel depletion modules, and it allows one to use diffusion and transport methods interchangeably in core neutronics calculations. This latter capability is especially important in the design of small modular cores. Additional unique features include the capability of updating the nuclear data file during a calculation; a detailed treatment of nuclide inventories and aggregate properties of burnable poisons, fission products, and actinides in the fuel; and the ability to make geometric changes such as control rod repositioning and fuel relocation in the course of a calculation. The detailed treatment of reactor fuel burnup, fission product creation and decay, as well as inventories of higher order actinides is a necessity when predicting the behavior of reactor fuel under increased burn conditions. The operation of the code system is illustrated by two actual problems.*

I. INTRODUCTION

The applied nuclear data, core-neutronics, depletion (DANDE) code system was initially developed for use in the analysis of advanced liquid-metal fast breeder reactor (LMFBR) concepts, but its flexibility allows application to other reactor types as well. The philosophy of the DANDE development has been to use standard, validated codes, files, and data libraries, linking them on a Los Alamos Class VI, Cray computer and guiding their interaction with a locally written controller. The result is the three-module code system shown in Fig. 1 consisting of data processing, core neutronics, and depletion modules. In Fig. 1 the modules are shown as rectangles, and the circles in between represent standard files[1] for transferring data between modules. Thus, any appropriate code that can operate in the standard file environment can be used in the code modules.

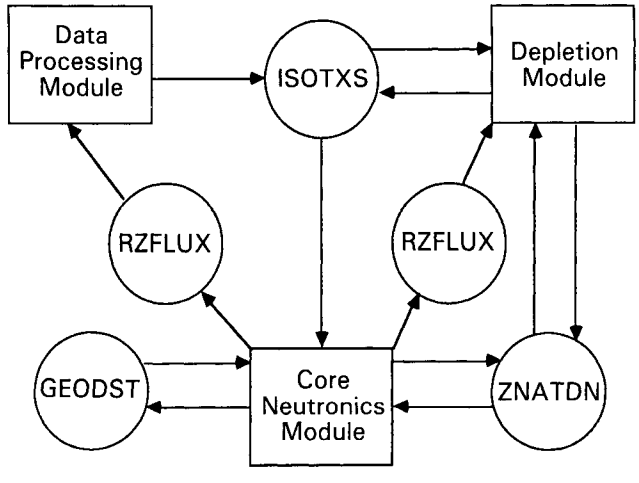

Fig. 1. DANDE code system for reactor core analysis.

Currently the data processing module consists of the TRANSX code[2] operating on a fine-group library generated by the NJOY code[3] from the evaluated nuclear data file[4] (ENDF/B-V). TRANSX produces neutron, photon, or coupled transport cross-section tables in the standard ISOTXS format. The code contains options for adjoint tables, mixtures, self-shielding/Doppler corrections, group collapse, cell homogenization, thermal upscatter, prompt or steady-state fission, transport corrections, elastic removal corrections, and flexible response function edits. As indicated in Fig. 1, fine-group weighting fluxes for group collapse computed in the core neutronics module are transferred to TRANSX via the standard RZFLUX file. Normally, the fine-group core neutronics model contains one dimension less than the final coarse-group model. In calculations for the fast flux test facility (FFTF) experiment discussed in Sec. IV, for example, fluxes from a two-dimensional, cylindrical, 80-group diffusion calculation were used in TRANSX to produce 12-group cross sections for the final three-dimensional hexagonal-Z model. During the course of a long time-depletion calculation with control rod and/or fuel repositioning, it may be necessary to recalculate the fine-group core model and rerun the data processing module to produce an updated ISOTXS file. This can be done with the controller. On the other hand, because ISOTXS is a standard file, ISOTXS files produced with codes other than TRANSX from outside Los Alamos can also be used.

The codes currently being used in the core neutronics model include the DIF3D diffusion code[5] (finite difference and nodal options in hexagonal and orthogonal geometries) and the TWODANT[6] (cylindrical geometry) and TWOHEX[7] (hexagonal geometry) discrete ordinates transport codes. The large, three-dimensional diffusion calculations discussed in Sec. VI run most efficiently on the Los Alamos largest Cray machines (1.8- or 3.0-M word storage), with the core neutronics calculation taking ~3 min per time step. The running times for two-dimensional problems using the S_n codes are comparable to those for three-dimensional problems using the diffusion code.

The CINDER-3 code,[8] an enhanced version of the CINDER-2 code,[9-12] is the only code used to date for the DANDE depletion module. Using data from the ISOTXS file and its own library data file,[12] the RZFLUX, and ZNATDN files produced by the core neutronics module, this code does inventory calculations with extensive fission product and actinide chains and provides updated nuclear densities for the principal nuclides in the ZNATDN file. The nonexplicit actinides and fission products are grouped into two aggregates, respectively; densities for each are placed on the ZNATDN file; and microscopic cross sections for each are placed on the ISOTXS file in preparation for the core calculation for the next time step. A total of 223 fission products and 46 actinides in 186 chains are used in the CINDER-3 calculation; burnable poisons (e.g., boron, samarium, and europium) are also handled in detail.

The local controller used to manipulate and/or monitor the three modules is written in CTL, a language developed at Los Alamos. CTL is used as FORTRAN would be to loop through the time steps in a depletion problem, calling in the various codes and files in the proper sequence. Geometric changes, such as control rod repositioning and fuel relocation, can be made between depletion time steps by deleting the GEODST file and supplying the core neutronics code with a new INPUT file reflecting the changes.

II. DATA PROCESSING MODULE

In most of our work to date, the DANDE data processing module, TRANSX, has used two fine-group libraries, both of which were generated by the NJOY code using basic nuclear data from ENDF/B-V. The first of these,[2] MATXS6, is an 80-neutron × 24-photon group library intended for fast reactor analysis but is also appropriate for fusion studies and shielding calculations. This library features extensive self-shielded cross sections for temperatures from 300 K to as high as 5000 K for some materials. MATXS6 currently contains data for ~100 nuclides, but data for additional materials are constantly being added as the need arises. MATXS6 has been used in DANDE code applications, which include LMFBR advanced concept studies and LCCEWG-5 calculations[13] discussed in Sec. VI.

The other library[2] used, MATXS7, is a 69-group neutron-only library designed for light water reactor problems. It includes self-shielded cross sections for the important actinides. Thermal scattering data are given for all materials, with bound scattering for the important moderators. The group structure has 42 thermal groups extending up to 4.00 eV. MATXS7 was used in the DANDE application to the Omega West Reactor (OWR) fuel element depletion problem described in Sec. VI.

As an example of the use of the TRANSX code in the DANDE data processing module, consider the production of the ISOTXS file for the LCCEWG-5 experiment discussed in Sec. VI. The processing path used is shown in Fig. 2. As indicated in the figure and mentioned above, the basic library used was MATXS6, the fine-group energy boundaries of which are given in Table I. Also given in Table I are the collapsed 12-group energy boundaries for the ISOTXS data file used in the final benchmark calculation.

Note in Fig. 2 that TRANSX must be run in two passes before the final 12-group ISOTXS file is produced. The purpose of the first pass is to provide an 80-group ISOTXS file for the two-dimensional flux calculation. The RZFLUX file produced is then used

TABLE I

Boundaries for 80-Group Structure
(12-Group Boundaries Indicated)

Group	Energy (eV)	Group	Energy (eV)
1	2.0000×10^{7} [a]	41	1.5034×10^{4} [a]
2	1.6905×10^{7}	42	1.3268×10^{4}
3	1.4918×10^{7}	43	1.1709×10^{4}
4	1.3499×10^{7}	44	1.0333×10^{4}
5	1.1912×10^{7}	45	9.1188×10^{3}
6	1.0000×10^{7}	46	8.0473×10^{3}
7	7.7880×10^{6}	47	7.1017×10^{3}
8	6.0653×10^{6}	48	6.2673×10^{3}
9	4.7237×10^{6}	49	5.5308×10^{3} [a]
10	3.6788×10^{6} [a]	50	4.8810×10^{3}
11	2.8650×10^{6}	51	4.3074×10^{3}
12	2.2313×10^{6}	52	3.8013×10^{3}
13	1.7377×10^{6}	53	3.3546×10^{3}
14	1.3534×10^{6} [a]	54	2.9604×10^{3}
15	1.1943×10^{6}	55	2.6126×10^{3}
16	1.0540×10^{6}	56	2.3056×10^{3}
17	9.3014×10^{5}	57	2.0347×10^{3} [a]
18	8.2085×10^{5}	58	1.7956×10^{3}
19	7.2440×10^{5}	59	1.5846×10^{3}
20	6.3928×10^{5}	60	1.3984×10^{3}
21	5.6416×10^{5}	61	1.2341×10^{3}
22	4.9787×10^{5} [a]	62	1.0891×10^{3}
23	4.3937×10^{5}	63	9.6112×10^{2}
24	3.8774×10^{5}	64	7.4852×10^{2} [a]
25	3.0197×10^{5} [a]	65	5.8295×10^{2}
26	2.3518×10^{5}	66	4.5400×10^{2}
27	1.8316×10^{5}	67	3.5358×10^{2}
28	1.4264×10^{5}	68	2.7536×10^{2} [a]
29	1.1109×10^{5} [a]	69	1.6702×10^{2}
30	8.6527×10^{4}	70	1.0130×10^{2}
31	6.7379×10^{4}	71	6.1442×10^{1}
32	5.2475×10^{4}	72	3.7267×10^{1}
33	4.0868×10^{4} [a]	73	2.2603×10^{1}
34	3.1828×10^{4}	74	1.3710×10^{1}
35	2.8088×10^{4}	75	8.3153×10^{0}
36	2.6058×10^{4}	76	5.0435×10^{0}
37	2.4788×10^{4}	77	3.0590×10^{0}
38	2.1875×10^{4}	78	1.1254×10^{0}
39	1.9305×10^{4}	79	4.1399×10^{-1}
40	1.7036×10^{4}	80	1.5230×10^{-1}
		81	$1.3888 \times 10^{-4} Emin$ [a]

[a]Twelve-group boundaries.

in the second TRANSX pass, which results in the 12-group ISOTXS file used in three-dimensional calculations. Normally, a default 80-group flux is employed in the first TRANSX pass, but in the case of preparation of the data file for LCCEWG-5, 80-group initial fluxes were available from preliminary FFTF calculations.

The 12-group ISOTXS file produced from the second TRANSX pass is ready for use in the core neutronics and depletion modules for three-dimensional FFTF cycle-1 depletion calculations. As is indicated in Figs. 1 and 2, this file could be updated during depletion steps by suitable application of the CTL controller. In fact only one 12-group ISOTXS file was generated for LCCEWG-5.

III. CORE NEUTRONICS MODULE

Any core neutronics code that operates in the standard file environment can be used in the core neutronics module. To date we have used DIF3D, TWODANT, and TWOHEX in DANDE calculations. The principal calculations reported here were made with the diffusion code DIF3D; comparison transport calculations were made with TWOHEX.

DIF3D was developed at Argonne National Laboratory and is a computer code that uses the mesh-centered, finite-difference approximation to obtain numerical solutions of the multigroup diffusion equations in one, two, or three dimensions for fast reactor applications. The code was written to employ the rigorous strategies of the PDQ-7 code,[14] and significant efforts were expended during development to provide efficient, yet flexible, data management and data structures.

Incorporated in DIF3D for the solution of two- and three-dimensional hexagonal geometry problems is a nodal option that uses input data virtually identical to that of the finite-difference option. Comparison of these two options for a typical LMFBR core design has shown that the accuracy of the nodal solution is superior to that of a standard (6-mesh cells per hexagon, 5-cm axial mesh spacing) finite difference calculation and that this improved accuracy is also achieved with a significant reduction in computational cost for a three-dimensional calculation. In the course of preliminary calculations for LCCEWG-5, the largest problem we ran on our Cray machines was a one-third-core model of the FFTF core in hexagonal-Z geometry with 13 axial planes and 80 groups. This problem ran in 12 min. More typical full-core models with 17 planes and 12 groups run in 3 to 4 min on the Cray machines. These problems run efficiently only on our machines having 1.8- or 3.0-M word storage.

TWODANT, developed at Los Alamos, is a code package for two-dimensional, diffusion-accelerated, neutral-particle transport. It is designed to solve the two-dimensional, time-independent, multigroup discrete ordinates form of the Boltzmann transport equation.

We have employed TWODANT in preliminary FFTF studies using the R-Z model in Fig. 3, with

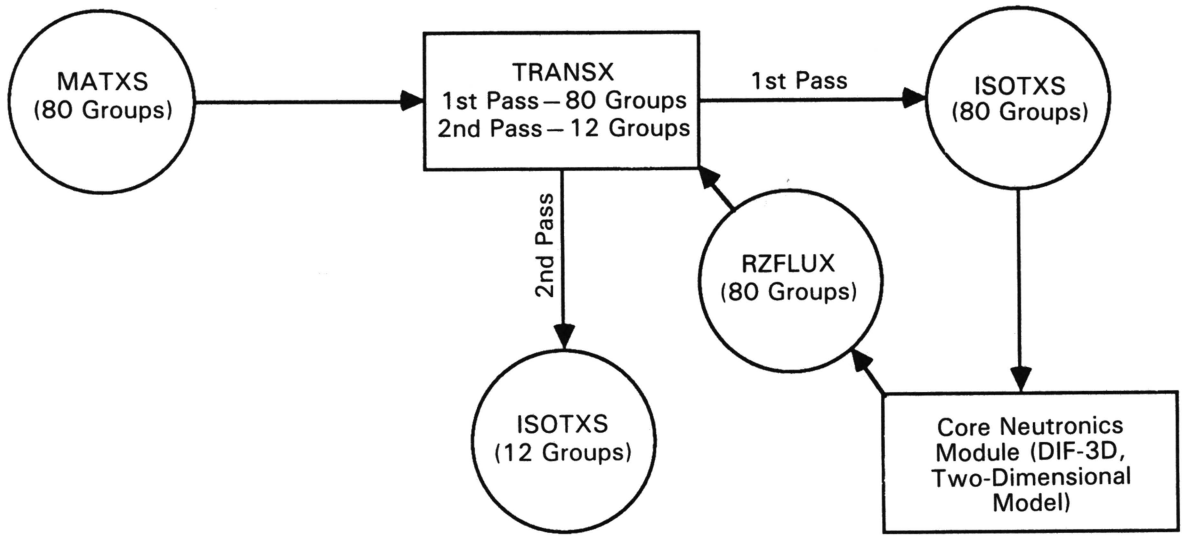

Fig. 2. DANDE data processing module configuration to produce the ISOTXS file for LCCEWG-5.

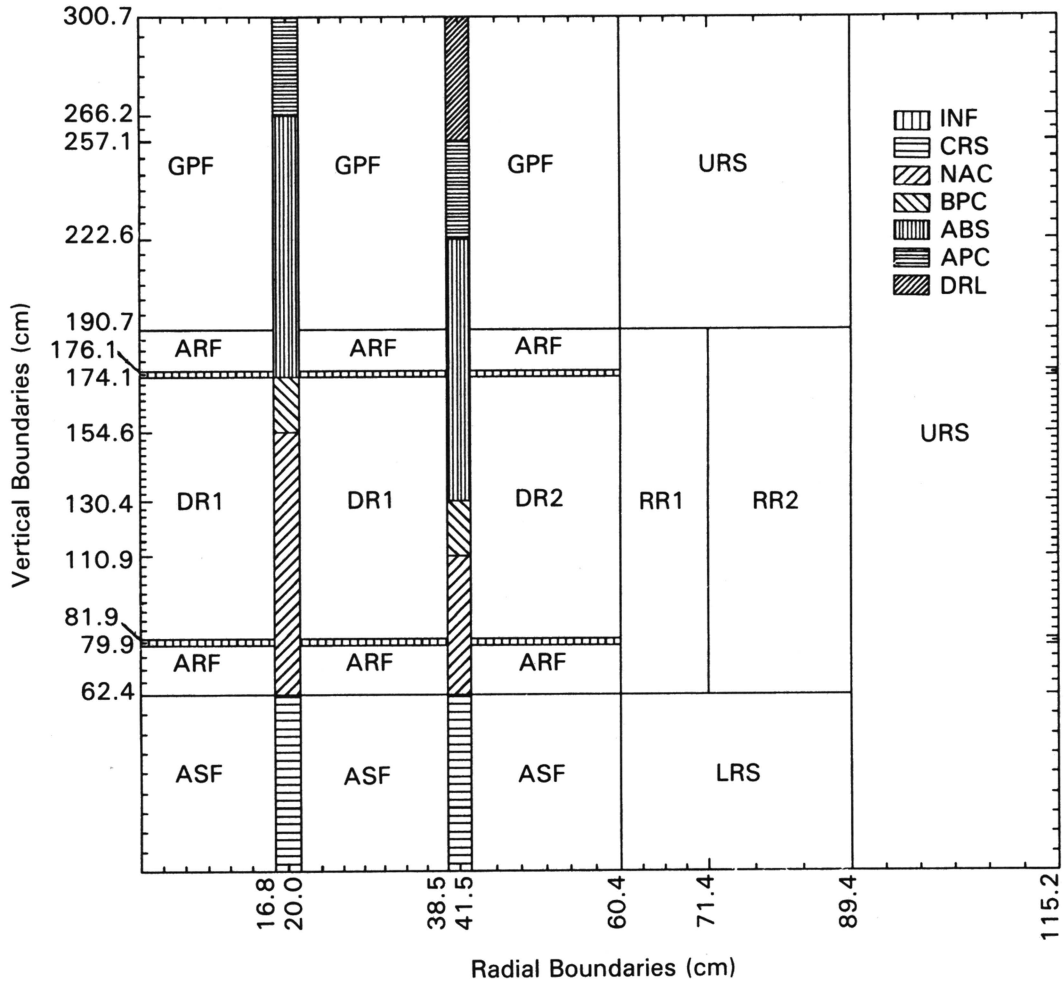

Fig. 3. FFTF/HPC *R-Z* model. Control assemblies are inserted about halfway into core. Tables II and III identify the reactor regions given in the legend. The control assembly is labeled ABS and the fuel regions are labeled DR1 and DR2. Major tick marks give region boundaries. Minor tick marks indicate number of points per region.

TABLE II

Region Vertical Boundaries After Homogenization

Number	Vertical Height (cm)	Region Description	Region Designation
1	62.4	Axial shield – fuel	ASF
1	62.4	Lower radial shield	LRS
1	62.4	Control assembly shield	CRS
2	79.86	Axial reflector – fuel	ARF
3	81.91	Insulator – fuel	INF
4	110.91	Sodium channel – control assemblies inserted halfway	NAC
5	130.41	Below poison channel – control assemblies inserted halfway	BPC
6	154.55	Sodium channel – safety assemblies withdrawn	NAC
7	174.05	Various fuel, characterizer, and experimental assemblies	[a]
7	174.05	Below poison channel – safety assemblies withdrawn	BPC
8	176.1	Insulator – fuel	INF
9	190.69	Axial reflector – fuel	ARF
10	222.55	Absorber – control assemblies inserted halfway	ABS
11	257.1	Above poison channel assemblies inserted halfway	APC
12	266.19	Absorber – safety assemblies withdrawn	ABS
13	300.74	Gas plenum – fuel region	GPF
13	300.74	Above poison channel of safety assemblies	APC
13	300.74	Driveline – control assemblies	DRL
13	300.74	Upper radial shield	URS

[a]Included are fuel types – F31, F32, F41, F42 (homogenized fuel DR1, DR2, DR1A); in-core shim assemblies (ICS); vibration open test assemblies (VOT); blanket test assemblies – SR1, SR2, W18, and W42; absorber test assemblies – HA3 and HA6; and reactor characterizer assemblies – CH1, CH2, CH3, CH4, and CH5.

region descriptions as given in Tables II and III, to compare both transport and high order (P_3) scattering in our calculations. The 80-group RZFLUX file from a TWODANT calculation was used in TRANSX to produce a P_3 ISOTXS file for comparing diffusion and discrete ordinates methods.

TWOHEX is also a Los Alamos code that solves the two-dimensional multigroup form of the neutral-particle, steady-state Boltzmann equation but on an equilateral triangular mesh in the x-y plane. The discrete ordinates form of the approximation is used for treating the angular variation of the particle distribution, and a linear characteristic/nodal scheme is used for spatial discretization. A standard inner (within-group) iteration, outer (energy-group-dependent source) iteration technique is applied. Both inner and outer iterations are accelerated using the Chebyshev acceleration method.[15]

Two-dimensional model DIF3D-TWOHEX comparisons were made in the course of the FFTF cycle-1 experimental studies. In these problems the vertical height was represented by a vertical buckling obtained by matching the two-dimensional with the three-dimensional DIF3D eigenvalues. Results are discussed in Sec. VI.

IV. DEPLETION MODULE

The code currently used for the DANDE depletion module is the CINDER-3 code, an enhanced version of the CINDER-2 code, and thus a member of the generic CINDER (Refs. 9, 10, and 11) nuclide inventory code family. CINDER resolves the coupled system of decay/reaction equations into a collection of

TABLE III

Radii for R-Z Homogenization at $Z = 81.91$ cm

Number	Inner Radius	Outer Radius	Region Name	Region Designation
1	0.0	16.76	Driver-1	DR1
2	16.76	20.03	Safety assembly	NAC
3	20.03	38.53	Driver-1	DR1
4	38.53	41.54	Control assembly	NAC
5	41.54	60.43	Driver-2	DR2
6	60.43	71.39	Radial reflector-1	RR1
7	71.39	89.36	Radial reflector-2	RR2
8	89.36	115.25	Shield	URS

linear chains using a Markov model. The linear chains can then be solved analytically and evaluated numerically.

Versions of CINDER have been incorporated into reactor physics codes, such as PDQ-HARMONY (Ref. 16) and EPRI-CELL (Ref. 17), for 20 yr or more. Typically, in the past, fission product neutron absorption has been treated by describing only a few major absorbers and/or groupings of fission product neutron absorption in one or more fictitious "lumps" generated independently of the spatial physics code. Neutron absorption in higher actinides (americium and curium) has often been ignored. In DANDE, however, three-dimensional physics calculations of the core neutronics module are performed with accurate actinide inventory; aggregate fission product and higher actinide reaction data are rapidly calculated by CINDER-3 for each volume element by summing the calculated values of all contributing nuclides.

The data processing and core neutronics modules provide initial nuclide atom densities (ZNATDN file), energy-group fluxes (RZFLUX file), and resonance self-shielded cross sections for abundant, explicitly treated nuclides (ISOTXS file) for each volume element. CINDER-3 returns end-of-time-step (EOS) atom densities of the explicit nuclides, and it groups nonexplicit fission product and actinide quantities for use in the next-time-step calculation of the core neutronics module. These aggregate quantities, accumulated separately for nonexplicit fission products and actinides, include atom densities and cross sections for (n,n), (n,n'), $(n,2n)$, (n,γ), fission, and total neutron absorption in the energy-group structure specified in the ISOTXS file. The data for all individual fission products and actinides are written to another file and are thus available for further exposure in the next call to the depletion module.

CINDER-3, shown schematically in Fig. 4, combines the functions of the CINDER-2 nuclide inventory code and its ENDF/B-V based data library with the TOAFEW-V (Ref. 12) collapsing code that uses a library of 154-group cross sections processed from ENDF/B-V augmented with $(n,2n)$ cross sections from Hanford Engineering Development Laboratory model calculations.[18] All calculations use the chain library, which contains the basic nuclear data describing the various nuclide couplings by fission yield, radioactive decay, and neutron absorption. Inventories within each region at the EOS are calculated using the energy group fluxes, nuclide atom densities, and group cross sections associated with the region at the beginning of the time step, as indicated in Fig. 4 by the RZFLUX, ZNATDN, and ISOTXS standard files, respectively.

V. CTL

The core neutronics module and the depletion module of the DANDE system communicate via numerous files. Often the application requires that fuel rods be repositioned or that fuel elements be changed between depletion time steps. Running multistep problems by hand is extremely tedious and error prone. Therefore, a controller written in CTL is composed for each application, allowing the problem to be run in interactive or production mode.

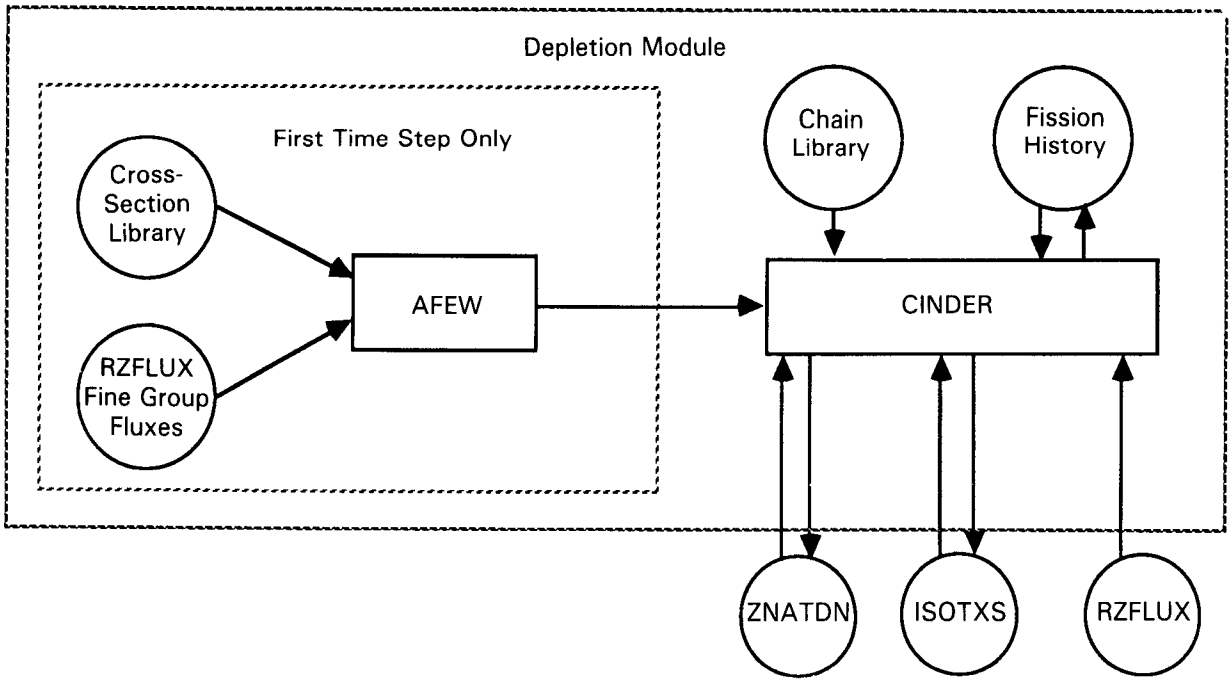

Fig. 4. CINDER-3 code package in DANDE depletion module.

The power and flexibility of CTL permit other forms of control strategy. For example, it is possible to retrieve the value of k_{eff} using built-in CTL functions. A reactor model can be constructed that runs continuously close to criticality by testing the k_{eff} after each time step and moving the control rods if the value of k_{eff} drops below a certain test value. Similarly, tests can be inserted that require fuel elements to be relocated at appropriate times. Fuel relocation strategies, however, require that the CINDER history file be reordered to correspond to the new configuration. At this time, reordering is not automatic to the DANDE system.

VI. DANDE VALIDATION

Although the DANDE code has been used in a number of applications at Los Alamos, two examples were chosen for this report to illustrate the operation of the code system and to compare with experimental and other calculational results. The two problems used are (a) the FFTF cycle-1 depletion experiment and (b) an OWR fuel element depletion experiment.

VI.A. The FFTF Cycle-1 Depletion Experiment

Los Alamos participation during the past 5 yr in the large core code evaluation working group (LCCEWG) provided us with the opportunity of validating the DANDE code system by calculating the LCCEWG fifth benchmark problem. The LCCEWG was a group of representatives from several laboratories funded by the U.S. Department of Energy (DOE) whose function had been to validate codes used in reactor design analysis. LCCEWG-5 is based on measurements made in the FFTF, a 400-MW(thermal) sodium-cooled fast reactor located near Richland,

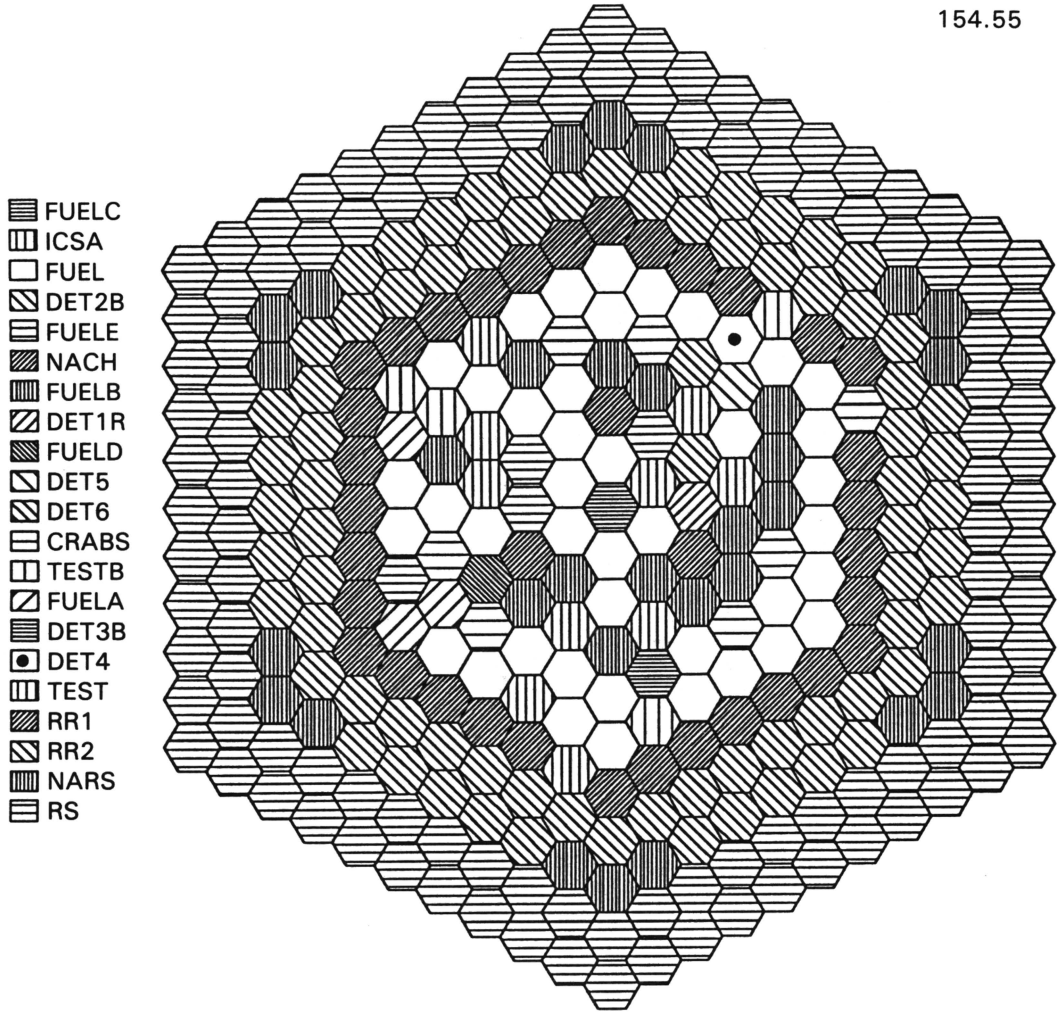

Fig. 5. FFTF midcore plan of calculational model for BOC-1A. Table IV identifies the reactor region abbreviations given in the legend.

Washington, and operated for DOE by Westinghouse Hanford Company. The benchmark includes two experiments:

1. the high power characterizer (HPC) experiment, in which several prototypic assemblies containing extensive dosimetry were irradiated for 8 full-power days
2. the cycle-1 depletion experiment in which pellet burnup measurements were made on fuel from two driver fuel assemblies removed at the end of cycle-1 operation.

The HPC calculations with DANDE produced results in excellent agreement with the experimentally measured data. These comparisons have been described in detail in previous DANDE documentation[19,20] and will not be presented here.

The cycle-1 depletion calculations were run in three parts, as indicated in the benchmark specifications:

1. beginning of life (BOL) to beginning of cycle 1A (BOC-1A), in which different assemblies received different exposures followed by 120 days of shutdown
2. BOC-1A to end of cycle 1A (EOC-1A) (34.1-day exposure followed by 94-day shutdown)
3. BOC-1B to EOC-1B (101.9-day exposure).

To obtain the starting model for FFTF cycle-1A depletion (BOC-1A), a six time-step DANDE run was made to estimate explicit nuclide, fission product aggregate, and individual fission product densities. The explicit-nuclide and aggregate fission product densities were transferred between the core neutronics and depletion modules via ZNATDN, the standard file[1] for explicit nuclide densities; the individual nonexplicit nuclide chain densities, however, remained in the depletion module and were updated in each time step.

The six time steps used in the approach to BOC-1A included cumulative irradiation times of 10, 15, 19, 24, and 32.4 full-power days, followed by a shutdown time of 120 days. The midcore plan of the model used in the approach to BOC-1A is shown in Fig. 5, and region descriptions and exposures are given in Table IV. The exposure each assembly received is indicated by a letter of the alphabet, with the exception of those receiving 32.4 full-power days to which no letter is assigned. Otherwise, those with a final letter "A" received 24 days; those with "B," 19 days; those with "C," 15 days; those with "D," 10 days; and those with "E," 0 days. The resulting k_{eff} from calculations of the approach to BOC-1A was 0.98358.

The FFTF operating history for the cycle-1 depletion experiment is given in Table V, and results for the cycle-1 three-dimensional, diffusion/depletion calculations (DIF3D in the core calculational module of DANDE) are shown in Table VI. Cycle 1A was run in two time steps, 17 and 17.1 days, respectively; and cycle 1B was run in four 16.95-day time steps. A shutdown period of 94 days was assumed between EOC-1A and BOC-1B. The control assembly bank was proportionately withdrawn for intermediate time steps. The reactivity gain between subcycles was the sum of 0.0005 in k_{eff} for the 94-day cooling time and 0.0013 for the additional 1.3-cm control rod bank

TABLE IV

Designations of Midcore Regions for LCCEWG-5 FFTF Cycle-1 Model

Region	Assembly Type[a]	Exposure (days)
FUEL	Fuel types 3.1, 3.2, 4.2	32.4
FUELA	Fuel types 3.1	24.0
FUELB	Fuel types 3.1, 3.2, 4.1, 4.2	19.0
FUELC	Fuel type 3.2	15.0
FUELD	Fuel type 3.2	10.0
FUELE	Fuel types 4.1, 4.2	0.0
ICSA	In-core shim assembly	---
NACH	Safety rod sodium channel	---
CRABS	Control rod absorber	---
DET1R	Depletion test 1-R	32.4
DET2B	Depletion test 2	19.0
DET3B	Depletion test 3	19.0
DET4	Depletion test 4	32.4
DET5	Depletion test 5	32.4
DET6	Depletion test 6	32.4
TEST	Test assemblies	---
TESTB	Blanket test assemblies	19.0
RR1	Radial reflector #1	---
RR2	Radial reflector #2	---
RS	Radial shield	---
NARS	50% sodium, 50% radial shield	---

[a]In actual DIF3D runs, different fuel and test assemblies were separately identified.

TABLE V

Depletion Steps of Cycle 1-A and Cycle 1-B Combined

Rod Position (cm)	Exposure (days)	Cumulative Exposure (days)	Cooling Time (days)	Elapsed Time (days)
42.6	17.0	17.0	0.0	17.0
47.7	17.1	34.1	0.0	34.1
53.1	0.0	34.1	94.0	128.1
54.4	16.95	51.05	0.0	145.05
63.4	16.95	68.00	0.0	162.00
72.4	16.95	84.95	0.0	178.95
81.3	16.95	101.90	0.0	195.90

TABLE VI

Cycle-1 Results, Three-Dimensional Calculations

Total Exposure (days)	Cooling Time (days)	Rod Position (cm Withdrawn)	k_{eff}	Comment
0.0	0.0	42.6	0.98358	BOC-1A
34.1	0.0	53.0	0.98344	EOC-1A
34.1	94.0	54.4	0.98527	BOC-1B
101.9	0.0	81.3	0.98353	EOC-1B

withdrawal. The final k_{eff} of 0.98353 for EOC-1B compared with 0.98358 for BOC-1A indicates the calculated reactivity loss/control bank worth to be essentially "in balance." The discrepancy amounts to only ~0.02 cents per full-power day.

The approximate 16-mk bias obtained with diffusion calculations has been observed by others.[21] For comparison with a discrete ordinates calculation, a two-dimensional hexagonal calculation was run with DIF3D in which buckling was adjusted to give a value of k_{eff} equal to the three-dimensional result. This buckling was then used in a calculation with the TWOHEX code, which resulted in a $k_{eff} = 0.99201$. Thus, the S_n method accounts for about half of the 16-mk bias.

VI.B. Calculation of the Actinide Nuclide Inventory of a Materials Test Reactor (MTR)-Type Spent Fuel Element

An OWR spent fuel element (identified as O-444) was recently used in a passive neutron signal measurement at Los Alamos. Calculations in support of the experimental measurements included using the EPRI-CELL code[17] coupled to CINDER-2 and DANDE. As the experimental results were not sufficiently accurate to determine which calculational method gave the best results, this section serves primarily as a comparison of the two approaches.

Element O-444 was used in the OWR core for an operational period exceeding 4 yr during which time it occupied seven different core grid positions. The reactor operated on a nominal 5 day/week, 8 h/day schedule, with quarterly 1-week shutdowns. The fuel of the element was subjected to varying flux levels and spectra varying with vertical position, core power level, spatial xenon distribution, control rod positions, core

TABLE VII

Power History of OWR Element 0-444

Report Period		δt	δt	Burnup, ^{235}U	Energy	Power	Power Density (W/cm^3)		
Start	Stop	(days)	(h)	(g)	(kWh)[a]	(W)	Minimum[b]	Maximum[b]	Average
3/31/80	6/06/80	67	1 608	3.32	75 727	47 094	50.96	195.6	135.2
6/06/80	9/05/80	91	2 184	4.27	97 396	44 595	48.26	185.2	128.0
9/05/80	11/26/80	82	1 968	3.64	83 026	42 188	45.65	175.2	121.1
11/26/80	2/13/81	48	1 152	3.11	70 937	61 578	66.63	255.8	176.7
2/13/81	4/24/81	70	1 680	2.87	65 463	38 966	42.16	161.8	111.8
4/24/81	9/12/81	141	3 384	7.26	165 596	48 935	52.95	203.2	140.5
9/12/81	12/18/81	97	2 328	5.10	116 328	49 969	54.07	207.5	143.4
12/18/81	3/12/82	84	2 016	3.62	82 570	40 957	44.32	170.1	117.6
3/12/82	6/11/82	91	2 184	4.67	106 520	48 773	52.78	202.6	140.0
6/11/82	8/13/82	6	1 512	4.39	100 133	66 226	71.66	275.1	190.1
8/13/82	11/05/82	84	2 016	5.66	129 101	64 038	69.29	266.0	183.8
11/05/82	4/01/83	147	3 528	7.98	182 019	51 593	55.83	214.3	148.1
4/01/83	6/24/83	84	2 016	5.53	126 136	62 568	67.70	259.9	179.6
6/24/83	8/26/83	63	1 512	3.51	80 061	52 950	57.30	219.9	152.0
8/26/83	11/23/83	89	2 136	4.65	106 063	49 655	53.73	206.2	142.5
11/23/83	3/09/84	107	2 568	7.88	179 738	69 992	75.73	290.7	200.9
3/09/84	5/11/84	63	1 512	4.70	107 204	70 902	76.72	294.5	203.5
5/11/84	2/01/86	631	15 144	0.0	0	0	0.0	0.0	0.0

[a]Assumes 22 809 kWh/g ^{235}U fissioned (200 MeV/fission).

[b]Maximum and minimum power densities relative to fuel average were taken from the vertical flux profile shown in Fig. 6. The maximum (144.7%) occurs at a height of 26.2 cm (10.3 in.) above the bottom of the 60-cm ($23\frac{5}{8}$-in.) fuel region. The minimum (37.7%) occurs at a height of 57.2 cm (22.5 in.). The minimum, average, and maximum exposures predicted are 124.6, 330.6, and 478.4 GWd/tU, respectively.

grid locations, and other considerations. The element burnup history and a measured vertical flux profile at core grid position 2B, shown in Fig. 6, were used at the locations of the minimum, maximum, and average flux; power was assumed to be constant during each of the time increments. A final cooling period was added to the history, accounting for decay from shutdown to the time of the planned measurement (February 1, 1986).

The cross sections and spectra used in the CINDER-2 calculation were obtained from an EPRI-CELL calculation of a pressurized water reactor (PWR) with a 2.56%-enriched UO_2 fuel at BOL, reflecting the OWR MTR-type fuel only in that they were calculated for a light water thermal reactor. The exposure history was as given in Table VII. The MATXS7, 69-group cross-section library was used as input to the data processing module for DANDE. Using methods described above, a 12-group set was produced for the CINDER-3 depletion calculations. The one-dimensional, infinite slab option of the DIF3D code was used for the neutronic calculations, as this proved to be an adequate modeling for the OWR fuel element. CINDER-3 was used for the depletion module.

Inventories calculated with the two methodologies are compared in Table VIII. Most of the large differences in inventory values are evidently due to the softness of the MTR spectrum, compared with that of the PWR, and the reduced epithermal contribution to radiative capture reactions calculated in DANDE. The largest differences in inventory occur for higher actinides produced via long absorption and decay paths.

The calculated inventory of radionuclides was used with the SOURCES neutron source code[22] to calculate the magnitude of the neutron sources due to the spontaneous fission (SF) of actinide nuclides and the interaction of their decay alpha particles in (α,n) reactions with aluminum. In this code, the $Al(\alpha,n)$ cross sections, taken from the measurements of Stelson and McGowan[23] and of Howard et al.,[24] are used with functional fits to the alpha stopping cross sections of Ziegler[25] to calculate (α,n) reaction rates. The SF neutron source data used in the code are described in Ref. 26.

TABLE VIII

Comparison of OWR Element 0-444 Actinide Nuclide Inventories Calculated with CINDER-2, Using PWR Data, and with DANDE

	Nuclide Atom Densities (Number/cm^3)								
	Minimum Power Density			Average Power Density			Maximum Power Density		
Nuclide	CINDER2	DANDE	Difference (%)	CINDER2	DANDE	Difference (%)	CINDER2	DANDE	Difference (%)
^{234}U	1.16+19[a]	1.20+19	1	1.01+19	1.12+19	11	8.78+18	1.04+1	18
^{235}U	1.35+21	1.36+21	1	9.09+20	9.28+20	2	6.06+20	6.33+20	4
^{236}U	4.89+19	3.95+19	−19	1.28+20	1.02+20	−20	1.81+20	1.45+20	−20
^{238}U	1.05+20	1.05+20	0	1.04+20	1.04+20	0	1.04+20	1.04+20	0
^{237}Np	7.26+16	1.48+17	104	5.83+17	1.07+18	84	1.39+18	2.35+18	69
^{238}Pu	2.19+15	2.84+15	30	5.36+16	6.03+16	13	2.10+17	2.12+17	1
^{239}Pu	1.62+17	2.19+17	35	2.92+17	4.51+17	54	3.39+17	5.43+17	60
^{240}Pu	1.81+16	1.19+16	−34	8.85+16	7.46+16	−16	1.39+17	1.45+17	4
^{241}Pu	2.19+15	8.38+14	−62	2.94+16	1.23+16	−58	6.64+16	3.24+16	−51
^{242}Pu	1.10+14	1.32+14	20	5.29+15	1.51+15	−72	2.27+16	7.04+15	−69
^{241}Am	2.80+14	1.19+14	−58	3.61+15	1.54+15	−57	7.78+15	3.91+15	−50
^{242}Am	6.75+06	1.55+06	−77	1.48+08	4.22+07	−72	3.33+08	1.17+08	−65
^{242m}Am	5.62+11	1.29+11	−77	1.24+13	3.51+12	−72	2.77+13	9.72+12	−65
^{243}Am	2.14+12	2.93+12	37	3.43+14	3.12+13	−91	2.63+15	1.93+14	−93
^{242}Cm	1.99+11	7.04+10	−65	9.10+12	2.36+12	−74	3.69+13	1.09+13	−70
^{243}Cm	7.68+09	1.86+09	−76	1.13+12	1.31+11	−88	7.84+12	9.62+11	−88
^{244}Cm	4.44+10	6.48+10	46	2.43+13	1.13+12	−53	3.43+14	9.09+12	−97
^{245}Cm	2.69+08	2.95+08	10	4.22+11	8.11+09	−98	9.21+12	6.71+10	−99
^{246}Cm	3.15+06	7.74+06	146	1.68+10	6.06+08	−96	6.69+11	6.92+09	−99

[a]Read as 1.16×10^{19}.

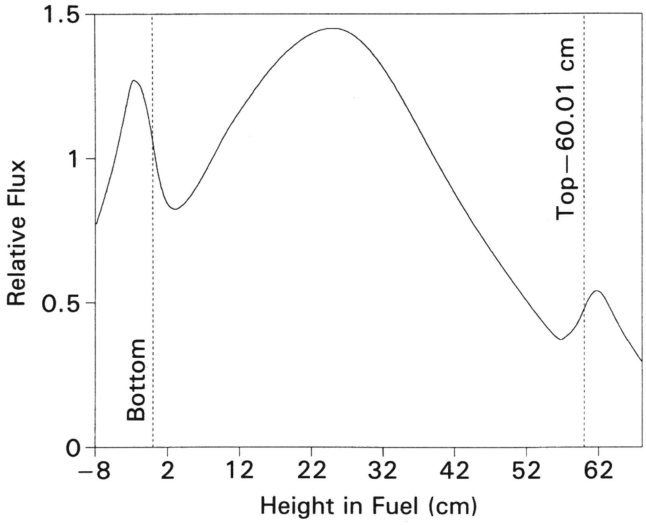

Fig. 6. Grid Position 2B—vertical flux profile relative to fuel average.

The calculated neutron source, dominated by ^{238}Pu, is not greatly different in the two calculations as shown in Table IX. The spontaneous-fission contribution, however, is somewhat reduced in the SOURCES result using the nuclide inventory from the DANDE calculation.

TABLE IX

Comparison of OWR Element 0-444 Intrinsic Neutron Source Obtained Using the SOURCES Code and Actinide Inventories Calculated with CINDER-2, Using PWR Data, and with DANDE

Nominal Exposure	Property	CINDER-2	DANDE
125 GWd/tU	SF n/s·cm^3	1.25−2[a]	9.58−3
	(α,n) n/s·cm^3	5.94−1	6.96−1
	Total n/s·cm^3	6.07−1	7.06−1
	% SF	2.06%	1.36%
326 GWd/tU	SF n/s·cm^3	1.79−1	1.19−1
	(α,n) n/s·cm^3	9.49+0	9.97+0
	Total n/s·cm^3	9.77+0	1.01+1
	% SF	2.86%	1.18%
466 GWd/tU	SF n/s·cm^3	2.11+0	4.14−1
	(α,n) n/s·cm^3	3.64+1	3.43+1
	Total n/s·cm^3	3.85+1	3.47+1
	% SF	5.48%	1.19%

[a]Read as 1.25×10^{-2}.

VII. SUMMARY

We have described the structure, operation, and validation of DANDE, a modular code system designed for reactor core neutronics and depletion analysis. The modules consist of standard data processing, core neutronics, and depletion codes, which are linked by standard files and which access standard data libraries, mainly based on ENDF/B-V.

We have included two examples in the paper in which DANDE was used in calculating actual experiments. Such extensive calculations illustrate the accuracy, flexibility, and speed with which DANDE can be applied in both fast and thermal reactor core design.

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