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AUTHOR(S): R. J. LaBauve, T-2
T. R. England, T-2
D. C. George, T-2
R. E. MacFarlane, T-2
W. B. Wilson, T-2

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DANDE-A LINKED CODE SYSTEM FOR CORE NEUTRONICS/DEPLETION ANALYSIS

by
R. J. LaBauve, T. R. England, D. C. George, R. E. MacFarlane, and W. B. Wilson
Applied Nuclear Science Group, Los Alamos National Laboratory

ABSTRACT

This report describes DANDE--a modular neutronics, depletion code system for reactor analysis. It consists of nuclear data processing, core physics, and fuel depletion modules, and 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 depletion, burnable poisons as well as 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 in this report by two sample problems.

I. INTRODUCTION

The DANDE (Applied Nuclear DAta, Core-Neutronics, DEpletion) 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 the 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.

Currently the data processing module consists of the TRANSX code[2] operating on a fine-group library generated by the NJOY[3] code from the ENDF/B-V[4] basic nuclear data file. 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 FFTF experiment discussed in Sec. VI, 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. In 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.

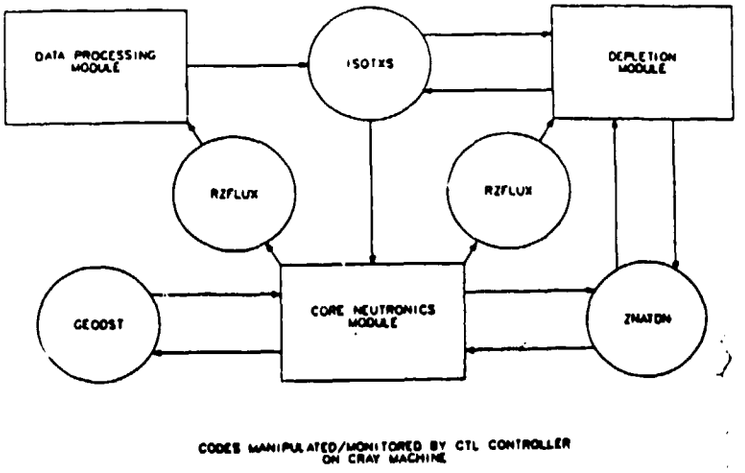

Fig. 1. DANDE code system for reactor core analysis.

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-M word storage), and the core neutronics calculation takes about three minutes 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 and the RZFLUX file produced by the core neutronics module, this code does summation calculations over the various fission-product and actinide chains and provides updated nuclear densities for the principal nuclides in the ZNATDN file. The non-explicit 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., B, Sm, Eu) 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 in a FORTRAN-like manner to loop through the time steps in a depletion problem, calling in the various codes and files in the proper sequence. Geometric changes (GEODST file), such as control rod repositioning and fuel relocation, can be made with CTL between depletion time steps.

II. DATA PROCESSING MODULE

In most of our work to date, we have used two fine-group libraries in the DANDE data processing module (TRANSX), both of which were generated by the NJOY code using basic nuclear data from ENDF/B-V. The first of these, MATXS6,[2] is an 80-neutron × 24-photon group library intended for fast reactor analysis but 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 about 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[13] calculations discussed in Sec. VI.

The other library used, MATXS7,[2] 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 OWR fuel element depletion problem described in Sec. VI.

Twelve-group ISOTXS files produced from TRANSX were used in the core neutronics and depletion modules for the calculations described in Sec. VI. Although, as is indicated in Fig. 1, these files could be updated during depletion steps by suitable application of the CTL controller; in fact only one 12-group ISOTXS file was generated for each case.

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 and 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.

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 to compare both transport and high order (P_3) scattering in our calculations.

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[9 11] summation code family. CINDER resolves the coupled system of decay equations into a collection of 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[16] and EPRI-CELL,[17] for 20 years 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 (Am and Cm) has often been ignored. In DANDE, however, three-dimensional physics calculations of the core neutronics module are performed with accurate actinide inventory; "lumped" 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, explictly-treated nuclides (ISOTXS file) for each volume element. CINDER-3 returns end-of-time-step atom densities of the explicit nuclides, and it groups non-explicit fission-product and actinide quantities for use in the next-time-step calculation of the core neutronics module. These aggregate quantities, accumulated separately for non-explicit fission products and actinides, include atom densities and cross sections for (n,n), (n,n'), (n,2n), (n,γ), and total neutron absorption in the energy-group structure specified in the ISOTXS file. The data for the individual fission-product and actinides are written to another file and are thus available for further exposure in the next call to the depletion module. Current versions of CINDER-3 use an ENDF/B-V data based library.[12]

V. CTL OPERATION

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 multi-step problems by hand is extremely tedious and error prone. Therefore, a controller written in the language CTL is composed for each application, allowing the problem to be run in interactive or production mode.

The power and flexibility of the CTL language permit other forms of control strategy. For example, it is possible to retrieve the value of k-effective using built-in CTL functions. A reactor model can be constructed that runs continuously close to criticality by testing the k-effective after each time step and moving the control rods if the value of k-effective 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 (1) The FFTF Cycle 1 depletion experiment and (2) the OWR fuel element depletion experiment.

A. The FFTF Cycle 1 Depletion Experiment

Los Alamos participation during the past five years 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 founded by the U.S. Department of Energy (DOE) whose function had been to validate codes used in reaction design analysis. LCCEWG-5 is based on measurements made in the Fast Flux Test Facility (FFTF), a 400-Mw(th) sodium cooled fast reactor located near Richland, Washington, and operated for the Department of Energy by Westinghouse Hanford Company (WHC). The benchmark includes two experiments:

(1) the high power characterizer (HPC) experiment, in which several prototypic as-assemblies containing extensive dosimetry were irradiated for eight full-power days; and

(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.

Only the DANDE calculations for Part 2 are described 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 EOC-1A (34.1d exposure followed by 94d shutdown);

(3) BOC-1B to EOC-1B (101.9d 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 lump, 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 irradiation times of 10, 15, 19, 24, and 32.4 full-power days, followed by a shutdown time of 120 days. The mid-core plan of the model used in the approach to BOC-1A is shown in Fig. 2 and region discriptions and exposures are given in Table I. 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 assinged. 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 in the approach to BOC-1A was 0.98358.

TABLE I

DESIGNATIONS OF MID-CORE REGIONS FOR LCCEWG-5 FFTF CYCLE-1 MODEL

Region	Assembly Type*	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	——

*In actual DIF3D runs, different fuel and test assemblies were separately identified.

The FFTF operating history for the Cycle 1 depletion experiment is givn in Table II and results for the Cycle 1 diffusion, three-dimensional, depletion calculations (DIF3D in the core calculational module of DANDE) are shown in Table III. 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 sub-cycles 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 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 about 0.02¢/full-power day.

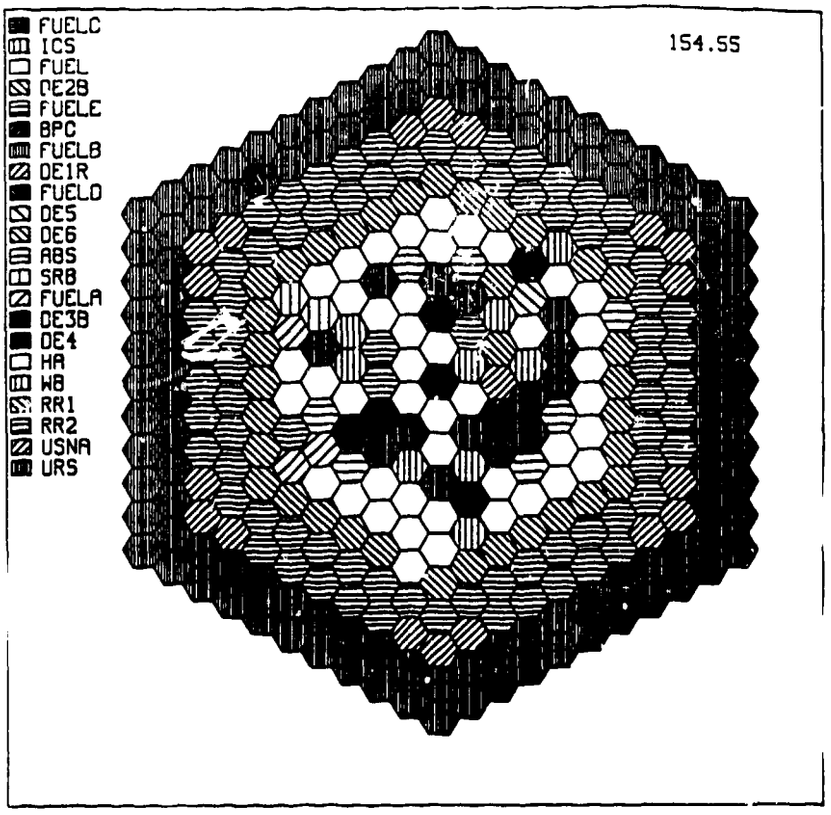

Fig. 2. FFTF mid-core plan of calculational model for BOX-1A. Table I identifies the reactor region abbreviations given in the legend.

TABLE II

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 III

CYCLE-1 RESULTS, 3-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

The approximate 16-milli-k bias obtained with diffusion calculations has been observed by others.[19] 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 Sn method accounts for about half of the 16-milli-k bias.

B. Calculation of the Actinide Nuclide Inventory of an Omega West Reactor (OWR) MTR-Type Spent Fuel Element.

An Omega West Reactor 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[20] 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 four years during which time it occupied seven different core grid positions. The reactor operated on a nominal 5-day/week, 8hour/day schedule, with quarterly 1-week shutdowns. The fuel of the element was subjected to varying flux levels and spectra due to verical position, core power level, spatial xenon distribution, control rod positions, core grid locations, and other considerations. The element burnup history and a measured vertical flux profile at core grid position 2B, shown in Fig. 3 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 that simulated the OWR by a PWR with 2.56%-enriched UO_2 fuel at beginning-of-life. 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 cylinder option of the DIF3D code was used for the neutronic calculations, as this proved to be an adequate modelling for the OWR fuel element. CINDER-3 was used for the depletion module.

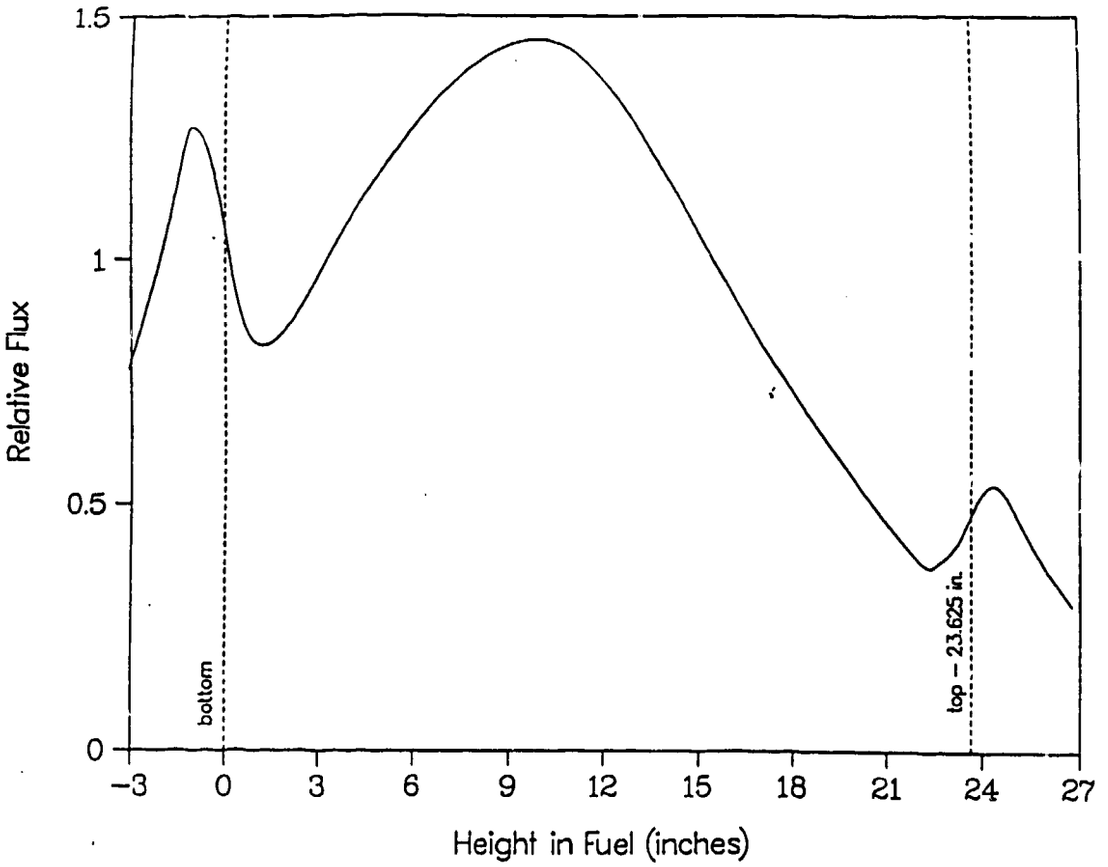

Fig. 3. Grid Position 2B - Vertical flux profile relative to fuel average.

Inventories calculated with the two methodologies are compared in Table IV. 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 radionucles was used with the SOURCES neutron source code[21] to calculate the magnitude of the neutron sources due to the SF of actinide nuclides and the interaction of their decay α-particles in (α,n) reactions with Al. In this code, the Al(α,n) cross sections, taken from the measurements of P. H. Stelson and F. K. McGowan[22] and of A. J. Howard et al.,[23] are used with functional fits to the α stopping cross sections of J. F. Ziegler[24] to calculate (α,n) reaction rates. The spontaneous-fission neutron source data used in the code is described in Ref. 25.

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

TABLE IV

COMPARISON OF OWR ELEMENT O-444 ACTINIDE NUCLIDE INVENTORIES CALCULATED WITH CINDER-2, USING PWR DATA, AND WITH DANDE

	Nuclide Atom Densities, #/cm³.								
	Minimum Power Density			Average Power Density			Maximum Power Density		
Nuclide	CINDER2	.DANDE.	%diff	CINDER2	.DANDE.	%diff	CINDER2	.DANDE.	%diff
^{234}U	1.16+19	1.20+19	1	1.01+19	1.12+19	11	8.78+18	1.04+19	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

TABLE V

COMPARISON OF OWR ELEMENT O-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-cm³	1.25-2	9.58-3
	(α,n) n/s-cm	5.94-1	6.96-1
	Total n/s-cm³	6.07-1	7.06-1
	% SF	2.06%	1.36%
326 GWd/tU	SF n/s-cm³	1.79-1	1.19-1
	(α,n) n/s-cm³	9.49+0	9.97+0
	Total n/s-cm³	9.77+0	1.01+1
	% SF	2.86%	1.18%
466 GWd/tU	SF n/s-cm³	2.11+0	4.14-1
	(α,n) n/s-cm³	3.64+1	3.43+1
	Total n/s-cm³	3.85+1	3.47+1
	% SF	5.48%	1.19%

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