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NUCLEAR SCIENCE COMMITTEE

BURNUP CREDIT CRITICALITY BENCHMARK  
Part I-B. Isotopic Prediction  
(Problem Specification)  
November 1992

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(Table 4 on page 4 has been revised).

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**Objective**

The objective of this part of the benchmark is to check the accuracy of the depletion codes used to predict the isotopic composition of the fuel as a function of burnup.

**Background**

Evaluating the reactivity of a spent fuel system has two fundamental requirements: (1) predicting the isotopic composition of the spent fuel and (2) analyzing the system reactivity based on these isotopes. Part I and Part I-A of this benchmark addressed the principal concern of this working group, the criticality calculation. However, the importance of the depletion calculation cannot be ignored. Depletion codes are often utilized to predict radiation source terms for shielding, and decay heat calculations. Validation sources for depletion codes include measurements of decay heat and chemical assay data. Chemical assay data are ideal for validating the ability of the depletion codes to accurately predict the quantities of specific nuclides in spent fuel as they are a direct measurement of these quantities.

Reference 1 describes one of a series of experiments designed to characterize spent fuel for light water reactors. The experiments were performed at the Materials Characterization Center (MCC) at Pacific Northwest Laboratories (PNL) as part of the United States Department of Energy (US/DOE) Office of Civilian Radioactive Waste Management (OCRWM) program. The spent fuel used in these measurements was designated as Approved Testing Material (ATM) - 104. The chemical assay data measured in these experiments are of particular value in validating the isotopic predictions used in burnup credit.

**Problem Specification**

This calculational benchmark problem will compare the computed nuclide inventories for a simple pin cell calculation. The fuel and operating specifications given in Tables 1-5 of this problem are based on data given in Ref. 1 and 2 for the Combustion Engineering (CE) 14 x 14 assembly designated as ATM-104. The fuel pin pitch has been modified for the pin-cell calculation in order to represent a fuel-to-moderator ratio equivalent to that in the two dimensional fuel assembly. Table 6 lists the measured data for ATM-104 at three burnups.

Participants should perform three independent calculations of the spent fuel inventory resulting from the power history data given in Table 3. Results for all nuclides listed in Table 7 should be compiled and forwarded to M. C. Brady either by electronic mail, computer diskette (Macintosh, DOS and tar formats acceptable on 3.5" diskettes, DOS only on 5.25" diskettes) or 8mm tapes written in tar format.

### References

1. R. J. Guenther, et al., Characterization of Spent Fuel Approved Testing Material--ATM-104, Pacific Northwest Laboratory report, PNL-5109-104, Richland, Washington (December 1991).
2. S. R. Bierman, Spent Reactor Fuel Benchmark Composition Data for Code Validation, Proceedings of the International Conference on Nuclear Criticality Safety - ICNC'91, September 9-13, 1991, Oxford, United Kingdom, p. II-113.

**Table 1. Physical data for isotopics calculation for PWR pin-cell**

Parameter	Data
Type fuel pellet	UO2
Fuel density, g-cm-3	10.045
Rod pitch, cm	1.5586
Rod OD, cm	1.118
Rod ID, cm	0.986
Pellet diameter, cm	0.9563
Active fuel length, cm	347.2
Effective fuel temperature, K	841
Clad temperature, K	620
Clad material	Zircalloy-2 (97.91 wt% Zr, 1.59 wt% Sn, 0.5 wt% Fe)
Water temperature, K	558
Water Density, av, g-cm-3	0.7569
Cycle 1 av boron concentration	331 ppm

**Table 2. Operating history data for isotopic calculation**

OPERATING CYCLE	BURN days	DOWN days	BORON %cycle 1
1	306.0	71	100
2	381.7	83.1	141.9
3	466.0	85	152.3
4	461.1	1870	148.8

BURN is the fuel irradiation time in days.

DOWN is the downtime in days between cycles except for cycle 4 where it includes the decay time from reactor to measurement (cooling time) of 1870 days.

BORON is the cycle-average boron concentration as a percent of the cycle 1 concentration.

Table 3. Specific power (kW/kgU) for the three cases

OPERATING CYCLE	POWER(a) kW/kgU	POWER(b) kW/kgU	POWER(c) kW/kgU
1	17.24	24.72	31.12
2	19.43	26.76	32.51
3	17.04	22.84	26.20
4	14.57	18.87	22.12

(a) Spent fuel sample 1 with a cumulative burnup of 27.35 GWd/MTU.

(b) Spent fuel sample 2 with a cumulative burnup of 37.12 GWd/MTU.

(c) Spent fuel sample 3 with a cumulative burnup of 44.34 GWd/MTU.

Table 4. Initial fuel number densities

Nuclide	Number Density
U-234	6.15165E-06
U-235	6.89220E-04
U-236	3.16265E-06
U-238	2.17104E-02
C-12	9.13357E-06
N-14	1.04072E-05
O	4.48178E-02

Table 5. Cycle 1 coolant number densities

Nuclide	Number Density
H-1	5.06153E-02
O-16	2.53076E-02
B-10	2.75612E-06
B-11	1.11890E-05

Table 6. Fuel radiochemical analyses results, mg/g fuel (UO<sub>2</sub> 2\$)  
from Ref.1

## Cumulative burnup

Nuclide	27.35 Gwd/MTU	37.12 Gwd/MTU	44.34 Gwd/MTU
U-234	1.6 E-01	1.4 E-01	1.2 E-01
U-235	8.47 E+00	5.17 E+00	3.54 E+00
U-236	3.14 E+00	3.53 E+00	3.69 E+00
U-238	8.425E+02	8.327E+02	8.249E+02
Pu-238	1.012E-01	1.893E-01	2.688E-01
Pu-239	4.264E+00	4.357E+00	4.357E+00
Pu-240	1.719E+00	2.239E+00	2.543E+00
Pu-241	6.812E-01	9.028E-01	1.020E+00
Pu-242	2.886E-01	5.761E-01	8.401E-01
Np-237	1.89 E-04*	2.51 E-04*	3.31 E-04*
Am-241	8.56 E-01*	1.18 E+00*	1.31 E+00*
Se-79	4.55 E-05*	6.036E-05*	6.49 E-05*
Sr-90	4.59 E+01*	5.9 E+01*	6.58 E+01*
Tc-99	9.59 E-03*	1.23 E-02*	1.35 E-02*
Sn-126	1.25 E-04*	1.82 E-04*	2.2 E-04*
Cs-135	4.16 E-04*	4.59 E-04*	4.95 E-04*
Cs-137	6.71 E+01*	9.01 E+01*	1.09 E+02*

\* These values are in mCi/g fuel (UO<sub>2</sub>)

**Table 7. Nuclides whose isotopic concentrations will be compared**

Actinides	Fission Products
U-234	Mo-95
U-235	Tc-99
U-236	Ru-101
U-238	Rh-103
Pu-238	Ag-109
Pu-239	Cs-133
Pu-240	Sm-147
Pu-241	Sm-149
Pu-242	Sm-150
Am-241	Sm-151
Am-243	Sm-152
Np-237	Nd-143
	Nd-145
	Eu-153
	Gd-155

**Table 8. Data to be included in results**

- 1 Date
- 2 Institute
- 3 Participants
- 4 Computer code(s)
- 5 Data library identification, origin, description (includes fission yields and decay data as well as cross-section data).
- 6 General results for all nuclides included in Table 7. Please list actinides first, followed by fission products in the order given in Table 7. \*\*Nuclide inventories should be given in units of mg/g-fuel, i.e., relative to the initial mass of UO<sub>2</sub> for the uranium and plutonium isotopes and as mCi/g-fuel for all other nuclides (e.g. as in Table 6).