

# BENCHMARKING AND VALIDATION OF MOCUP

K. Wang\*, T-P Lou, E. Greenspan and J. Vujic  
Department of Nuclear Engineering  
University of California  
Berkeley, CA 94720  
[gehud@nuc.berkeley.edu](mailto:gehud@nuc.berkeley.edu)

## ABSTRACT

The purpose of this work was to benchmark the MOCUP code for burnup analysis. Two well-documented benchmarks were used to validate MOCUP and the way we are applying it. One benchmark consists of three PWR pin-cell burnup problems. The other benchmark is a fast reactor (burner) burnup problem. From the comparisons of our MOCUP results with those obtained from measurement and/or other computer codes, it has been concluded that: (a) with few exceptions, the MOCUP results of isotopic compositions fall within the range of those calculated by different codes, (b) MOCUP results for the actinide concentration are in agreement with the measurement values to within 11%, and (c) the MOCUP predictions of reactivity change with burnup are in good agreement with the reported values. For example, for most of the actinides the deviations in concentration are less than 5%, and for all fission products studied, the deviation of MOCUP results from the measured values is less than 10% (an exception is  $^{149}\text{Sm}$ ).

## 1. INTRODUCTION

The utility program MOCUP<sup>1</sup> developed by Idaho National Engineering and Environment Laboratory is a linkage code that couples MCNP<sup>2</sup>, a generalized-geometry Monte Carlo (MC) transport code, and ORIGEN2<sup>3</sup>, an isotope generation and depletion code. MOCUP is extremely useful for analysts who perform isotope production, material transformation, and depletion and isotope analyses on complex, non-lattice geometric configurations. The main advantage of MC technique is that more accurate results for reactivity calculations and hence for burnup can be obtained due to realistic modeling of complex geometries and the use of continuous-energy cross sections. Due to lack of funding, MOCUP was not well documented and not well benchmarked.

Before using MOCUP in our routine research work, we have chosen two well-documented benchmarks to validate MOCUP and the way we are applying it. The MOCUP results were not included in the documented analysis<sup>4,5</sup> of any of these benchmark problems.

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\* The permanent address is: Department of Engineering Physics, Tsinghua University, Beijing, 100084, P.R.CHINA

The first benchmark problem is from the OECD/NEA Burnup Credit Computational Criticality Benchmark Phase I-B Results<sup>4</sup>, which was proposed to provide a comparison of the ability of different code systems and data libraries to perform depletion analysis for the prediction of spent fuel isotopic concentrations and included results representing 21 different sets of calculations submitted by 16 different organizations worldwide and were based on a limited set of nuclides determined to have the most important effect on the neutron multiplication factor of light-water-reactor spent fuel. This benchmark modeled a simple fuel pin-cell which was burned for four complete cycles including burn time and subsequent down time, and consisted of three cases corresponding to fuel samples taken from three different axial locations in the reference practical fuel pin, each with a different final burnup.

The second benchmark problem is from OECD document, Physics of Plutonium Recycling<sup>5</sup>, which was about a 600 MWe (1500 MWth) oxide burner reactor operating on a 125 EFPD cycle at 80% capacity factor. The reactor core was of a homogeneous layout with two radial enrichment zones and no radial blankets; axially, the core was about one meter high and had no axial blankets. The fuel was comprised of an annular mixed oxide pin of depleted uranium and multi-recycled LWR plutonium. Six organizations submitted their results obtained from different sets of calculation codes.

Section 2 and 3 of this paper, respectively, describe the thermal pin benchmark and the fast reactor benchmark along with our calculation results of MOCUP. Conclusions are made in Section 4.

## **2. THERMAL PIN BENCHMARKING OF MOCUP**

### **2.1 BENCHMARK SPECIFICATION**

The purpose of this calculational benchmark problem was to compare nuclide depletion concentrations computed by all participants for a simple pin-cell model.<sup>4</sup> The fuel pin-cell description is given in Table I. The fuel sample was burned for four complete cycles; the length of the burn time and subsequent down time for each cycle are given in Table II. This benchmark consists of three cases, each with a different total burnup; the specific power for each cycle and the final burnup are given in Table III for each of the three cases. Table IV lists the initial isotopic concentrations used for the fuel material for all three cases. Table V provides the isotopic composition of the moderator for cycle 1, and the boron concentrations for subsequent cycles should be modified by the cycle-specific relative boron concentrations given in Table II.

### **2.2 SOME IMPORTANT MOCUP PARAMETERS**

Time interval of running MCNP. The results presented in Section 2.3 were obtained by running MCNP in the time steps of 60 days. It was also found that the similar accuracy could be obtained by using the longer time steps (a half year) in combination with shorter time steps (up to 10 days) at the beginning of each cycle (after each downtime), in order to account the <sup>135</sup>Xe buildup. By

using the latter choice of time steps, the accuracy of the  $^{135}\text{Cs}$  concentration has been improved. Thus, we adopted the second method for our current research work.

Normalization of flux. The flux obtained from MCNP must be normalized with the practical thermal power. Either of the following two ways can be used:

a) When the IRF card in ORIGEN input (constant flux depletion mode) is used, the flux multiplier factor (FMT) is calculated by the following equations:

$$\nu = K_{\text{eff}} \times \frac{\text{Tloss} - \text{Cutoff} - \text{Cnrxn}}{\text{Floss}} \quad (1)$$

$$\text{FMT} = \frac{\nu \times P \times 10^6}{1.602 \times 10^{-13} \times K_{\text{eff}} \times Q} \quad (2)$$

where,  $\nu$  - Number of neutrons per fission;  $K_{\text{eff}}$  - Multiplication factor from MCNP; Tloss - Total loss of neutrons from MCNP; Cutoff - Cutoff neutrons from MCNP; Cnrxn - Neutrons created by (n, xn) from MCNP; Floss - Neutron loss by fission from MCNP. P - Thermal power (MW); Q - Recoverable energy per fission, 204.5 MeV/fission. This flux normalization method was used in the fast reactor benchmark problem described in Section 3.

b) When the IRP card in ORIGEN input (constant power depletion mode) is used, flux can be calculated by ORIGEN as follows:<sup>6</sup>

$$f = \frac{6.242 \times 10^{18} \times P}{\sum_i X_i^f s_i^f Q_i} \quad (3)$$

$$Q_i = 1.29927 \times 10^{-3} (Z^2 A^{0.5}) + 33.12 \quad (4)$$

where,  $\Phi$  - Neutron flux(n/cm<sup>2</sup>-s);  $X_i^f$  - Amount of fissile nuclide i(g-atom);  $\sigma_i^f$  - Microscopic fission cross section for nuclide i (barn);  $Q_i$  - Recoverable energy per fission for nuclide i (MeV/fission); Z - Atomic number; A - Atomic mass. This method was used in the thermal benchmark problem described in this section.

Length of time step of ORIGEN2.1. The length of 3 days was used as the ORIGEN time step in this thermal benchmark. In general, it should not be longer than 10 days. Otherwise, the calculated errors in the nuclide concentrations for isotopes: Pu, Am and Cm will be too large. The length of 10 days was used in the fast reactor benchmark.

Nuclides modeled in MCNP. The following 15 fissionable isotopes were included in the thermal benchmark:  $^{234}\text{U}$ ,  $^{235}\text{U}$ ,  $^{236}\text{U}$ ,  $^{238}\text{U}$ ,  $^{238}\text{Pu}$ ,  $^{239}\text{Pu}$ ,  $^{240}\text{Pu}$ ,  $^{241}\text{Pu}$ ,  $^{242}\text{Pu}$ ,  $^{241}\text{Am}$ ,  $^{242}\text{Am}$ ,  $^{243}\text{Am}$ ,  $^{237}\text{Np}$ ,  $^{238}\text{Np}$  and  $^{245}\text{Cm}$ . In addition,  $^{242}\text{Cm}$ ,  $^{243}\text{Cm}$ ,  $^{244}\text{Cm}$  and  $^{246}\text{Cm}$  were also included in the fast reactor benchmark. The following 28 fission products were included in the thermal benchmark:  $^{95}\text{Mo}$ ,  $^{99}\text{Tc}$ ,  $^{109}\text{Ag}$ ,  $^{101}\text{Ru}$ ,  $^{103}\text{Ru}$ ,  $^{133}\text{Cs}$ ,  $^{135}\text{Cs}$ ,  $^{147}\text{Sm}$ ,  $^{149}\text{Sm}$ ,  $^{150}\text{Sm}$ ,  $^{151}\text{Sm}$ ,  $^{152}\text{Sm}$ ,  $^{143}\text{Nd}$ ,  $^{145}\text{Nd}$ ,

$^{147}\text{Nd}$ ,  $^{151}\text{Eu}$ ,  $^{152}\text{Eu}$ ,  $^{153}\text{Eu}$ ,  $^{154}\text{Eu}$ ,  $^{155}\text{Eu}$ ,  $^{155}\text{Gd}$ ,  $^{157}\text{Gd}$ ,  $^{131}\text{Xe}$ ,  $^{133}\text{Xe}$ ,  $^{135}\text{Xe}$ ,  $^{103}\text{Rh}$ ,  $^{147}\text{Pm}$  and  $^{149}\text{Pm}$ . In addition,  $^{141}\text{Pr}$ ,  $^{105}\text{Pd}$ ,  $^{108}\text{Pd}$ ,  $^{129}\text{I}$ ,  $^{137}\text{Cs}$  and  $^{93}\text{Zr}$  were also included in the fast reactor benchmark.

## 2.3 COMPARISONS OF MOCUP RESULTS WITH BENCHMARK VALUES

In addition to the parameters described in Section 2.2, the reflective boundary conditions for MCNP and the ORIGEN2 cross section library for PWR with 33 GWd/MTU were used. The depletion of boron in the coolant was considered. Table VI, VII and VIII give the comparisons of the results of isotopic concentrations and Table IX shows the EOL  $k_{\infty}$ . Based on the results presented in these tables, the following conclusions can be made:

- (a) MOCUP results are in an agreement with the measured values of the actinide concentrations to within 11%; most deviations are less than 5%.
- (b) MOCUP results are in an agreement with the measured concentrations of all fission products studied to within 10%. An exception is  $^{149}\text{Sm}$  with deviations of up to 50%.
- (c) All MOCUP isotopic concentration results fall within the range of the results calculated by different sets of codes. That is, the relative errors of MOCUP results with the average calculated values are less than the standard deviation. However, there are some exceptions for certain burnup values, in the case of several isotopes of Am and Sm.
- (d) The  $k_{\infty}$  values calculated by MOCUP deviate from the benchmark values by less than 0.012.

## 3. FAST REACTOR BENCHMARKING OF MOCUP

### 3.1 BENCHMARK SPECIFICATION

The core sketch is shown in Figure 1. The BOL compositions are specified in Table X. Additional data are given in Table XI.

### 3.2 COMPARISONS OF MOCUP RESULTS WITH BENCHMARK VALUES

In addition to the parameters described in Section 2.2, the vacuum boundary conditions for MCNP and the ORIGEN2 cross section library for LMFBR with LWR-Pu/U/U/U were used. MCNP was run at the following effective full power days (EFPD): 0, 250, 375 and 625. The comparisons of some BOL results are given in Table XII. Table XIII shows the results of isotopic composition variation and reactivity loss. The following observations can be made, based on the presented results:

- (a) The MOCUP calculated  $k_{\text{eff}}$  and neutron balance components fall within the range of the reported results.
- (b) The MOCUP prediction of reactivity loss with burnup and inner core and outer core isotopic composition variation are also within or almost within the range of the corresponding results given in the benchmark.

## 4. CONCLUSIONS

Based on the results of the thermal pin-cell and the fast reactor (burner) benchmarks, it is concluded that MOCUP can give the burnup results of reactivity swing and isotopic concentration variations which are in good agreement with those obtained from measurement and/or other codes. However, the accuracy of the results depends on several parameters that must be properly chosen (the time intervals for running MCNP, the normalization of flux, the length of the time steps in ORIGEN). In addition, more nuclides may need to be modeled in MCNP to get more accurate reactivity results.

## REFERENCES

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Table I. Physical Data for Benchmark Problem Pin-cell Calculation<sup>4</sup>

Parameter	Data
Type of Fuel Pellet	UO <sub>2</sub>
Fuel Density, g/cm <sup>3</sup>	10.045
Rod Pitch, cm	1.5586
Outer Diameter of rod, cm	1.118
Inner Diameter of rod, cm	0.986
Fuel Diameter, cm	0.9563
Active Fuel Length, cm	347.2
Effective Fuel Temperature, K	841
Clad Temperature, K	620
Clad Material	Zircaloy-2(97.91wt%Zr, 1.59wt%Sn, 0.5wt%Fe)
Water Temperature, K	558
Water Density, g/cm <sup>3</sup>	0.7569

Table II. Operating History Data for Benchmark Problem Pin-cell Calculation<sup>4</sup>

Operating Cycle	Burntime (days)	Downtime (days)	Born Concentration (ppm)	Boron Concentration (% of cycle 1)
1	306.0	71.0	331.0	100.0
2	381.7	83.1	469.7	141.9
3	466.0	85.0	504.1	152.3
4	461.1	1870.0	492.5	148.8

Table III. Specific Power for the Three Benchmark cases<sup>4</sup>

Operating Cycle	Specific Power(kW/kgU)		
	Case A (Final Burnup= 27.35GWd/MTU)	Case B (Final Burnup= 37.12GWd/MTU)	Case C (Final Burnup= 44.34GWd/MTU)
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

Table IV. Initial Fuel Composition and Number Densities<sup>4</sup>

Nuclide	<sup>234</sup> U	<sup>235</sup> U	<sup>236</sup> U	<sup>238</sup> U
Number Density (atoms/b-cm)	6.15165x10 <sup>-6</sup>	6.89220x10 <sup>-4</sup>	3.16265x10 <sup>-6</sup>	2.17104x10 <sup>-2</sup>
Nuclide	<sup>12</sup> C	<sup>14</sup> N	<sup>16</sup> O	
Number Density (atoms/b-cm)	9.13357x10 <sup>-6</sup>	1.04072x10 <sup>-5</sup>	4.48178x10 <sup>-2</sup>	

Table V. Beginning of Cycle 1 coolant Number Densities<sup>4</sup>

Nuclide	<sup>1</sup> H	<sup>16</sup> O	<sup>10</sup> B	<sup>11</sup> B
Number Density (atoms/b-cm)	5.06153x10 <sup>-2</sup>	2.53076x10 <sup>-2</sup>	2.75612x10 <sup>-6</sup>	1.11890x10 <sup>-5</sup>

Table VI. Comparisons of Isotopic Concentrations(mg/g UO<sub>2</sub>) for Case A  
(27.35GWd/MTU Burnup)

Isotope	Measurement Value	Average Value	Standard Deviation of Col. 3 (%)	MOCUP Results	Error of Col. 5 with Col.2(%)	Error of Col. 5 with Col.3(%)
<sup>234</sup> U	1.600x10 <sup>-1</sup>	1.590x10 <sup>-1</sup>	5.19	1.5611 x10 <sup>-1</sup>	-2.43	-1.82
<sup>235</sup> U	8.470	8.190	2.98	8.4275	-0.50	2.90
<sup>236</sup> U	3.140	3.224	2.91	3.1460	0.19	-2.42
<sup>238</sup> U	8.425x10 <sup>+2</sup>	8.375x10 <sup>+2</sup>	0.12	8.3761x10 <sup>+2</sup>	-0.58	0.01
<sup>238</sup> Pu	1.012x10 <sup>-1</sup>	9.027x10 <sup>-2</sup>	15.68	9.2807x10 <sup>-2</sup>	-8.29	2.81
<sup>239</sup> Pu	4.264	4.230	5.16	4.1036	-3.76	-2.99
<sup>240</sup> Pu	1.719	1.710	3.95	1.6842	-2.03	-1.51
<sup>241</sup> Pu	6.812x10 <sup>-1</sup>	6.697x10 <sup>-1</sup>	6.45	6.8976x10 <sup>-1</sup>	1.26	3.00
<sup>242</sup> Pu	2.886x10 <sup>-1</sup>	2.761x10 <sup>-1</sup>	8.69	2.8698x10 <sup>-1</sup>	-0.56	3.94
<sup>241</sup> Am		2.426x10 <sup>-1</sup>	4.22	2.4250x10 <sup>-1</sup>		-0.04
<sup>243</sup> Am		4.101x10 <sup>-2</sup>	11.31	3.9537x10 <sup>-2</sup>		-3.59
<sup>237</sup> Np	2.680x10 <sup>-1</sup>	2.912x10 <sup>-1</sup>	8.61	2.6676x10 <sup>-1</sup>	-0.46	-8.39
<sup>95</sup> Mo		5.666x10 <sup>-1</sup>	1.17	5.6028x10 <sup>-1</sup>		-1.12
<sup>99</sup> Tc		5.985x10 <sup>-1</sup>	5.17	5.9757x10 <sup>-1</sup>		-0.16
<sup>101</sup> Ru		5.637x10 <sup>-1</sup>	1.03	5.6355x10 <sup>-1</sup>		-0.03
<sup>103</sup> Rh		3.492x10 <sup>-1</sup>	4.57	3.4761x10 <sup>-1</sup>		-0.46
<sup>109</sup> Ag		5.396x10 <sup>-2</sup>	11.03	5.3361x10 <sup>-2</sup>		-1.11
<sup>133</sup> Cs	8.500x10 <sup>-1</sup>	8.415x10 <sup>-1</sup>	4.87	8.4288x10 <sup>-1</sup>	-0.84	0.16
<sup>135</sup> Cs	3.600x10 <sup>-1</sup>	3.821x10 <sup>-1</sup>	2.49	3.8658x10 <sup>-1</sup>	7.38	1.17
<sup>143</sup> Nd	6.130x10 <sup>-1</sup>	6.232x10 <sup>-1</sup>	2.76	6.1430x10 <sup>-1</sup>	0.21	-1.43
<sup>145</sup> Nd	5.100x10 <sup>-1</sup>	5.066x10 <sup>-1</sup>	1.02	5.0698x10 <sup>-1</sup>	-0.59	0.07
<sup>147</sup> Sm		1.806x10 <sup>-1</sup>	6.03	1.6275x10 <sup>-1</sup>		-9.89
<sup>149</sup> Sm	2.900x10 <sup>-3</sup>	2.054x10 <sup>-3</sup>	14.14	1.9915x10 <sup>-3</sup>	-31.33	-3.04
<sup>150</sup> Sm	2.070x10 <sup>-1</sup>	1.953x10 <sup>-1</sup>	5.30	2.1025x10 <sup>-1</sup>	1.57	7.66
<sup>151</sup> Sm		9.742x10 <sup>-3</sup>	22.41	9.6462x10 <sup>-3</sup>		-0.98
<sup>152</sup> Sm	8.700x10 <sup>-2</sup>	9.394x10 <sup>-2</sup>	7.20	8.6684x10 <sup>-2</sup>	-0.36	-7.72
<sup>153</sup> Eu	7.900x10 <sup>-2</sup>	7.655x10 <sup>-2</sup>	7.90	8.1485x10 <sup>-2</sup>	3.15	6.45
<sup>155</sup> Gd		3.879x10 <sup>-3</sup>	33.45	4.0300x10 <sup>-3</sup>		3.89

Table VII. Comparisons of Isotopic Concentrations(mg/g UO<sub>2</sub>) for Case B  
(37.12GWd/MTU Burnup)

Isotope	Measurement Value	Average Value	Standard Deviation of Col. 3 (%)	MOCUP Results	Error of Col. 5 with Col.2(%)	Error of Col. 5 with Col.3(%)
<sup>234</sup> U	1.400x10 <sup>-1</sup>	1.363x10 <sup>-1</sup>	7.08	1.3331x10 <sup>-1</sup>	-4.78	-2.20
<sup>235</sup> U	5.170	4.879	6.01	4.9255	-4.73	0.95
<sup>236</sup> U	3.530	3.633	2.72	3.5762	1.31	-1.56
<sup>238</sup> U	8.327x10 <sup>+2</sup>	8.304x10 <sup>+2</sup>	0.17	8.3046x10 <sup>+2</sup>	-0.27	0.01
<sup>238</sup> Pu	1.893x10 <sup>-1</sup>	1.746x10 <sup>-1</sup>	14.80	1.6950x10 <sup>-1</sup>	-10.46	-2.92
<sup>239</sup> Pu	4.357	4.314	6.08	4.2756	-1.87	-0.89
<sup>240</sup> Pu	2.239	2.189	4.27	2.1852	-2.40	-0.17
<sup>241</sup> Pu	9.028x10 <sup>-1</sup>	8.859x10 <sup>-1</sup>	5.97	8.5309x10 <sup>-1</sup>	-5.51	-3.70
<sup>242</sup> Pu	5.761x10 <sup>-1</sup>	5.593x10 <sup>-1</sup>	8.28	5.6241x10 <sup>-1</sup>	-2.38	0.56
<sup>241</sup> Am		3.119x10 <sup>-1</sup>	4.35	2.9460x10 <sup>-1</sup>		-5.55
<sup>243</sup> Am		1.137x10 <sup>-1</sup>	10.41	9.5145x10 <sup>-2</sup>		-16.32
<sup>237</sup> Np	3.560x10 <sup>-1</sup>	4.183x10 <sup>-1</sup>	8.86	3.8220x10 <sup>-1</sup>	7.36	-8.63
<sup>95</sup> Mo		7.333x10 <sup>-1</sup>	1.30	7.2860x10 <sup>-1</sup>		-0.64
<sup>99</sup> Tc		7.745x10 <sup>-1</sup>	3.57	7.8220x10 <sup>-1</sup>		0.99
<sup>101</sup> Ru		7.611x10 <sup>-1</sup>	1.05	7.6273x10 <sup>-1</sup>		0.21
<sup>103</sup> Rh		4.436x10 <sup>-1</sup>	5.15	4.4074x10 <sup>-1</sup>		-0.65
<sup>109</sup> Ag		8.237x10 <sup>-2</sup>	10.61	8.0589x10 <sup>-2</sup>		-2.16
<sup>133</sup> Cs	1.090	1.085	4.90	1.0852	-0.44	0.02
<sup>135</sup> Cs	4.000x10 <sup>-1</sup>	4.148x10 <sup>-1</sup>	2.98	4.1604x10 <sup>-1</sup>	4.01	0.30
<sup>143</sup> Nd	7.160x10 <sup>-1</sup>	7.292x10 <sup>-1</sup>	3.93	7.1175x10 <sup>-1</sup>	-0.59	-2.39
<sup>145</sup> Nd	6.530x10 <sup>-1</sup>	6.454x10 <sup>-1</sup>	1.25	6.4923x10 <sup>-1</sup>	-0.58	0.59
<sup>147</sup> Sm		2.010x10 <sup>-1</sup>	7.95	1.7613x10 <sup>-1</sup>		-12.37
<sup>149</sup> Sm	3.000x10 <sup>-3</sup>	2.208x10 <sup>-3</sup>	15.01	2.0576x10 <sup>-3</sup>	-31.41	-6.81
<sup>150</sup> Sm	2.710x10 <sup>-1</sup>	2.738x10 <sup>-1</sup>	7.07	2.9822x10 <sup>-1</sup>	10.05	8.92
<sup>151</sup> Sm		1.092x10 <sup>-2</sup>	21.72	9.5884x10 <sup>-3</sup>		-12.19
<sup>152</sup> Sm	1.040x10 <sup>-1</sup>	1.195x10 <sup>-1</sup>	9.01	1.0975x10 <sup>-1</sup>	5.52	-8.16
<sup>153</sup> Eu	1.090x10 <sup>-1</sup>	1.139x10 <sup>-1</sup>	8.19	1.1988x10 <sup>-1</sup>	9.98	5.25
<sup>155</sup> Gd		6.676x10 <sup>-3</sup>	33.28	6.7335x10 <sup>-3</sup>		0.86



Table VIII. Comparisons of Isotopic Concentrations(mg/g UO<sub>2</sub>) for Case C  
(44.34GWd/MTU Burnup)

Isotope	Measurement Value	Average Value	Standard Deviation of Col. 3 (%)	MOCUP Results	Error of Col. 5 with Col.2(%)	Error of Col. 5 with Col.3(%)
<sup>234</sup> U	1.200x10 <sup>-1</sup>	1.215x10 <sup>-1</sup>	8.99	1.1945x10 <sup>-1</sup>	-0.46	-1.69
<sup>235</sup> U	3.540	3.201	8.12	3.2615	-7.87	1.89
<sup>236</sup> U	3.690	3.769	2.60	3.7162	0.71	-1.40
<sup>238</sup> U	8.249x10 <sup>+2</sup>	8.247x10 <sup>+2</sup>	0.21	8.2480x10 <sup>+2</sup>	-0.01	0.01
<sup>238</sup> Pu	2.688x10 <sup>-1</sup>	2.452x10 <sup>-1</sup>	13.86	2.4147x10 <sup>-1</sup>	-10.17	-1.52
<sup>239</sup> Pu	4.357	4.303	7.12	4.0566	-6.89	-5.73
<sup>240</sup> Pu	2.543	2.437	5.27	2.4383	-4.12	0.05
<sup>241</sup> Pu	1.020	9.892x10 <sup>-1</sup>	6.86	9.7377x10 <sup>-1</sup>	-4.53	-1.56
<sup>242</sup> Pu	8.401x10 <sup>-1</sup>	7.985x10 <sup>-1</sup>	8.39	8.1602x10 <sup>-1</sup>	-2.87	2.19
<sup>241</sup> Am		3.403x10 <sup>-1</sup>	5.29	3.2639x10 <sup>-1</sup>		-4.09
<sup>243</sup> Am		1.917x10 <sup>-1</sup>	10.40	1.5251x10 <sup>-1</sup>		-20.44
<sup>237</sup> Np	4.680x10 <sup>-1</sup>	5.005x10 <sup>-1</sup>	9.42	4.5338x10 <sup>-1</sup>	-3.12	-9.42
<sup>95</sup> Mo		8.440x10 <sup>-1</sup>	1.85	8.4205x10 <sup>-1</sup>		-0.23
<sup>99</sup> Tc		8.958x10 <sup>-1</sup>	4.21	9.0798x10 <sup>-1</sup>		1.36
<sup>101</sup> Ru		9.021x10 <sup>-1</sup>	1.76	9.0841x10 <sup>-1</sup>		0.70
<sup>103</sup> Rh		4.099x10 <sup>-1</sup>	5.40	4.9139x10 <sup>-1</sup>		19.88
<sup>109</sup> Ag		1.036x10 <sup>-1</sup>	10.21	1.0218x10 <sup>-1</sup>		-1.37
<sup>133</sup> Cs	1.240	1.244	5.60	1.2423	0.19	-0.13
<sup>135</sup> Cs	4.300x10 <sup>-1</sup>	4.318x10 <sup>-1</sup>	3.63	4.4194x10 <sup>-1</sup>	2.78	2.35
<sup>143</sup> Nd	7.630x10 <sup>-1</sup>	7.748x10 <sup>-1</sup>	4.51	7.5649x10 <sup>-1</sup>	-0.85	-2.36
<sup>145</sup> Nd	7.440x10 <sup>-1</sup>	7.339x10 <sup>-1</sup>	1.46	7.4198x10 <sup>-1</sup>	-0.27	1.10
<sup>147</sup> Sm		2.070x10 <sup>-1</sup>	9.12	1.7816x10 <sup>-1</sup>		-13.93
<sup>149</sup> Sm	4.700x10 <sup>-3</sup>	2.336x10 <sup>-3</sup>	15.61	2.2334x10 <sup>-3</sup>	-52.48	-4.39
<sup>150</sup> Sm	3.610x10 <sup>-1</sup>	3.311x10 <sup>-1</sup>	8.50	3.6496x10 <sup>-1</sup>	1.10	10.23
<sup>151</sup> Sm		1.171x10 <sup>-2</sup>	22.31	1.0994x10 <sup>-2</sup>		-6.12
<sup>152</sup> Sm	1.210x10 <sup>-1</sup>	1.355x10 <sup>-1</sup>	9.68	1.2364x10 <sup>-1</sup>	2.18	-8.76
<sup>153</sup> Eu	1.480x10 <sup>-1</sup>	1.397x10 <sup>-1</sup>	8.52	1.4628x10 <sup>-1</sup>	-1.16	4.71
<sup>155</sup> Gd		8.849x10 <sup>-3</sup>	32.97	8.9863x10 <sup>-3</sup>		1.55

Table IX. Comparisons of EOL  $k_{\infty}$  for Three Cases

Burnup (GWd/MTU)	Computer code	$k_{\infty}$ with calculated concentrations, $k_{\infty,C}$	$k_{\infty}$ with measured concentrations, $k_{\infty,M}$	$\rho_C - \rho_M^a$	$k_{\infty}$ with average concentrations, $k_{\infty,A}$	$\rho_C - \rho_A$
27.35	MOCUP	1.00567 <sup>b</sup>	1.00399	0.0017	1.00103	0.0046
	CASMO-3	1.00934	1.01842	-0.0088	1.01721	-0.0077
37.12	MOCUP	0.92079	0.92823	-0.0087	0.91906	0.0020
	CASMO-3	0.89869	0.92193	-0.0280	0.91776	-0.0231
44.34	MOCUP	0.85399	0.86263	-0.0117	0.86257	-0.0116
	CASMO-3	0.82784	0.85320	-0.0359	0.85474	-0.0380

<sup>a</sup>  $\rho$  denotes reactivity.

<sup>b</sup> The statistical uncertainties of all the  $k_{\infty}$  from MOCUP are less than 0.001.

Table X. Initial Atomic Number Density(atoms/barn-cm) for Fast Reactor Benchmark<sup>5</sup>

Inner core					
<sup>235</sup> U	<sup>238</sup> U	<sup>238</sup> Pu	<sup>239</sup> Pu	<sup>240</sup> Pu	
9.409x10 <sup>-6</sup>	3.754 x10 <sup>-3</sup>	8.683 x10 <sup>-5</sup>	6.037 x10 <sup>-4</sup>	4.105 x10 <sup>-4</sup>	
<sup>241</sup> Pu	<sup>242</sup> Pu	<sup>241</sup> Am	Fe	Cr	
1.990 x10 <sup>-4</sup>	2.180 x10 <sup>-4</sup>	1.990 x10 <sup>-5</sup>	1.231 x10 <sup>-2</sup>	3.541 x10 <sup>-3</sup>	
Ni	Mo	O	Na	Mn	
2.583 x10 <sup>-3</sup>	3.105 x10 <sup>-4</sup>	1.057 x10 <sup>-2</sup>	7.389 x10 <sup>-3</sup>	2.957 x10 <sup>-4</sup>	
Outer core					
<sup>235</sup> U	<sup>238</sup> U	<sup>238</sup> Pu	<sup>239</sup> Pu	<sup>240</sup> Pu	
7.899x10 <sup>-6</sup>	3.152 x10 <sup>-3</sup>	1.223 x10 <sup>-4</sup>	8.503 x10 <sup>-4</sup>	5.782 x10 <sup>-4</sup>	
<sup>241</sup> Pu	<sup>242</sup> Pu	<sup>241</sup> Am	Fe	Cr	
2.803 x10 <sup>-4</sup>	3.071 x10 <sup>-4</sup>	2.803 x10 <sup>-5</sup>	1.231 x10 <sup>-2</sup>	3.541 x10 <sup>-3</sup>	
Ni	Mo	O	Na	Mn	
2.583 x10 <sup>-3</sup>	3.105 x10 <sup>-4</sup>	1.061 x10 <sup>-2</sup>	7.389 x10 <sup>-3</sup>	2.957 x10 <sup>-4</sup>	
Axial and radial reflector(shielding)					
Fe	Cr	Ni	Mo	Na	Mn
2.662 x10 <sup>-2</sup>	7.662 x10 <sup>-3</sup>	5.588 x10 <sup>-3</sup>	6.717 x10 <sup>-4</sup>	1.093 x10 <sup>-2</sup>	6.398 x10 <sup>-4</sup>
(Rod) Follower					
Fe	Cr	Ni	Mo	Na	Mn
7.987 x10 <sup>-3</sup>	2.299 x10 <sup>-3</sup>	1.676 x10 <sup>-3</sup>	2.015 x10 <sup>-4</sup>	1.863 x10 <sup>-2</sup>	1.920 x10 <sup>-4</sup>

Table XI. Physical Data of Fast Reactor Benchmark

Parameter	Data
Sub-assembly lattice dimension, cm	15.14
Number of pins/sub-assembly	331(221 fuel pins,110 pins with no fuel)
External clad diameter, cm	0.655
Pellet diameter, cm	0.550
Central hole diameter, cm	0.200
Nature and density of fuel	Mixed UO <sub>2</sub> (10.46g/cc)-PuO <sub>1.98</sub> (10.94g/cc)
Uranium isotopic composition, at%	0.25U-235, 99.75U-238
Plutonium isotopic composition, at%	5.6Pu-238, 39.1Pu-239, 26.7Pu-240, 13.0Pu-241, 14.3Pu-242, 1.3Am-241
Pu/(U+Pu) ratio for inner core, mass%	28.85
Pu/(U+Pu) ratio for outer core, mass%	40.64
Density of steel(hex-tube and cladding), g/cc	7.95
Composition of steel, mass%	64.75Fe, 17.00Cr, 14.00Ni, 2.75Mo, 1.50Mn
Volume fraction of fuel sub-assembly, %	22.96Fuel, 23.11Steel, 33.89Sodium
Number of sub-assemblies in inner core	128
Number of sub-assemblies in outer core	112
Volume fraction of reflector sub-assembly, %	50.0Steel, 50.0Sodium
Volume fraction of follower sub-assembly, %	15.0Steel, 85.0Sodium
Thermal power, MW	1500
Electrical Power, MW	600
Load factor	0.80
Residence time of fuel sub-assemblies, EFPD	625
Fuel temperature, C	1227
Temperature of cladding, tube and sodium, C	470

Table XII. Comparisons of Some BOL Results

Sort	MOCUP results	Range of reported values	Sort	MOCUP results	Range of reported values
k-eff	1.11955 (0.00170) <sup>a</sup>	1.10660-1.13488			
Critical balance(%)					
Absorption	90.64	88.5-92.0	Leakage	9.36	8.0-11.5
Absorption normalized to 1.0					
U-235	0.0037	0.0037-0.0394	O	0.0024	0.0016-0.0030
U-238	0.2041	0.2027-0.2139	Fe	0.0948	0.0746-0.0925
Pu-238	0.0327	0.0290-0.0349	Cr	0.0391	0.0263-0.0379
Pu-239	0.2771	0.2786-0.2916	Ni	0.0374	0.0358-0.0409
Pu-240	0.0756	0.0674-0.0838	Mo	0.0532	0.0478-0.0547
Pu-241	0.1164	0.1155-0.1237	Mn	0.0167	0.0230-0.0330
Pu-242	0.0314	0.0034-0.0325	Na	0.0071	0.0069-0.0078
Am-241	0.0080	0.0080-0.0090			

<sup>a</sup> The value in parentheses is the statistical uncertainties of MCNP.

Table XIII. Comparisons of Reactivity Loss and Isotopic Composition Variation

Sort	MOCUP	ANL (USA)	CEA (FRANCE)	PNC(J2) (JAPAN)	PNC(J3,2) (JAPAN)	PSI (SWIZERLAND)
Reactivity loss of BOL-EOL(% of $\Delta k/kk'$ )						
$\Delta \rho \times 100$ %	12.44	12.85	13.27	13.60	13.39	13.06
Isotopic composition variation of EOL-BOL( $\Delta kg$ )						
U-235	-5.61	-5.6	-5.9	-5.8	-5.7	-5.5
U-238	-394.5	-420	-411	-392	-390	-384
Pu-238	-49.0	-50	-45	-50	-47	-43.4
Pu-239	-160.9	-149	-174	-170	-131	-173
Pu-240	-34.7	-38	-21	-32	-13	-34
Pu-241	-136.5	-133	-139	-133	-122	-137
Pu-242	-30.5	-29	-42	-31	-20	-25
Am-241	9.58	9.1	7.5	8.3	9.5	8.6
Am-243	31.2	31	44	33	34	33
Cm-242	4.63	3.7	5.2	4.8	4.5	4.1
Cm-244	4.48	4.1	7.4	5.3	5.3	5.4

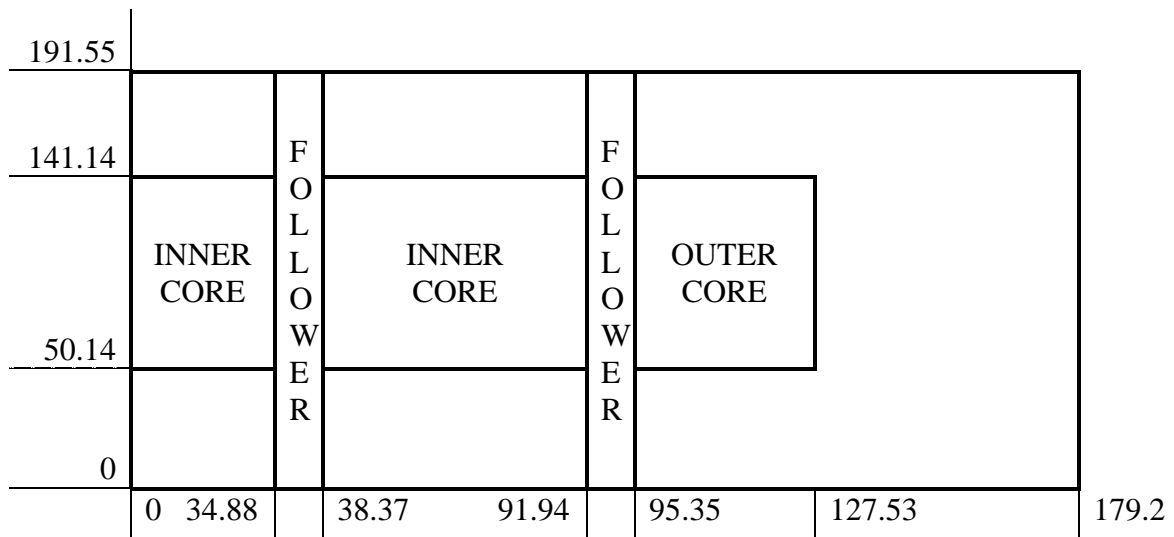


Figure 1. R-Z Geometry Sketch of Fast Reactor Benchmark. The Unspecified Region is Reflector. Unit: cm.