Nuclear Energy & Infrastructure Systems Division - Energy Sciences & Technology Dept.

Building 130
Phone 631 344-2604
Fax 631 344-3957
diamond@bnl.gov

managed by Brookhaven Science Associates
for the U.S. Department of Energy

Memo

date: *June 24, 2004*

to: *Files*

from: *D. Diamond, A. Hanson, J. Saccheri*

subject: *ACR-700 CVR Calculations*

INTRODUCTION

This memo is to document progress on Task 1 of the project "Confirmatory Analysis of Nuclear Phenomena for ACR-700 Safety Evaluation." The objective of Task 1 is to provide detailed analysis of safety-related ACR-700 phenomena and to assess modeling needs for further analyses. This is to support the NRC staff's technical review activities, and their associated efforts to adapt and qualify an audit capability that will simulate operating states, transients, and accidents.

The first step in this process is to use rigorous computer models to calculate the coolant void reactivity (CVR) for an isolated fuel bundle. The objective is to provide quantitative information on the contributions to the CVR at the lattice physics level from different physics effects, to determine the effect of different modeling approximations, and, by comparing results with those from AECL, improve our understanding of the validation of the vendor's nuclear analysis methods. After this work is completed, further analyses will be performed modeling larger portions of the core, e.g., color sets (a 2x2 array of fuel cells), and/or the entire core.

METHODOLOGY

ACR-700 fuel bundle calculations have been carried out using the MCNP [1], MONTEBURNS [2], and ORIGEN2 [3] computer codes. MCNP provides the continuous energy Monte Carlo analysis of the fuel bundle neutronics for a given composition and geometry. The depletion and change of inventory are computed with ORIGEN2. MONTEBURNS is used as an automated interface between MCNP and ORIGEN2 to calculate the inventories and burnup over time. It uses the local neutron spectra from MCNP to determine one-group nuclear reaction cross sections used in ORIGEN2 to calculate the buildup of fission products and actinides and the burnup of fuel and poison materials in each predefined region. After a given time step, MONTEBURNS takes the inventory as calculated by ORIGEN2 and generates the compositions needed to run MCNP at the new time step. This process is repeated for a user determined number of time steps.

Results were obtained from MONTEBURNS at 1, 311, and 631 days, the time steps at which data was available from AECL [4]. MCNP was used at these time steps to calculate the multiplication factor (k or actually k_∞) for the system. CVR is calculated from the multiplication factor with and without coolant in the bundle: $CVR = 1/k_{cooled} - 1/k_{voided}$.

A set of evaluated neutron cross sections for many stable isotopes and a limited number of fission products is distributed with the MCNP computer code. This set of cross sections lacks many of the fission products that are needed for certain reactor analyses. Most of the fission products included in the inventories calculated by AECL (Appendix B of [4]) are not included. In addition, this set does not include dysprosium, which is a burnable poison in the ACR-700. Therefore the set of neutron cross sections in use at BNL for MCNP was enhanced by adding nuclides that are needed to analyze the ACR-700.

There were three changes made to the library. The first enhancement was to include cross sections for dysprosium. These cross sections were generated at ORNL by Luiz Leal using the NJOY computer code and were supplied to BNL by Donald Carlson at the NRC. The second source of data was from the University of Texas. More than 1000 files were downloaded and included from this source. The ~1000 files included many nuclides evaluated at 19 different temperatures. The final source of data was from M.I.T. and was generated for inclusion with the MCODE computer code. There were approximately 270 files from this source that were added to the standard MCNP library in use at BNL.

The selection of the specific cross section files for use in the MCNP models along with the scattering kernels was based on the temperatures for the different regions as described in Reference [4]. Many of the fission product files were evaluated only at one specific temperature so data at those temperatures had to be used. The major actinides, the dysprosium isotopes, and the moderator and coolant materials have been evaluated at several temperatures making possible the selection of files at temperatures close to those reported in Tables 4-1 and 4-2 of Reference [4].

The fuel bundle was modeled in two dimensions within a square fuel cell with periodic boundary conditions as shown in Figure 1. (Later calculations may be done in three-dimensions to determine the effect of end fittings and reactivity control devices.) The fuel bundle has one central pin with natural uranium and dysprosium as a burnable poison. Around the central pin is a set of seven fuel pins with slightly enriched U. The central pin and the first ring of pins have a fuel pellet radius of 0.631 cm. The first ring of fuel elements are on a pitch of 1.73 cm relative to the central element. There are two outer rings with a pellet radius of 0.536 cm. The third ring has 14 fuel elements, and the outer ring has 21 fuel elements. Ring three has a pitch of 3.075 cm and ring four has a pitch of 4.385 cm. The space between the pins is filled with light water. The fuel is clad in Zircaloy-4.

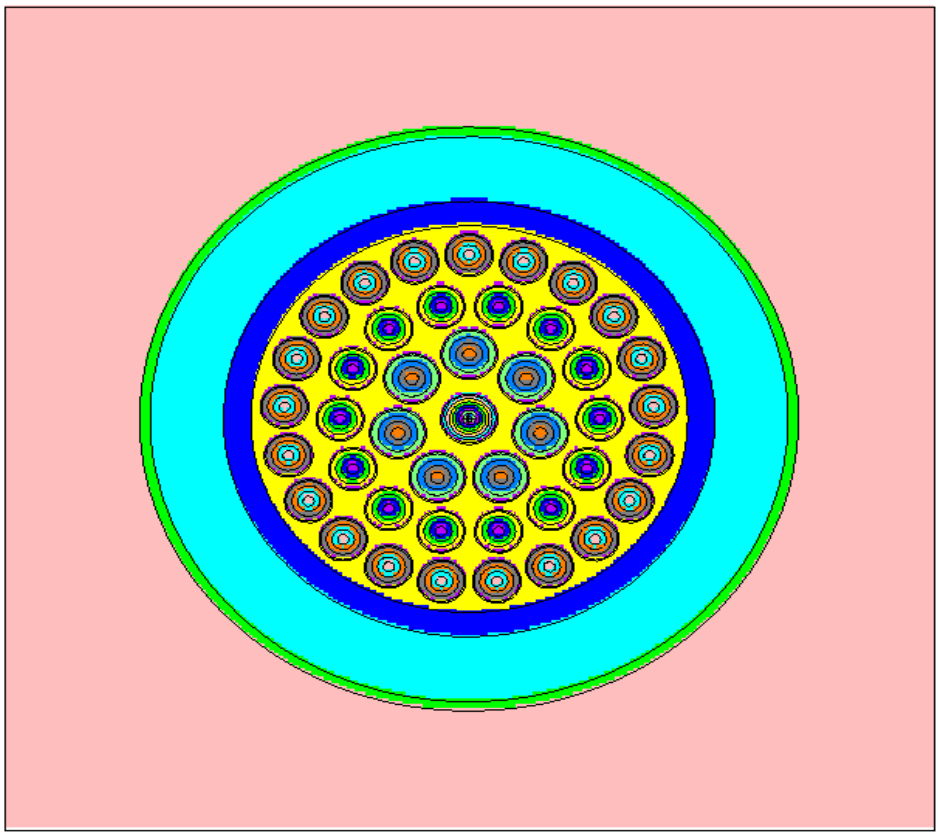

Figure 1 MCNP Fuel Cell Model for ACR-700

The pressure tube that contains the fuel pins is made of Zr-2.5% Nb. This tube is surrounded by a gap filled with CO_2. The CO_2 is retained in a calandria tube, made of Zircaloy-2. Outside of this is the D_2O moderator.
The geometric model has the central fuel pellet divided into eight concentric regions with equal thickness. The pellets in the three outer rings were divided into four concentric regions. The burnup analysis was done for each region.

Two different fuel bundles were considered; one with the design that had been documented by AECL [4] and one with a newer design that had been proposed as of mid-2003. The former used

2.0 w/o[a] enriched fuel in the outer rings and 4.6 w/o[a] Dy in the center element, whereas the latter used 2.1 w/o U-235 in the fuel and 7.6 w/o Dy. The reason for analyzing the older design was to compare burnup inventories that AECL provided for this design; inventories that are not yet available for the current design. For the 2 w/o enrichment design, k was calculated with MCNP using the inventories determined by AECL [4] and using those determined using MCNP/MONTEBURNS/ORIGEN2.

RESULTS

Original Design Table 1 shows, for the original design (i.e., 2 w/o U-235), the mean values of k_∞ calculated by MCNP for the cooled and voided conditions as well as the standard error. Results are shown for beginning-of-cycle (BOC) as well as at three other times during the life of a bundle. The BNL results are both using the AECL generated inventories and those generated using MONTEBURNS. Some results for k_∞ were available from AECL documents/presentations and these are shown in the table. Where results were not available NA is marked. The AECL results were from WIMS-AECL (deterministic) calculations and the standard error is not relevant as it is for the Monte Carlo analysis. The differences between the AECL and BNL values of k_∞ are significant but it cannot be said whether they are due to differences in computer codes, fuel cell modeling, or input specifications for the fuel bundle or a combination of all three. An example of modeling is the number of annuli used to represent the fuel in each ring and an example of input is whether 100% heavy water was used in the moderator or water of some lesser purity. What would be significant would be a direct comparison between the AECL and BNL values of CVR for the identical conditions. Unfortunately, information from AECL to make that comparison is not yet available.

The values of CVR calculated by MCNP shown in Table 1 are also shown in Figure 2. Those marked as "AECL" were calculated using the inventories provided by AECL in Reference [4] and those marked "BNL" used MONTEBURNS to calculate the burnup. The results show that the CVR for this design is initially positive at low burnup and then becomes negative as burnup increases.

What is significant as well is whether the burnup dependence is calculated similarly by MONTEBURNS and WIMS-AECL. Figure 2 shows that this is true up to 311 days but the results at 631 days disagree by more than the standard deviation. Another comparison of the burnup analysis for the bundle with 2 w/o enriched fuel is given in Table 2. The table shows specific important nuclides (inventories) calculated by MONTEBURNS vs those calculated by WIMS-AECL. The table provides inventories in each of the four rings for three points in time. As time proceeds the differences become larger, however, without knowing anything about the AECL calculations, it is not possible to speculate on what causes the differences.

---

[a] Weight per cents are defined by AECL to be relative to unity U weight. Hence, 4.6 w/o Dy in U corresponds to 3.9% in UO_2.

Table 1 Multiplication Factors and CVR for Original Design (2.0 w/o U-235)

Source	Burnup	k_∞ (cooled)	std error, pcm	k_∞ (void)	std error, pcm	CVR, mk	std error, mk
BNL	BOC	1.25341	15	1.25502	16	1.0	0.1
AECL	BOC	1.24848	NA	NA	NA	NA	NA
BNL	1 day	1.21501	15	1.21716	16	1.4	0.2
AECL	1 day	1.21004	NA	NA	NA	NA	NA
BNL w AECL inventory	1 day	1.21558	15	1.21781	17	1.5	.2
BNL	311 days	1.05730	15	1.05340	16	-3.5	0.2
AECL	311 days	1.05343	NA	NA	NA	NA	NA
BNL w AECL inventory	311 days	1.06379	15	1.05972	16	-3.6	0.2
BNL	631 days	0.91988	15	0.91448	15	-6.42	0.2
AECL	631 days	0.91099	NA	NA	NA	NA	NA
BNL w AECL inventory	631 days	0.92444	15	.91974	15	-5.5	0.2

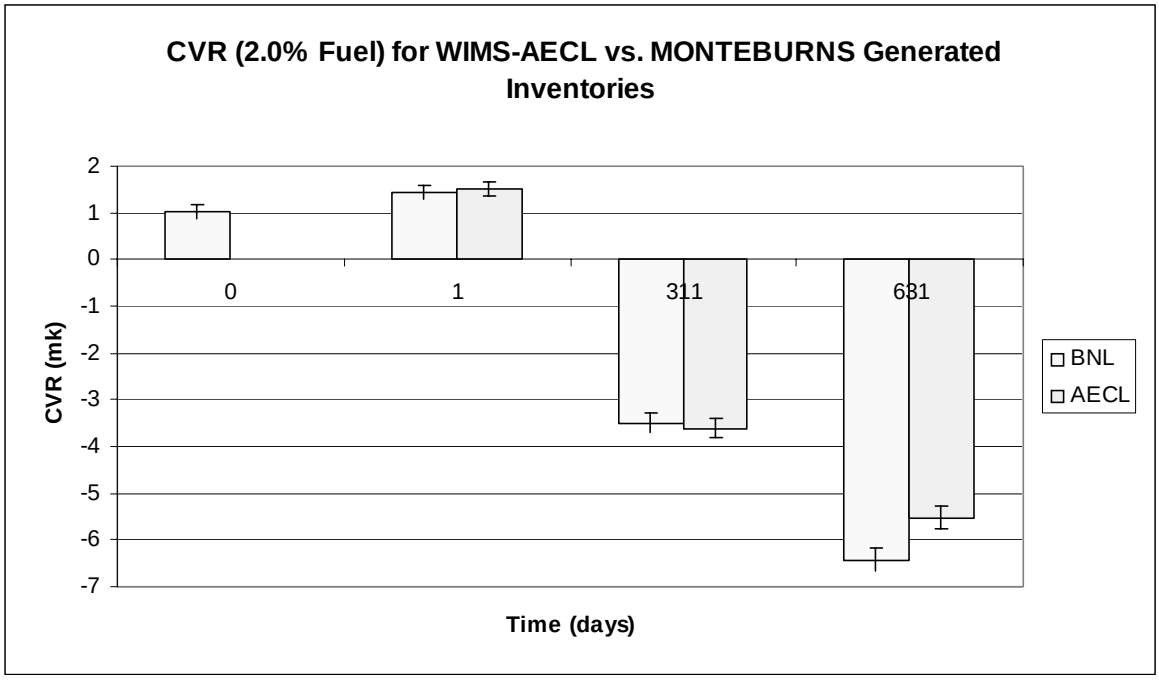

Figure 2. CVR Calculated by MCNP Using BNL and AECL Inventories

Table 2a Comparison of Selected Isotopes; WIMS vs MONTEBURNS Generated Inventories, After 1 Day of Irradiation

	wt fraction		%Deviation
	WIMS	**MB**	**(MB-WIMS)/WIMS**
Central Pin			
XE135	3.36E-08	3.32E-08	-1.30
DY160	8.98E-04	8.99E-04	0.06
DY161	7.30E-03	7.30E-03	0.00
DY162	9.86E-03	9.92E-03	0.63
DY163	9.74E-03	9.74E-03	0.00
DY164	1.11E-02	1.11E-02	-0.02
U235	6.02E-03	6.02E-03	-0.01
U238	8.41E-01	8.41E-01	0.00
PU239	1.36E-06	1.28E-06	-5.83
Ring 2			
XE135	9.17E-08	9.30E-08	1.44
U235	1.76E-02	1.76E-02	-0.01
U238	8.64E-01	8.64E-01	0.00
PU239	1.74E-06	1.58E-06	-9.06
Ring 3			
XE135	9.42E-08	9.55E-08	1.42
U235	1.76E-02	1.76E-02	0.00
U238	8.64E-01	8.64E-01	0.00
PU239	2.02E-06	1.89E-06	-6.38
Ring 4			
XE135	9.63E-08	9.74E-08	1.18
U235	1.76E-02	1.76E-02	-0.01
U238	8.64E-01	8.64E-01	0.00
PU239	2.59E-06	2.44E-06	-5.73

Table 2b Comparison of Selected Isotopes; WIMS vs MONTEBURNS Generated Inventories, After 311 Days of Irradiation

	wt fraction		
	WIMS	**MB**	**%Deviation**
			(MB-WIMS)/WIMS
Central Pin			
XE135	6.47E-08	6.84E-08	5.71
DY160	7.05E-04	7.81E-04	10.82
DY161	5.34E-03	5.40E-03	1.20
DY162	1.01E-02	1.04E-02	3.20
DY163	9.82E-03	9.72E-03	-1.03
DY164	6.27E-03	5.72E-03	-8.79
U235	4.62E-03	4.59E-03	-0.69
U238	8.37E-01	8.37E-01	-0.01
PU239	2.23E-03	2.25E-03	1.03
Ring 2			
XE135	1.07E-07	1.10E-07	2.77
U235	1.17E-02	1.16E-02	-1.07
U238	8.59E-01	8.59E-01	0.01
PU239	2.41E-03	2.34E-03	-2.99
Ring 3			
XE135	9.88E-08	1.02E-07	3.69
U235	1.02E-02	1.00E-02	-1.47
U238	8.58E-01	8.58E-01	0.00
PU239	2.45E-03	2.44E-03	-0.50
Ring 4			
XE135	8.61E-08	9.24E-08	7.42
U235	7.76E-03	7.64E-03	-1.61
U238	8.57E-01	8.57E-01	-0.01
PU239	2.58E-03	2.58E-03	0.02

Table 2c Comparison of Selected Isotopes; WIMS vs MONTEBURNS Generated Inventories, After 631 Days of Irradiation

	wt fraction		
	WIMS	**MB**	**%Deviation**
			(MB-WIMS)/WIMS
Central Pin			
XE135	7.28E-08	8.11E-08	11.48
DY160	5.29E-04	6.57E-04	24.18
DY161	3.58E-03	3.65E-03	1.78
DY162	9.68E-03	1.04E-02	6.99
DY163	9.90E-03	9.69E-03	-2.12
DY164	3.42E-03	2.87E-03	-16.14
U235	3.24E-03	3.18E-03	-1.95
U238	8.33E-01	8.32E-01	-0.06
PU239	3.19E-03	3.26E-03	2.47
Ring 2			
XE135	9.43E-08	1.01E-07	7.09
U235	7.08E-03	6.87E-03	-2.89
U238	8.54E-01	8.53E-01	-0.02
PU239	3.15E-03	3.14E-03	-0.20
Ring 3			
XE135	7.91E-08	8.60E-08	8.69
U235	5.02E-03	4.84E-03	-3.58
U238	8.52E-01	8.51E-01	-0.05
PU239	2.90E-03	2.97E-03	2.44
Ring 4			
XE135	6.24E-08	6.90E-08	10.49
U235	2.69E-03	2.60E-03	-3.43
U238	8.49E-01	8.48E-01	-0.07
PU239	2.77E-03	2.85E-03	3.06

Current Design Table 3 shows results for the current design (2.1 w/o U-235). The CVR is negative at BOC and one day for this design (as opposed to the original design) and becomes more negative with burnup. One data point is available from AECL and several from the Canadian Nuclear Safety Commission (CNSC) [5]. The data from CNSC based on MCNP utilized burnup from a WIMS-AECL calculation and no standard error was provided for the individual calculations of multiplication factor. The other source of data from CNSC utilized the HELIOS lattice physics code. Results are also shown graphically in Figure 3 for the cases calculated by MCNP at both BNL and CNSC.

It can be seen that the BNL MCNP results give a much larger negative CVR than obtained by AECL and CNSC for both BOC and at midburnup. The CNSC calculations using MCNP and HELIOS are consistent. The reason for this discrepancy can only be uncovered by looking into how AECL and CNSC carried out their calculations and making additional comparisons. For example, the BNL analysis uses multiple regions to model burnup within fuel pellets, the AECL analysis uses a single region and the CNSC model is not known. Further work could be done by investigating differences with codes used at these other installations (including not just AECL and CNSC, but also Purdue where similar calculations are underway) and at BNL using the DRAGON code. Preliminary results using DRAGON had not been satisfactory and there is a need to expend resources if that path is to be pursued.

To illustrate the difficulty in interpreting the differences note that for the 2.0 w/o case the differences in CVR between using the BNL and the AECL generated inventories are the result of the burnup calculation since both use MCNP to calculate CVR. The results show differences that are not large. However, in the 2.1 w/o case the differences in CVR calculated at BNL and CNSC both using MCNP are much larger and the suspected problem in this case would be the burnup calculation.

Figures 4, 5, and 6 show reaction rates, cooled and voided, at 0, 311, and 631 days to help understand the physics of the CVR. Each figure shows results for each of the four rings in the cluster. Due to the increase in number of fuel elements as one goes from the center "ring" (one element) to the three other rings (7, 14, and 21 elements), there is always an increase in reaction rate going toward the outside (not to be confused with the volumetric reaction rate). What is of interest on the graphs is to see how the rate changes when going from a cooled to voided condition as that directly determines a component of the CVR.

Figure 4a shows that at BOC the effect of void is to decrease the ^{235}U fission rate but only significantly in the outside ring. Similarly Figure 4b shows that the effect of void is to increase the capture rate in ^{238}U in the outer ring. Both of these negative effects are further enhanced by the increase in absorption in the Dy in the center element with the net effect being a negative CVR. The increase in Dy reaction rate with voiding at zero burnup is shown in Figure 7 as a function of annular region within the fuel element.

The same effects are seen at 311 and 631 days. Figures 5a and 6a have the change in fission rate but now include ^{239}Pu as well as ^{235}U. Figures 5b and 6b provide the capture rates in the important

U isotopes and Figure 4c and 5c are added to show similar results for the important Pu isotopes. All results show negative contributions to the CVR. Figures 8 and 9 show the corresponding changes in Dy reaction rate at 311 and 631 days, respectively. They are shown for each of the eight annular regions used to calculate the burnup in the central element.

Figure 10 shows the calculated multiplication factor vs void fraction. Although the calculations described above showed that the CVR for an isolated fuel cell was negative, it was of interest to know if it was negative for all void fractions. As can be seen from the graph the void reactivity coefficient (the slope of the curve in the figure) does not become positive. However, it can be seen that the value of the coefficient is low at small and large values of void fraction.

Table 3. Multiplication Factors and CVR for Current Design (2.1 w/o U-235)

Source	**Burnup**	**k_∞ (cooled)**	**std error, pcm**	**k_∞ (voided)**	**std error, pcm**	**CVR, mk**	**std error, mk**
BNL	BOC	1.25638	15	1.25102	16	-3.4	0.1
CNSC (MCNP)	BOC	1.25503	-	1.25388	-	-0.7	0.2
CNSC (HELIOS)	BOC	1.25206	NA	1.25125	NA	-0.5	NA
BNL	1 day	1.21787	17	1.21347	16	-3.0	0.2
BNL	311days (10 MWd/kg)	1.06086	15	1.05217	16	-7.8	0.2
AECL	“Midburn up”	1.06558	NA	1.06245	NA	-2.8	NA
CNSC (MCNP)	12 MWd/kg	1.03582	-	1.03261	-	-3.0	0.3
CNSC (HELIOS)	12 MWd/kg	1.03445	NA	1.03111	NA	-3.1	NA
BNL	631 days	0.92460	15	0.91548	15	-10.8	0.2

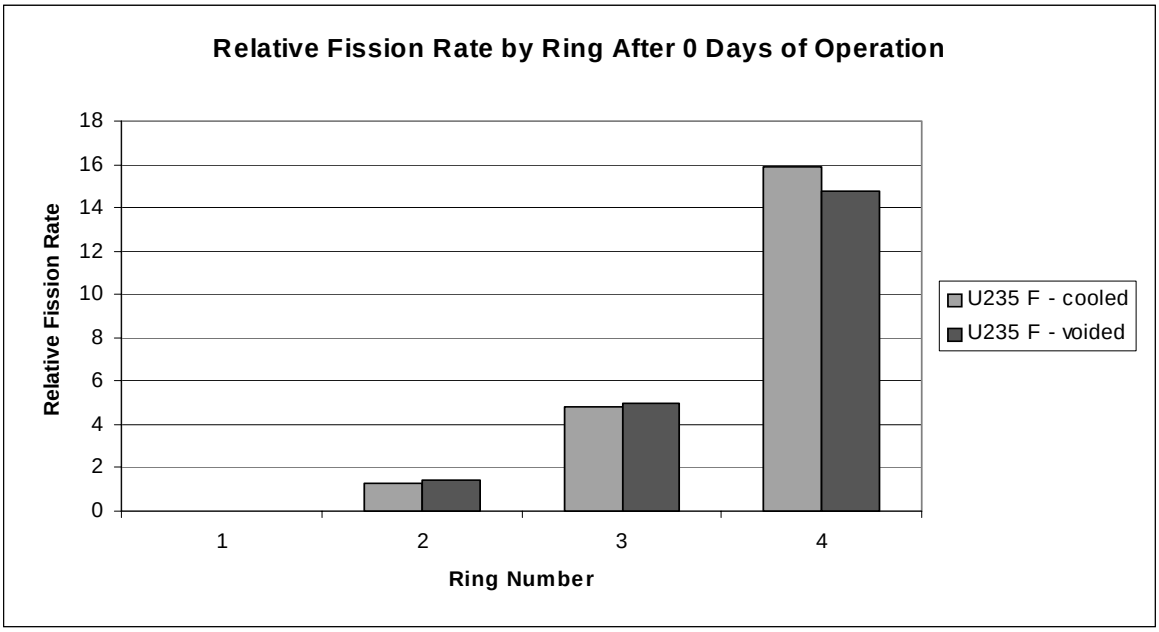

Figure 4a Relative Reaction Rates at Zero Burnup - Fission

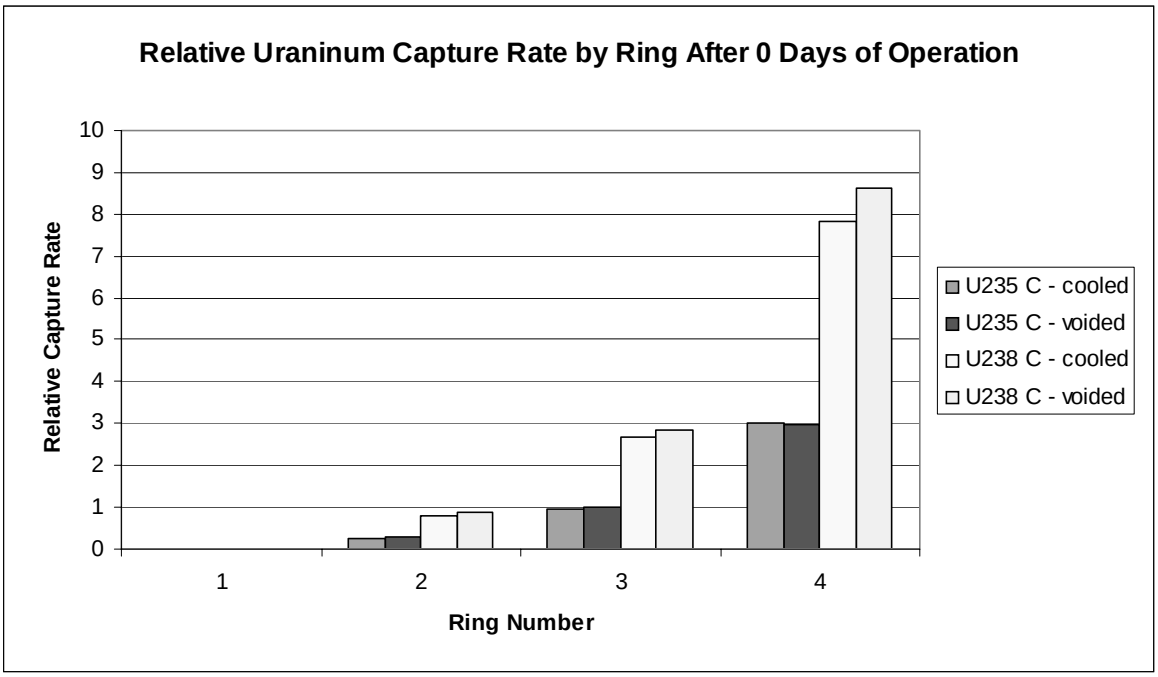

Figure 4b Relative Reaction Rates at Zero Burnp - Uranium Capture

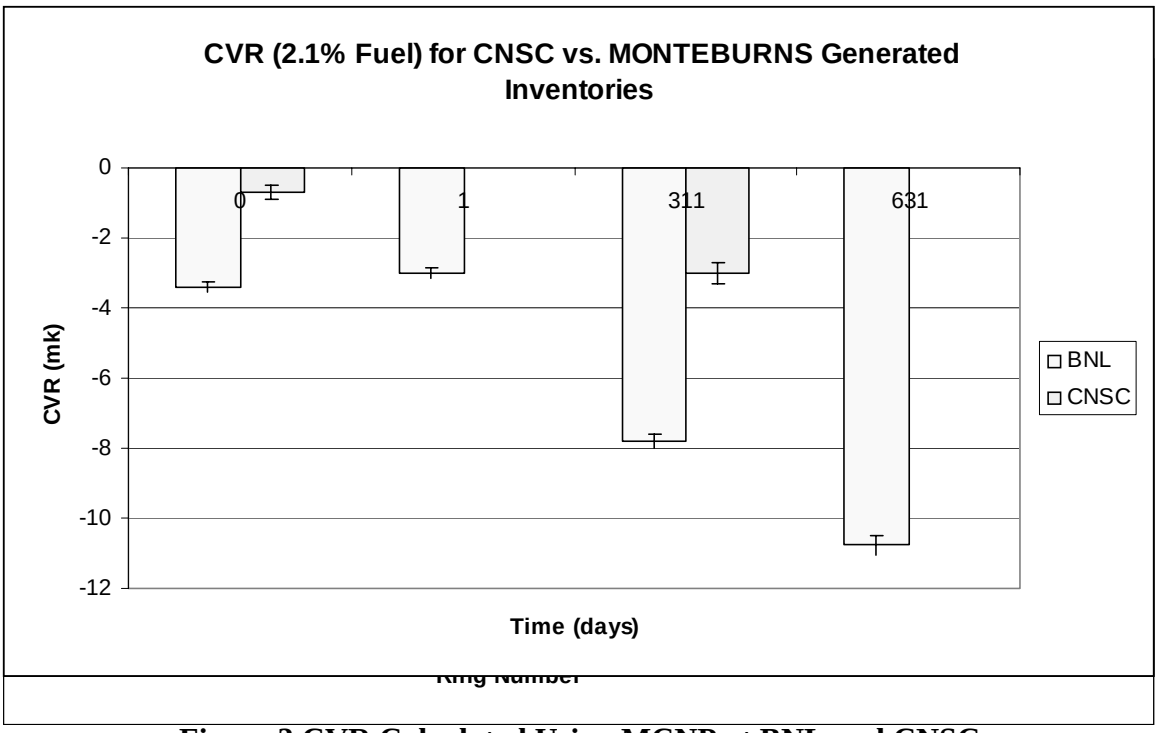

Figure 3 CVR Calculated Using MCNP at BNL and CNSC

Figure 5a Relative Reaction Rates at 311 Days - Fission

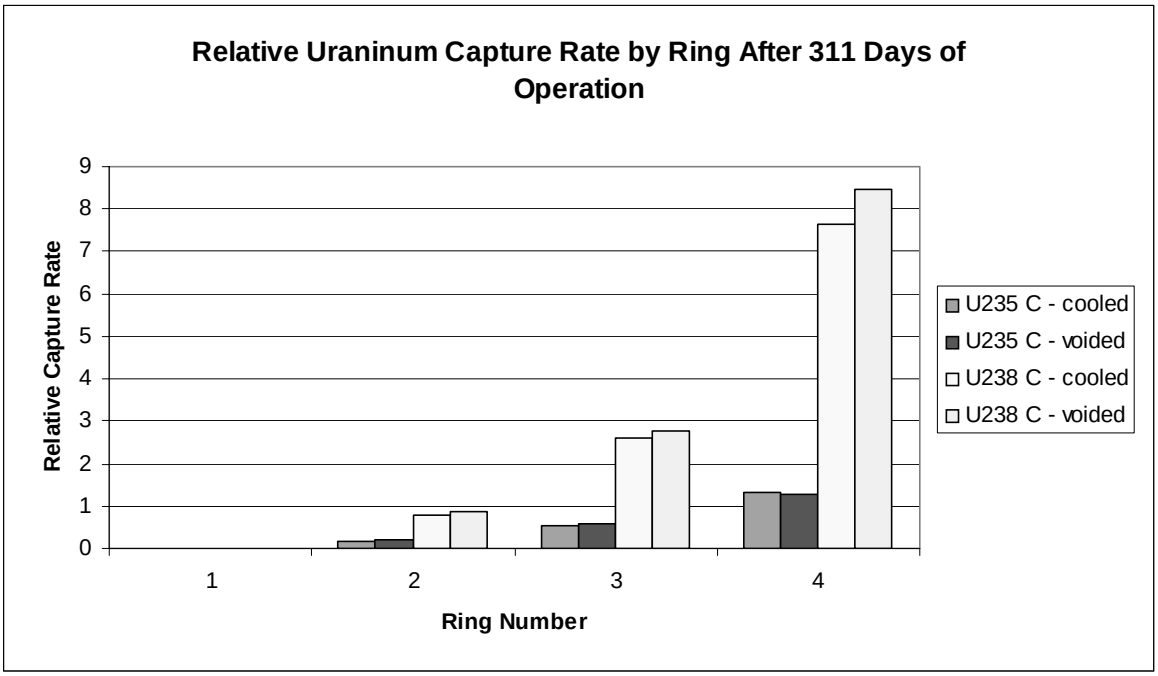

Figure 5b Relative Reaction Rates at 311 Days - Uranium Capture

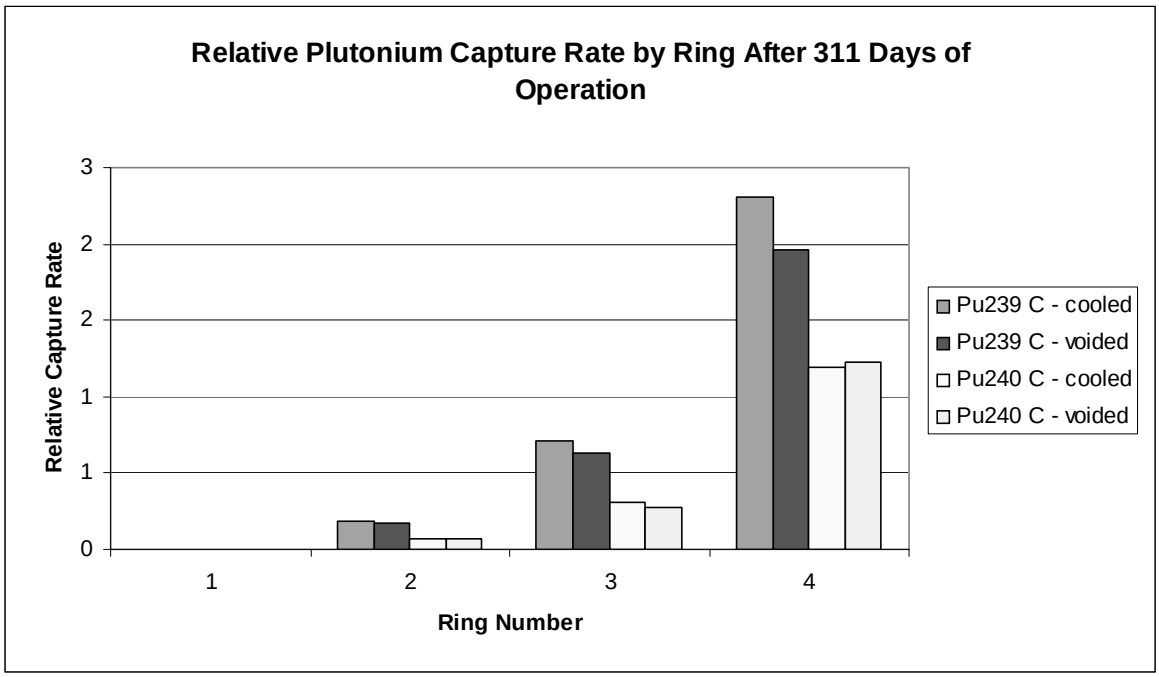

Figure 5c Relative Reaction Rates at 311 Days - Plutonium Capture

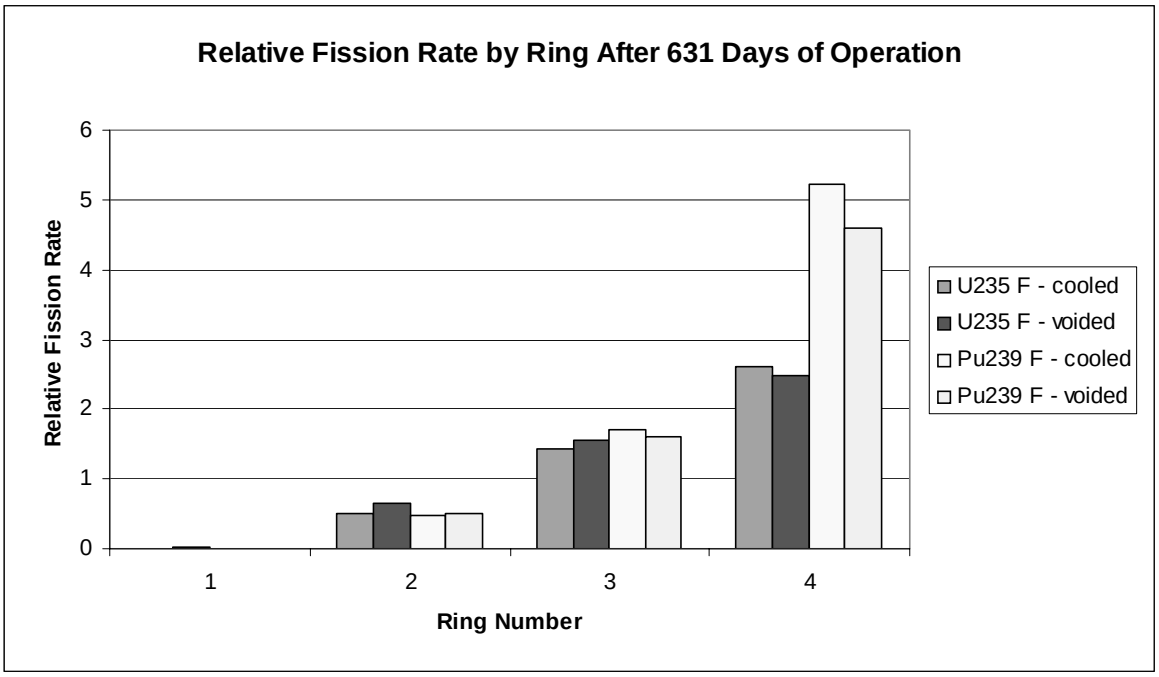

Figure 6a Relative Reaction Rates at 631 Days - Fission

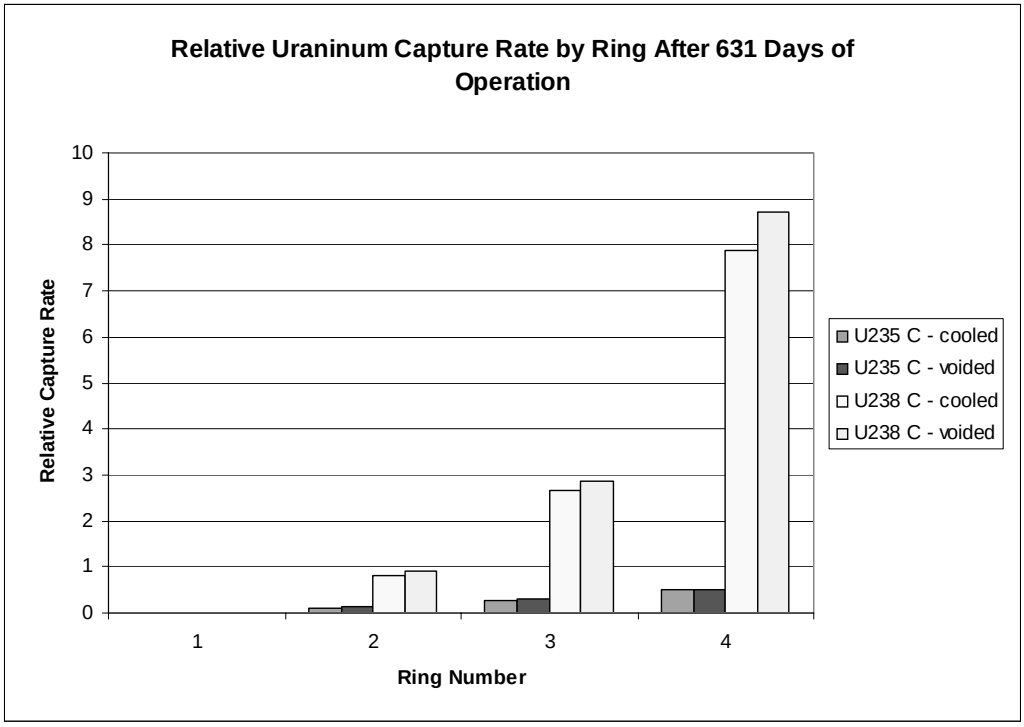

Figure 6b Relative Reaction Rates at 631 Days - Uranium Capture

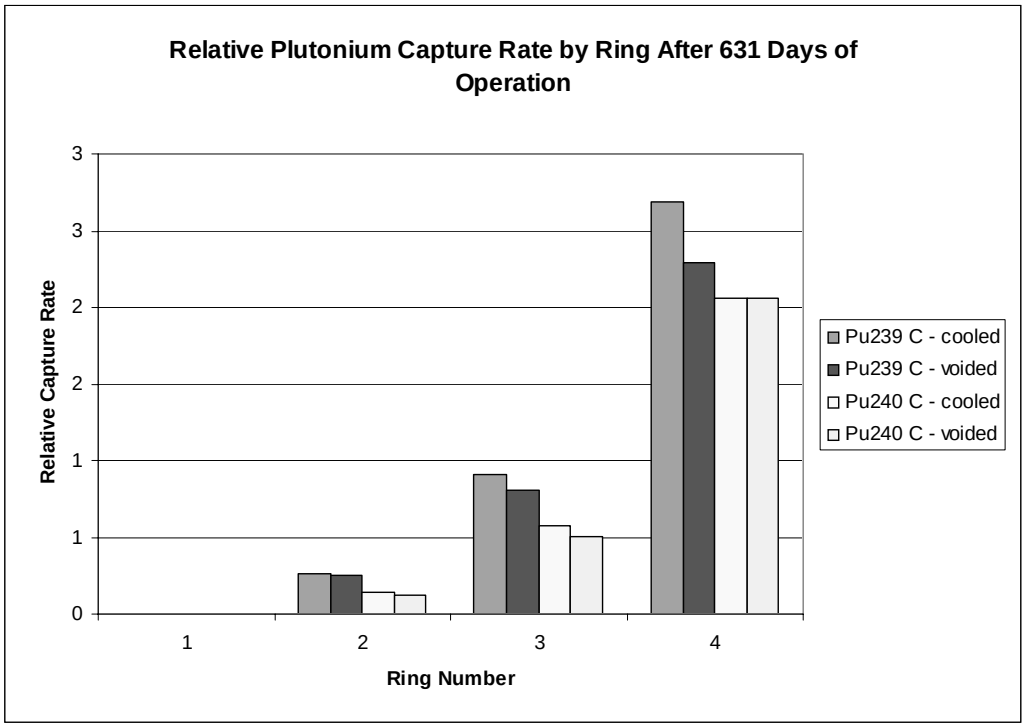

Figure 6c Relative Reaction Rates at 631 Days - Plutonium Capture

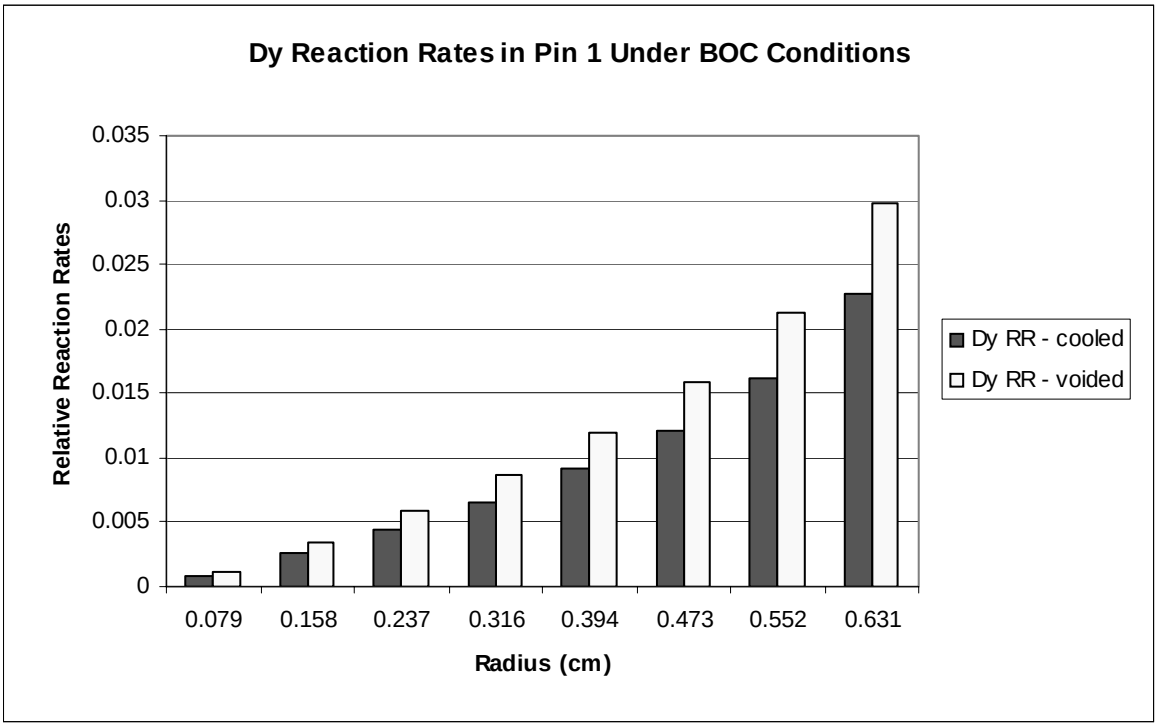

Figure 7 Dysprosium Reaction Rates at Zero Burnup

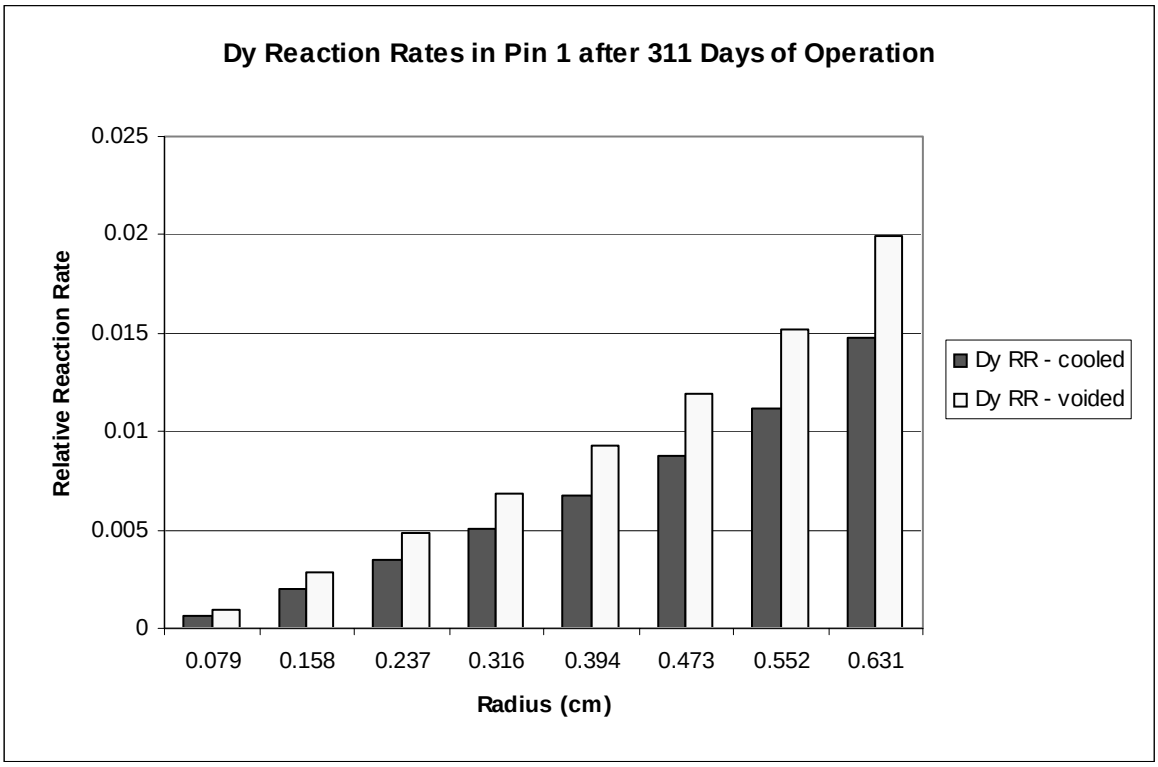

Figure 8 Dysprosium Reaction Rates at 311 Days

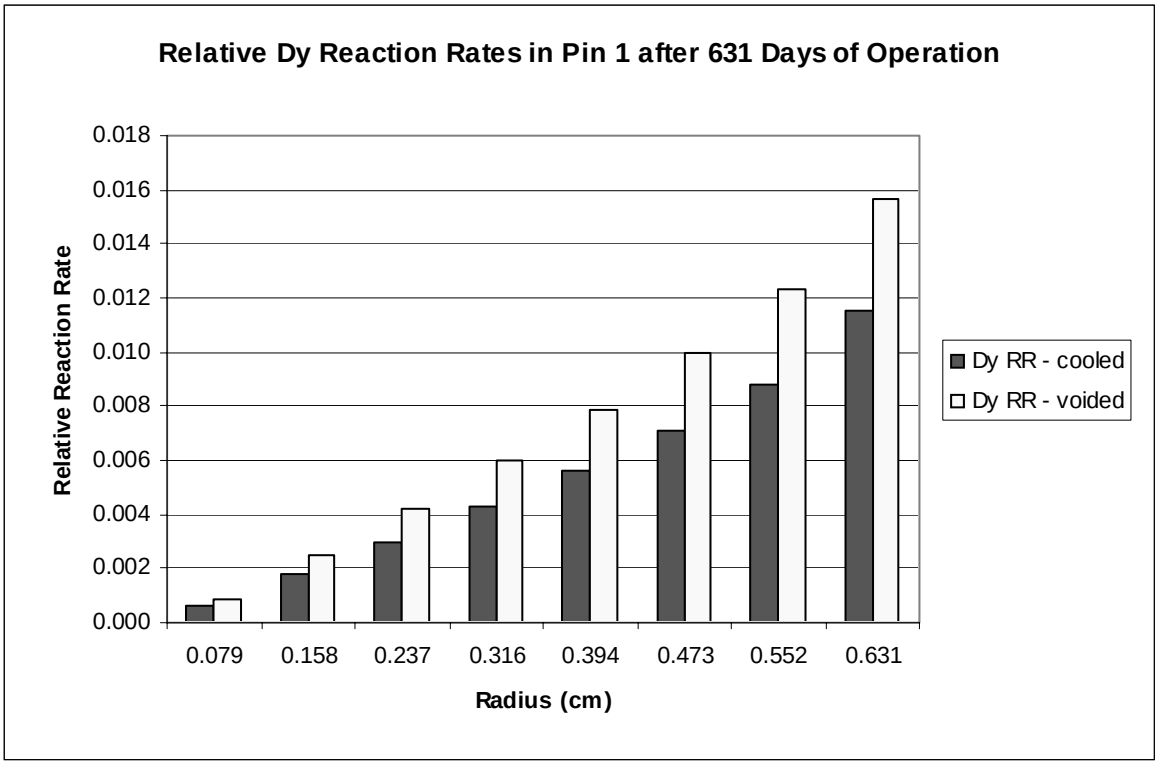

Figure 9 Dysprosium Reaction Rates at 631 Days

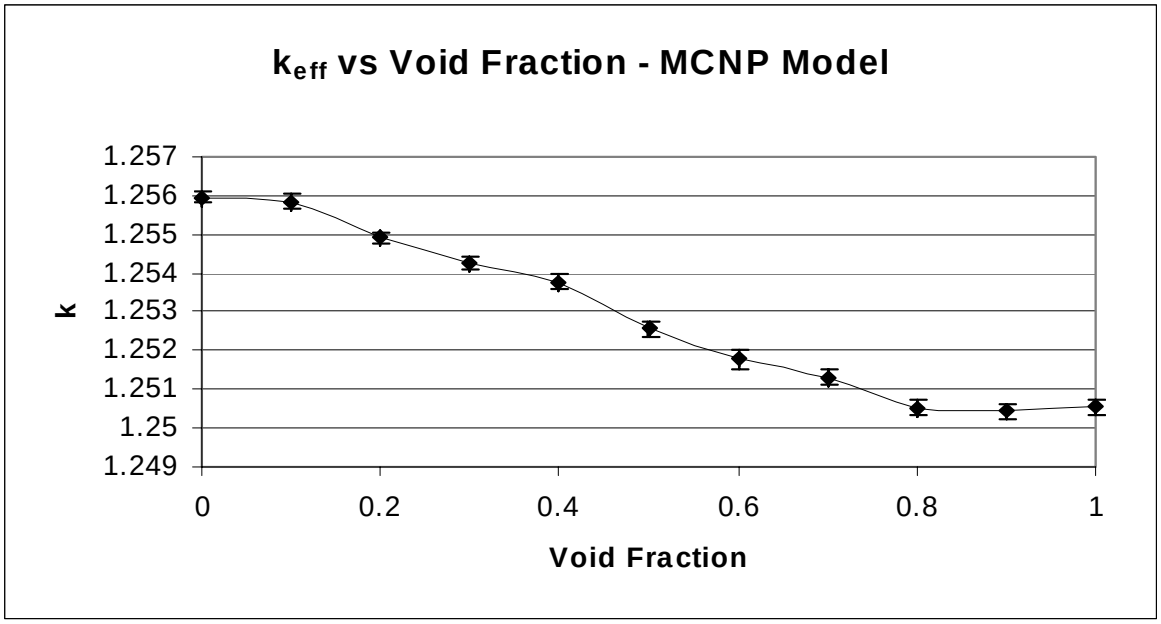

Figure 10 Multiplication Factor vs Void Fraction

REFERENCES

1. J. F. Breismeister (Ed.), "MCNP – A General Monte Carlo N-Particle Transport Code, Version 4b," LA-12625, Los Alamos National Laboratory, March 1997.

2. H. R. Trellue, "Development of MONTEBURNS: A Code that Links MCNP and ORIGEN in an Automated Fashion for Burnup Calculations," Los Alamos National Laboratory, LA-13514-T, December 1998.

3. A.G. Croff, "A User Manual for the ORIGEN2 Computer Code," ORNL/TM-7175, Oak Ridge National Laboratory, 1980.

4. O. Michaela, "Assessment Document; ACR-700 Reactor Physics Design," 10810-03300-ASD-001 Revision 2, Atomic Energy of Canada, June 6, 2003.

5. V. Khotylev and R. J. J. Stamm'ler, "Coolant Void Reactivity of ACR-700 Fuel," to be presented at the ANS Conference November 2004.