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Methodology For The Weapons-Grade MOX Fuel Burnup Analysis In The Advanced Test Reactor

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ABSTRACT

A UNIX BASH (Bourne Again SHell) script CMO has been written and validated at the Idaho National Laboratory (INL) to couple the Monte Carlo transport code MCNP with the depletion and buildup code ORIGEN-2 (CMO). The new Monte Carlo burnup analysis methodology in this paper consists of MCNP coupling through CMO with ORIGEN-2, and is therefore called the MCWO. MCWO is a fully automated tool that links the Monte Carlo transport code MCNP with the radioactive decay and burnup code ORIGEN-2.

MCWO is capable of handling a large number of fuel burnup and material loading specifications, Advanced Test Reactor (ATR) lobe powers, and irradiation time intervals. MCWO processes user input that specifies the system geometry, initial material compositions, feed/removal specifications, and other code-specific parameters. Calculated results from MCNP, ORIGEN-2, and data process module calculations are output in succession as MCWO executes. The principal function of MCWO is to transfer one-group cross-section and flux values from MCNP to ORIGEN-2, and then transfer the resulting material compositions (after irradiation and/or decay) from ORIGEN-2 back to MCNP in a repeated, cyclic fashion.

The basic requirements of MCWO are a working MCNP input file and some additional input parameters; all interaction with ORIGEN-2 as well as other calculations are performed by CMO. This paper presents the MCWO-calculated results for the Reduced Enrichment Research and Test Reactor (RERTR) experiments RERTR-1 and RERTR-2 as well as the Weapons-Grade Mixed Oxide (WG-MOX) fuel testing in ATR. Calculations performed for the WG-MOX test irradiation, which is managed by the Oak Ridge National Laboratory (ORNL), supports the DOE Fissile Materials Disposition Program (FMDP). The MCWO-calculated results are compared with measured data.

CONTENTS

TABLES

CONTENTS (continued)

FIGURES

Methodology for the Weapons-Grade MOX Fuel Burnup Analysis in the Advanced Test Reactor

1. INTRODUCTION

As computational power continues to increase, it becomes more practical to utilize Monte Carlo methods to perform burnup calculations. The UNIX Bourne Again SHell (BASH) script called CMO has been developed at the Idaho National Laboratory (INL) to couple the Monte Carlo transport code MCNP[1] with the depletion and buildup code ORIGEN-2[2] (CMO). The Monte Carlo burnup analysis methodology developed in this paper consists of MCNP coupling through CMO with ORIGEN-2, and is called the MCWO.[3,4] The primary functions of MCNP are to calculate one-group cross-sections and fluxes that are used by ORIGEN-2 in burnup calculations and to provide criticality and neutron economy information if requested. After burnup calculations are performed by ORIGEN-2, CMO passes isotopic compositions of materials back to MCNP to begin another burnup cycle.

CMO consists of a UNIX BASH script file that executes MCNP, ORIGEN-2, and the FORTRAN77 data processing programs *m2o.f* and *o2m.f*, which manipulate the input and output from MCNP and ORIGEN-2 to form a completely automated nuclear fuel burnup and material depletion tool - MCWO.

2. DESCRIPTION OF MCWO

In the last few years, interest in burnup calculations using Monte Carlo methods has increased. Existing burnup codes, such as PDQ, use diffusion theory to calculate the neutronics information. PDQ has worked well for the INL's Advanced Test Reactor (ATR) core safety and physics analyses. However, diffusion theory does not produce accurate results in burnup problems that include strong absorbers or large voids. Also, diffusion theory codes are geometry-limited (rectangular, hexagonal, cylindrical, and spherical coordinates). Monte Carlo methods are ideal for analyzing very heterogeneous reactors and/or lattices/assemblies in which considerable burnable poisons are used. The key feature of this “exact” modeling is that it permits reactor physics analysis without resorting to energy and spatial homogenization of neutron cross sections.

The BASH script CMO integrates the FORTRAN programs m2o.f, and o2m.f. The detailed source files of CMO (gft00), m2o.f (rerm2o.f), and o2m.f (rero2m.f) are listed in Appendix A. The input to MCWO burnup analysis code begins with a working MCNP input file. Other input includes material feed information and other code-specific variables used to perform burnup calculations in ORIGEN-2 concurrently with flux/cross-section calculations in MCNP. CMO is designed to link the Monte Carlo transport code MCNP with the radioactive decay and burnup code ORIGEN-2. MCWO produces a large number of criticality and burnup results based on various material feed specifications, ATR power(s), and irradiation time intervals. The program processes user input that specifies the system geometry, initial material compositions, feed/removal specifications, and other code-specific parameters. CMO is the primary interaction

mechanism between MCNP and ORIGEN-2. MCNP provides one-group microscopic cross sections and fluxes to ORIGEN-2 for burnup calculations, and ORIGEN-2 provides material compositions for MCNP. After ORIGEN-2 and MCNP have completed a depletion step, results are written into the ORIGEN-2 input file first, and the isotopic compositions obtained from ORIGEN-2 are used to generate a new MCNP input file for the next burn step. Various results from MCNP, ORIGEN-2, and other calculations are then output successively as the code runs.

MCWO performs MCNP and ORIGEN-2 runs for each user-specified time step. If the material composition burnup/decay/buildup may change significantly over time, user can easily specify a smaller time step. For each MCNP calculation step, MCNP updates the fission power distribution and burnup-dependent cross sections for each fuel pin. This data is then transferred by CMO to ORIGEN-2 for cell-wise depletion calculations. The MCNP-generated reaction rates are integrated over the continuous-energy nuclear data and the space within the region. Any odd or regular shaped region within the MCNP model can be depleted (on average) with reaction rate data that may provide better accuracy than the few-group data used in the commercial LWR industry. In this study, only the cross sections of the U-Pu actinides were updated versus burnup in the ORIGEN-2 calculations.

2.1. Description of MCNP Code

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by surfaces. The Monte Carlo technique is a statistical method in which estimates for system characteristics are obtained through multiple computer simulations of the behavior of individual particles in a system.

2.2. Description of ORIGEN-2 code

ORIGEN-2 performs burnup calculations for MCWO using the matrix exponential method to calculate time-dependent formation, destruction, and decay concurrently. These calculations require (1) the initial compositions and amounts of material, (2) one-group microscopic cross sections for each isotope, (3) material feed and removal rates (if desired), (4) the length of the irradiation period(s), and (5) the flux or power of the irradiation.

The ORIGEN-2 input must specify the location of the ORIGEN-2 libraries (both decay and cross-section) in the user's file space or in the directory of another user on the system that has the library files. The initial cross-section libraries provided by ORIGEN-2 are listed in Table 1.

Table 1. Initial cross-section libraries provided by ORIGEN-2

Library	Character Identifier	Number Identifier		
		Activation product	Actinide	Fission product
PWR: ^{235}U-enriched UO_2 with a burnup of 33,000 MWd/t	PWRU	204	205	206
PWR: ^{235}U-enriched UO_2 in a self-generated Pu recycle reactor	PWRPUU	207	208	209
PWR: Pu-enriched UO_2 in a self-generated Pu recycle reactor	PWRPUPU	210	211	212
BWR: ^{235}U-enriched UO_2	BWRU	251	252	253
BWR: ^{235}U-enriched fuel in a self-generated Pu recycle reactor	BWRPUU	254	255	256
BWR: Pu-enriched fuel in a self-generated Pu recycle reactor	BWRPUPU	257	258	259
CANDU: Natural	CANDUNAU	401	402	403
CANDU: Slightly Enriched	CANDUSEU	404	405	406
LMFBR: Advanced Oxide, LWR-Pu/U/U/U Core	AMOPUUUC	407	408	409
Axial Blanket	AMOPUUUA	321	322	323
Radial Blanket	AMOPUUUR	324	325	326
LMFBR: Early Oxide, LWR-Pu/U/U/U Core	EMOPUUUC	327	328	329
Axial Blanket	EMOPUUUA	301	302	303
Radial Blanket	EMOPUUUR	304	305	306
LMFBR: Advanced Oxide, recycle-Pu/U/U/U Core	AMORUUUC	311	312	313
Axial Blanket	AMORUUUA	314	315	316
Radial Blanket	AMORUUUR	317	318	319
LMFBR: Advanced Oxide, LWR-Pu/U/U/Th Core	AMOPUUTC	331	332	333
Axial Blanket	AMOPUUTA	334	335	336
Radial Blanket	AMOPUUTR	337	338	339
LMFBR: Advanced Oxide, LWR-Pu/Th/Th/Th Core	AMOPTTTC	341	342	343
Axial Blanket	AMOPTTTA	344	345	346
Radial Blanket	AMOPTTTR	347	348	349
LMFBR: Advanced Oxide, 14% denatured 233U/Th/Th/Th Core	AMO1TTTC	361	362	363
Axial Blanket	AMO1TTTA	364	365	366
Radial Blanket	AMO1TTTR	367	368	369
LMFBR: Advanced Oxide, 44% denatured 233U/Th/Th/Th Core	AMO2TTTC	371	372	373
Axial Blanket	AMO2TTTA	374	375	376
Radial Blanket	AMO2TTTR	377	378	379
ATR core (Beryllium)	ATRXS	204	908	909
High temperature gas cooled reactor (Graphite)	HTGRXS	204	405	406
PWR: ^{235}U-enriched UO_2 with a extend burnup	PWRUS	601	602	603
BWR: ^{235}U-enriched UO_2 with a extend burnup	BWRUS	604	605	606

The cross sections of ^{149}Sm and ^{135}Xe chains and fission products from fuel irradiation as provided in the ORIGEN-2 library were used in the fuel cycle analysis. In this study, we only calculated and updated the burnup dependent one-group cross section of nuclides whose reactions are important to criticality for reactors under study.

3. RESULTS AND DISCUSSIONS

The MCWO methodology was used to analyze the Reduced Enrichment for Research and Test Reactors (RERTR) fuel experiment and Weapons-Grade Mixed-Oxide (WG-MOX) test irradiation. There are four major tallies used in the MCNP model calculation process. The first tally in the model computes the neutron flux (particles/cm^2) averaged over the target cells. The second tally calculates the cell average fission reaction rate. The third tally calculates the neutron energy deposition (MeV/g) averaged over the target cells. And the fourth tally calculates the prompt gamma energy deposition (MeV/g) averaged over the target cells, which also includes the capture gamma and inelastic gamma energy deposition in the test assembly.

The MCNP-calculated heat rate tally normalization factor is defined to be:

= (fission neutron / fission) x (fission / MeV) x (W / MW)
= (2.42) x (1/201.09) x $1.0X10^6$
= 12,034 per total core MW.

A value of 201.09 MeV/fission[5] is used in the above normalization. Within this report, all of the MCNP-calculated fission and total heat rate distributions are based on a typical middle of cycle condition. MCNP-calculated tallies were normalized using an NW-lobe power of 18.0 MW and SE-lobe/SW-lobe powers of 23.0 MW.

3.1 RERTR-1 and -2 experiments in ATR

The Reduced Enrichment Research and Test Reactor (RERTR) program has developed and designed the high density low-enriched uranium (LEU, < 20%) fuels. The RERTR fuels testing are being irradiated in the Advanced Test Reactor (ATR). The RERTR-1 and RERTR-2 irradiation vehicles were irradiated in the small SE and SW I-positions (see Figure 1). The capsule basket contains 8 independent experiments, designated as capsules (from top to bottom) A through H in RERTR-1 and Z through S in RERTR-2. Each capsule is designed to hold 4 micro-plates, for a total of 32 micro-plates per capsule basket.

The MCWO methodology was used to analyze the RERTR experiments. There are four major tallies used in the MCNP model calculation process. The first tally in the model computes the neutron flux (particles/cm2) averaged over the target cells. The second tally calculates the cell average fission reaction rate. The third tally calculates the neutron energy (MeV/g) averaged over the target cells. And the fourth tally calculates the prompt gamma energy deposition (MeV/g) averaged over the target cells, which also includes the capture gamma and inelastic gamma energy deposition in the test assembly.

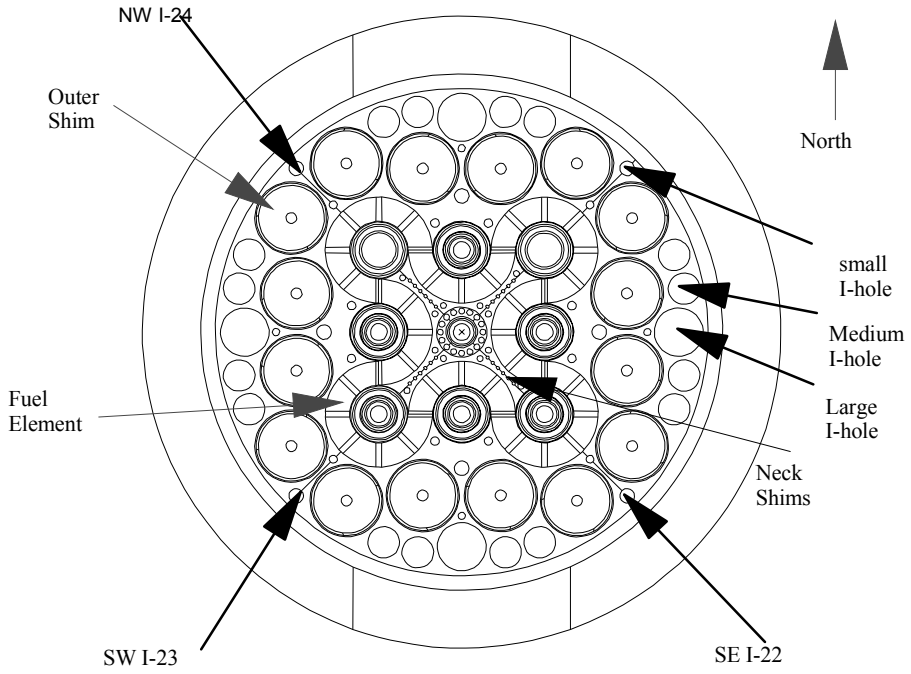

Figure 1. ATR MCNP core model cross-section view.

All the MCNP-calculated fission and total heat rate distributions in this report were based on a typical middle of cycle condition, which was used to extrapolate from the beginning of cycle (BOC) to end of cycle (EOC) for each irradiation cycle. MCNP-calculated fission tallies were normalized using SE-lobe and SW-lobe powers of 23.2 MW.

MCWO methodology provided the important fuel test parameters, linear heat generation rates and burnups, as demonstrated during the completed irradiation for RERTR-1 (from Cycle 114B to 114C at the SE small I-irradiation position) and RERTR-2 (from Cycle 114B to 116B at the SW small I-irradiation position). MCWO was used to track fuel burnup and heat rates as functions of irradiation time. Temperature distributions[6] were needed to make sure that the RERTR fuel microplates (with a volume of 0.19 cc) met the ATR safety requirements. For the RERTR experiments irradiated in the ATR small I-hole positions, the MCNP calculations (running with Fixed-Source mode with 3 parallel tasks, nps = 2.5 x 10^8) required approximately 1500 minutes CPU time on a DELL-650 XEON-2-CPU 3.06 GHz workstation to achieve one standard deviation (1σ, about 3.5 %) in the cell fission tallies.

MCWO was used for accurately determining fuel stack power and neutron flux distributions in the RERTR fuel micro-plates. The ORIGEN-2 ATRXS.lib in Table 1 was chosen as the reference library in the following MCWO calculations. In irradiation of RERTR-1, the effective full power days (EFPDs) for Cycles 114B and 114C were 51.1 and 43.3, respectively, at the SE I-22 position. To achieve higher burnup, the longer EFPDs of RERTR-2 for Cycles 114B, 114C,

115B, 115C, 116A, and 116B are 51.1, 43.33, 36.2, 48.4, 12.8, and 22.2, respectively, at the SW I-23 position. All of the capsules were visually examined in the transfer canal at the ATR during the shuffling and transfer to ANL-E for post irradiation examination (PIE). No anomalous indications were seen. The initial micro-plate fuel loading is listed in APPENDIX B. The MCWO-calculated burnup distributions are summarized in Table 2.

Table 2. MCWO-calculated and measured ^{235}U burnup distributions in the RERTR-1 and RERTR-2 fuel micro-plates

ID	RERTR-1 at the end of Cycle 114C			ID	RERTR-2 at the end of Cycle 116B		
	MCWO-calculated[a] ^{235}U burnup (%)	Measured[b] ^{235}U burnup (%)	C/M		MCWO-calculated ^{235}U burnup (%)	Measured ^{235}U burnup (%)	C/M
A-1	40.67%			Z-1	62.27%		
A-2	39.13%			Z-2	61.40%		
A-3	38.09%	32.90%	1.16	Z-3	60.32%	59.45%	1.01
A-4	38.57%			Z-4	60.92%		
B-1	40.21%			Y-1	63.39%		
B-2	39.07%			Y-2	62.88%		
B-3	38.85%			Y-3	62.68%		
B-4	39.45%			Y-4	63.51%		
C-1	42.91%			X-1	67.13%		
C-2	42.27%			X-2	66.72%		
C-3	41.71%			X-3	65.49%		
C-4	40.93%			X-4	66.04%		
D-1	40.72%			W-1	66.17%		
D-2	40.85%			W-2	65.31%		
D-3	40.66%	42.75%	0.95	W-3	64.99%	70.85%	0.92
D-4	41.17%			W-4	65.85%		
E-1	41.25%			V-1	66.22%		
E-2	40.71%			V-2	65.63%		
E-3	41.29%			V-3	65.79%		
E-4	41.17%			V-4	66.58%		
F-1	41.87%			U-1	65.88%		
F-2	41.46%			U-2	64.77%		
F-3	41.39%			U-3	65.18%		
F-4	41.47%			U-4	65.78%		
G-1	40.76%			T-1	64.64%		
G-2	40.27%			T-2	63.58%		
G-3	41.21%			T-3	64.77%		
G-4	40.73%			T-4	64.96%		
H-1	39.16%	35.55%	1.10	S-1	63.04%		
H-2	39.97%			S-2	63.25%		
H-3	38.44%			S-3	62.20%		
H-4	39.04%			S-4	62.39%		

a. MCNP-calculated ^{235}U burnup with $1\sigma = 3.5\%$.
b. Measured ^{235}U burnup with $1\sigma = 5.0\%$.

The MCNP - input and output files are rer14b, rer14.o, rer14c; rer14c.o; rer15b, rer15b.o; rer16a, rer16a.o; and rer16b, rer16b.o. These MCNP input and output files are all stored on a CD-ROM. For comparison, some of the microplates measured burnups at ANL-E are also tabulated in Table 3. The MCWO-calculated ^{235}U burnup at the positions D3, H1, W3, and Z3 are in good agreement with the measured burnup. The ratio of the MCWO-calculated to measured (C/M) ^{235}U burnup at A3 (at the core top position) is about 1.16, which is still in the $\pm 2\sigma = 17\%$ uncertainty range.

A simple, uninstrumented test assembly containing RERTR fuel microplates was inserted into the ATR. Important neutronics parameters were computed using MCWO methods. These computations led to an experiment design with RERTR fuel microplates that met all safety design requirements. MCWO was used to perform the neutronics analysis of the RERTR fuel micro-plates in ATR. It is remarkable that the results matched so well considering the complicated ATR geometry and the uncertainty ($1\sigma = 8.5\%$) of the core power distribution in each lobe. Because LHGR is proportional to the burnup, this validates the accuracy of MCWO-calculated burnup and LHGR.

3.2 WG-MOX Test Irradiation in ATR

There are three MOX fuel test sections axially, with the center section at the core midplane, and three fuel capsules in each section, for a total of nine fuel capsules in the test assembly, which are all included in the ATR MCNP Core Model (ATRM) as shown in Figure 1. The WG-MOX test fuel pellet comprises five percent PuO_2 and 95% depleted UO_2. Each fuel capsule is 0.415 cm in radius and 15.24 cm in length and contains 15 MOX fuel pellets. Channel 1 capsules are located away from the ATR core center, behind the capsules in channels 2 and 3. The adjacent flux-wire channel X is closer to the core center, in front of the flux wires in channels Y and Z as shown in Figure 2.

The initial experiment phase (Phase-I irradiation), which contained nine MOX fuel capsules, was loaded into the NW I-24 position (see Figure 1) in January 1998. After 153.5 effective full power days (EFPDs) of irradiation in Phase-I,[7] a capsule pair was withdrawn from the ATR in September 1998 after having achieved an average discharge burnup of about 8.6 GWd/t. At the end of Phase-II[8] irradiation (226.9 EFPDs), an additional capsule pair was withdrawn in September 1999 after having achieved an average discharge burnup of about 21.5 GWd/t. At the end of Phase-III[9] irradiation (232.8 EFPDs), an additional capsule pair was withdrawn in September 2000, after having achieved an average discharge burnup of about 29.6 GWd/t. The maximum burnup to be achieved in this test was originally set at 30 GWd/t. It was subsequently decided that the WG-MOX fuel would be irradiated to a burnup of 50 GWd/t. At the end of Phase-IV-Part 1[10] irradiation, an additional capsule pair was withdrawn in March 2002, after having achieved an average discharge burnup of about 40.0 GWd/t. Post-Irradiation Examination (PIE) of these capsules has recently been completed at Oak Ridge National Laboratory (ORNL). Because of the ^{239}Pu depletion, the fuel pellet Linear Heat Generation Rate (LHGR) is quite low in the final Phase-IV-Parts 2 and 3 irradiations. To increase the LHGR, the MOX fuel test assembly was moved from NW I-24 with a lobe power of 18.0 MW to SW I-23 with a lobe power of 23.0 MW. The current PIEs involve three capsules withdrawn at the end of Phase-IV-Part 3 in October 2003 with an average burnup of 50.0 GWd/t.

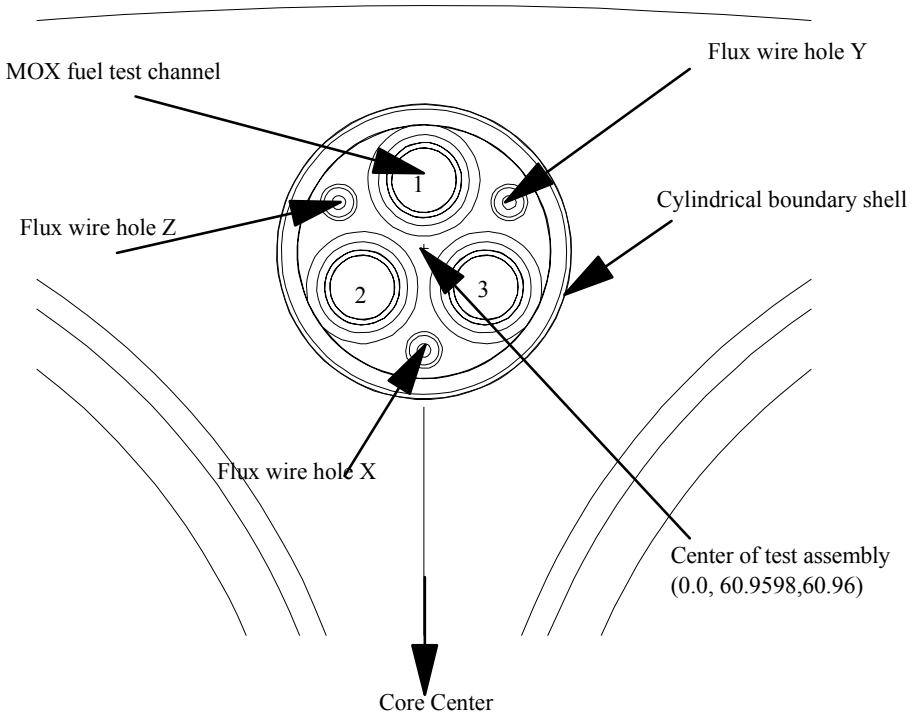

Figure 2. Detailed radial cross-sectional view of the WG-MOX fuel test assembly.

3.2.1 Determination of MOX Fuel Burnup by MCWO-MS Method

Fuel burnup is an important parameter needed for fuel performance evaluation. For the irradiated MOX fuel's Post-Irradiation Examination, the ^{148}Nd method was used to measure the burnup. The fission product ^{148}Nd is an ideal burnup indicator, when appropriate correction factors are applied. The verified Monte Carlo depletion tool (MCWO) used in this study can provide a burnup-dependent correction factor for the reactor parameters, such as capture-to-fission ratios, isotopic concentrations and compositions, fission power, and spectrum in a straightforward fashion. Furthermore, the correlation curve generated by MCWO can be coupled with the ^{239}Pu/Pu ratio measured by a Mass Spectrometer (in the new MCWO-MS[11] method) to obtain a best-estimate MOX fuel burnup. Mass Spectrometry (MS) can be calibrated to achieve a highly accurate measurement by eliminating the mass discrimination bias. Mass ratios can be obtained by MS with a precision of about 1%. The MCWO-MS tool only needs the MS-measured ^{239}Pu/Pu ratio, without the measured isotope ^{148}Nd concentration data, to determine the burnup accurately.

All the withdrawn capsule pairs in the MOX fuel test assembly had the same initial ^{239}Pu /Pu atom percent 93.81%. This decreases monotonically but not linearly with burnup. A good indicator of fuel burnup is the Fissions per Initial heavy Metal Atom (FIMA). This is simply the ratio of the number of fissions that have occurred in the fuel to the initial (zero burnup) inventory of heavy metal atoms (uranium plus plutonium) in the fuel. A FIMA value is determined as part

of the normal PIE burnup determination procedure. The burnup (GWd/t) is then obtained by multiplying the FIMA (%) by the conversion factor 9.60. FIMA MCWO-calculated ratios of ^{239}Pu/Pu are shown versus burnup in Figure 3. The MS measured ^{239}Pu/Pu ratios and ^{148}Nd measured burnup have a good agreement with the MCWO-MS generated correlation curve of the ^{239}Pu/Pu ratio and burnup as shown in Figure 3. The MCWO-MS estimated and ^{148}Nd corrected burnups agreed well within one uncertainty band ($1\sigma = \pm 5\%$). The MCWO-calculated ^{239}Pu/Pu ratio profile in Figure 3 shows that the buildup of ^{239}Pu from ^{238}U is almost equal to the ^{239}Pu depletion when the ^{239}Pu/Pu ratio reaches 20.6%.

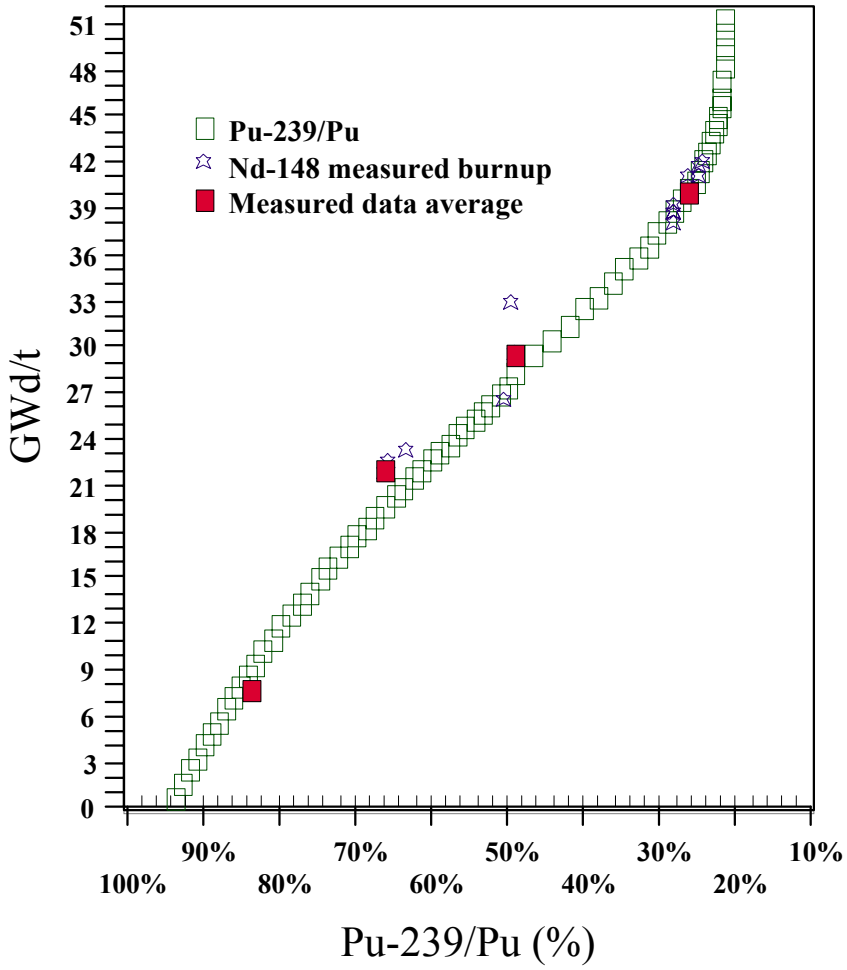

Figure 3. FIMA MCWO-calculated ^{239}Pu/Pu ratio profile and Mass-Spectrometer-measured ^{239}Pu/Pu ratio versus burnup.

4. CONCLUSIONS

MCWO fuel burnup methodology is only as good as the MCNP cross sections that are available to the user. If cross-section libraries do not exist for several fission products or actinides, or cross sections at the appropriate temperatures are not available, then MCWO results should be closely scrutinized. MCWO is also limited by the accuracy of the ORIGEN-2 fission product yields.

Acceptance of a code such as MCWO depends very strongly on its validation. Validation involves the benchmark of the code predictions to the in-pile experimental data and results of post-irradiation examinations (PIE). In addition to this report, in Ref. 11, a validation was made by comparing the MCWO-calculated concentration profiles with theVIMBURN[12] code, which has been validated against PIE data. The validated MCWO code can provide accurate neutronics characteristics of fuel burnup performance. In addition, the Monte Carlo burnup code MCWO has been successfully applied to the weapons-grade (WG)-MOX testing[13] in the ATR capsule neutronics design and irradiation as-run physics analyses. The measured burnups obtained by the neodymium method with a 1σ uncertainty band of ±5.0%[12] are plotted in Figure 3. The MCWO-calculated results show very good agreement with measured burnups at 9 and 22 GWd/t. The results at 30 GWd/t are within 8.3%.

The comparison of the results shows that the MCWO-calculated and measured data are in very good agreement with one another. However, more detailed benchmarking efforts also need to be performed. Work is ongoing to make the input/output of MCWO more user-friendly. Additionally, work is continuing on the benchmarking of MCWO with experimental and analytical burnup results, over a wide range of inputs.

5. IMPLEMENTATION OF MCWO

The MCWO executable can be run on almost any platform as long as the files discussed below are available in the working directory and the directory has access to MCNP and ORIGEN-2.

LINUX workstation - gscmox

To run MCWO on a LINUX system, the user must have a copy of the MCWO BASH script file *(see Appendix A)* and the executable programs generated by compiling the FORTRAN77 source files *rerm2o.f and rero2m.f (see Appendix A).* Additionally, the user must have access to both MCNP and ORIGEN-2 executables.

MCWO can be run by typing the following command at the LINUX prompt.
MCWO can then be run by typing the following command at the LINUX prompt.

```
%    gft00 01 02
     gft00 02 03
     gft00 03 04
     gft00 04 05
```

gft00 05 06

gft00 06 07

Computer Codes and Data Retention

The computer codes MCNP and ORIGEN-2 are contained in the INL listing of qualified codes. The archival MCNP and ORIGEN-2 source codes are retained on CD-ROM with labels of "MCNP" and "ORIGEN-2", respectively. The RERVV test assembly models, BASH script, FORTRAN codes, input, and output files are stored in GSCMOX:/datafls/rervv. The working directory will also be stored within the backup system. The same RERVV files, as well as the executable MCNP4C and ORIGEN-2 files are also retained on an attached CD-ROM (Title - RERVV).

6. REFERENCES

1. J. BRIESMEISTER (Editor), 'MCNP—A General Monte Carlo N-Particle Transport Code, Version 4C,' LA-13709-M, Los Alamos National Laboratory (2000).

2. A. G. CROFF, "ORIGEN-2: A Versatile Computer Code for Calculating the Nuclide Compositions and Characteristics of Nuclear Materials," Nuclear Technology, Vol. 62, pp. 335-352, 1983.

3. G. S. CHANG and J. M. RYSKAMP, "Depletion Analysis of Mixed Oxide Fuel Pins in Light Water Reactors and the Advanced Test Reactor," Nucl. Technol., Vol. 129, No. 3, p. 326-337 (2000).

4. G. S. CHANG, " MCWO - LINKING MCNP AND ORIGEN-2 FOR FUEL BURNUP ANALYSIS," *The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World,* Chattanooga, Tennessee, April 17–21, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005).

5. J. W. STERBENTZ letter to R. PEDERSEN, "Determination of the MeV/fission value for the ATR, " JWS-02-2002, June 25, 2002.

6. R. G. AMBROSEK, G. S. CHANG, "Improved Methodology for Temperature Predictions in Advanced Reactors," HTD-Vol. 316, 1995 National Heat Transfer Conference - Volume 14, p. 41-46, ASME 1995.

7. R. N. MORRIS, C. A. BALDWIN, B. S. COWELL, S. A. HODGE, et. al. "*MOX Average Power Early PIE: 8 GWd/MT Final Report,*" Oak Ridge National Laboratory, ORNL/MD/LTR-172, (November 1999).

8. R. N. MORRIS, C. A. BALDWIN, S. A. HODGE, L. J. OTT, C. M. MALONE, N. H. PACKAN, "*MOX Average Power Intermediate PIE: 21 GWd/MT Final Report,*" Oak Ridge National Laboratory, ORNL/MD/LTR-199, (December 2000).

9. R.N. MORRIS, C. A. BALDWIN, S. A. HODGE, N. H. PACKAN, "*MOX Average Power 30 GWd/MT PIE: Final Report*," Oak Ridge National Laboratory, ORNL/MD/LTR-212, (November 2001).

10. R.N. MORRIS, C. A. BALDWIN, N. H. PACKAN, "*MOX Average Power 40 GWd/MT PIE: Final Report*," Oak Ridge National Laboratory, Vol. 1, ORNL/MD/LTR-241, (August 2003).

11. G. S. CHANG, " Monte Carlo Analysis of Burnup-Dependent Pu Concentration Profiles in UO_2 and MOX fuel Pins," *Trans. Am. Nucl. Soc.*, **78** (1997).

12. A. SASAHARA, T. MATSUMURA, G. NICOLAOU, J. P. GLATZ, E. TOSCANO, and C. T. WALKER, " Post irradiation Examinations and Computational Analysis of High Burn-up UOX and MOX Spent Fuels for Interim Dry Storage," 10th Pacific Basin Nuclear Conference, Kobe, Japan, p. 1072-1080, 20-25 October, 1996.

13. G. S. Chang, "ATR WG-MOX FUEL PELLET BURNUP MEASUREMENT BY MONTE CARLO – MASS SPECTROMETRIC METHOD," Proceedings of the International Conference on the New Frontiers of Nuclear Technology: Reactor Physics, Safety and High-Performance Computing, The ANS 2002 RPD Topical Meeting, Seoul, Korea, October 7-10, 2002.

APPENDIX A

LINUX BASH script (gft00) and FORTRAN source code m2o.f (rerm2o.f) and o2m.f (rero2m.f) for RERTR-1 and RERTR-2

The LINUX BASH script - gft00

```
 1 grep '^                .......E' u001$1.o > tmox
 2 cp u001$1.o tt2
 3 sed -e '1,/        masses/d'   tt2 > tt3
 4 sed -e '11,$d'    tt3 > tt4
 5 grep E tt4 > tt5
 6 sed -e '1,/           volumes/d'   tt2 > tt6
 7 sed -e '11,$d'    tt6 > tt7
 8 grep E tt7 > tt8
 9 cat  tt8 tt5       > tt9
10 mv   tmox          f4.in
11 mv   tt9           f7m.in
12 rm  tt?
13 rerm2o.x < ftinp.$1
14 mv obfmw.f1   obfmw.$2
15 mv  file.???        ../ftrerd1/.
16 cd ../ftrerd1
17 int.ed
18 sub.ed
19 gordrer1  $1 $2
20 rero2m.x < goinp.00
21 mv file.???  ./rd$1/.
22 #rm r???$2.o
23 rm r???.int
24 rm r*.sub
25 mv obc.re4 ../rerd1/obc4.$2
26 mv obm.re4 ../rerd1/obm4.$2
27 cd ../rerd1
```

MCNP to ORIGEN-2 data processing Fortran program rerm2o.f

```
      program rerm2o
      integer matn(200),nmat(200),nn,pt(40),tlyid(200,50)
      character*8 intfile,cellf,subfile,midf,matf,tlyf,f7mf
     1           ,f4mwpta
      dimension xtotal(200),yact1(200,50),yact2(200,50),
     1    yact3(200,50),yact4(200,50),f7pa(200),day(6)
     1    ,f7pw(200),f7s(200),af7s(200)
      character*83 hhlt(50),hhact(50),hhfp(50),hhfp2(50)
      dimension total(200),matnum(200),flux(200),f7(200),f4(200)
      dimension gtly(200,50),tly(200,50),sum(200),fm(200),fv(200)
      dimension tlyilt(200,50),tlyifp(200,50)
      character*8  hhint(6)
      character*114  hhfm
      character*23 hhmov
      character*58 hsult(50)
      character*28 hsuact(50)
      character*58 hsufp(50)
      character*82 hhline(50)
      character*13 cella(50),cellt(50),celact(50),celfp(50)
      character*3  decid,hirp,hirf,mov
      character*6 mid1(50),midilt(50),midiact(50),midifp(50)
       hirp="IRP"
       hirf="IRF"
       decid="DEC"
       hhint(1)=" 1 2 4 2"
       hhint(2)=" 2 3 4 0"
       hhint(3)=" 3 4 4 0"
       hhint(4)=" 4 5 4 0"
       hhint(5)=" 5 6 4 0"
       hhint(6)=" 1 2 4 0"
       hhmov="MOV   6   1   0   1.0"
      read(5,13)days,atrmw,rmwpcc,dec,atmo2,atmal
c      write(6,13)days,atrmw,rmwpcc,dec,atmo2,atmal
      read(5,10)f7mf
      read(5,10)matf
      read(5,10)tlyf
      read(5,10)intfile
      read(5,10)subfile
      read(5,10)f4mwpta
   13 format(2f10.4,e10.3,3f10.4)
c  13 format(2f10.6,1pe10.3,3f10.6)
       decay=dec+days
c      ir=0 IRF, ir=1 IRP
      read(5,16) ilt,iact,ifp,ir,icells,isubr,isrcel,ieven
c      write(6,16) ilt,iact,ifp,ir,icells,isubr,isrcel,ieven
   16 format(8i5)
      itat=ilt+iact+ifp
      open(unit=10,file=f7mf,form='formatted',status='old')
      open(unit=11,file=matf,form='formatted',status='old')
      open(unit=12,file=tlyf,form='formatted',status='old')
      open(unit=13,file=intfile,status='new')
      open(unit=14,file=subfile,status='new')
      open(unit=15,file=f4mwpta,status='new')
```

```
   10 format(a8)
   19 format(4a3)
c     If (ilt.gt.0) read(10,11) (midilt(i),i=1,ilt)
c     if (iact.gt.0) read(10,11) (midiact(i),i=1,iact)
c     if (ifp.gt.0) read(10,11) (midifp(i),i=1,ifp)
      do 906 j=1,icells
      read(12,12)     f4(j)
  906  continue
      do 917 j=1,icells
      read(12,12)     f7(j)
  917  continue
      if (ilt.eq.0) goto 603
      do 903 j=1,icells
      do 903 i=1,ilt
      read(12,12) tlyilt(j,i)
       tlyilt(j,i)=tlyilt(j,i)/f4(j)
  903  continue
  603  continue
       if (iact.eq.0) goto 604
      do 911 j=1,icells
      do 911 i=1,iact
      read(12,12) yact1(j,i)
       yact1(j,i)=yact1(j,i)/f4(j)
  911  continue
      do 912 j=1,icells
      do 912 i=1,iact
      read(12,12) yact2(j,i)
       yact2(j,i)=yact2(j,i)/f4(j)
  912  continue
      do 913 j=1,icells
      do 913 i=1,iact
      read(12,12) yact3(j,i)
       yact3(j,i)=yact3(j,i)/f4(j)
  913  continue
      do 904 j=1,icells
      do 904 i=1,iact
      read(12,12) yact4(j,i)
       yact4(j,i)=yact4(j,i)/f4(j)
  904  continue
  604  continue
       if (ifp.eq.0) goto 605
      do 905 j=1,icells
      do 905 i=1,ifp
      read(12,12) tlyifp(j,i)
       tlyifp(j,i)=tlyifp(j,i)/f4(j)
  905  continue
  605  continue
   27 format(a80)
   11 format(a6)
   12 format(16x,1pe12.5)
       nmat(1)=1000
        if (ilt.eq.0) goto 606
      do 381  i=1,ilt
        read(11,625)hhlt(i)
        hsult(i)=hhlt(i)(24:82)
        cellt(i)=hhlt(i)(1:13)
```

```
381 continue
606 continue
      if (iact.eq.0) goto 607
    do 382  i=1,iact
      read(11,625)hhact(i)
      hsuact(i)=hhact(i)(54:82)
      celact(i)=hhact(i)(1:13)
382 continue
607 continue
      if (ifp.eq.0) goto 608
    do 383  i=1,ifp
      read(11,625)hhfp(i)
      read(11,625)hhfp2(i)
      hsufp(i)=hhfp(i)(24:82)
      celfp(i)=hhfp(i)(1:13)
383 continue
608 continue
625 format(a83)
     do 950 j=1,icells
      if (ilt.eq.0) goto 611
    do 921 k=1,ilt
     write(14,120) cellt(k),tlyilt(j,k),hsult(k)
921   continue
611   continue
      if (iact.eq.0) goto 612
    do 922 k=1,iact
    write(14,121)celact(k),yact1(j,k),yact2(j,k),yact3(j,k),
   1        yact4(j,k),hsuact(k)
922   continue
612   continue
      if (ifp.eq.0) goto 613
    do 923 k=1,ifp
     write(14,120) celfp(k),tlyifp(j,k),hsufp(k)
     write(14,625) hhfp2(k)
923   continue
613   continue
950   continue
121   format(a13,1pe10.3,1pe10.3,1pe10.3,1pe10.3,a28)
120   format(a13,1pe10.3,a58)
610 format(i5)
620 format(i5,a75)
615 format(i5)
630 format(a5,1x,i4,1x,1pe11.4,1x,a56)
635 format(a5)
     kd=5
     do 935 i=1,5
     day(i)=days/kd
     kd=kd-1
935   continue
     day(6)=decay
       if (ir.gt.0) then
        ncells=icells-(isubr*(isrcel-1))
       icc=icells/7
        icc=icc*7+1
    do 901 j=1,icc,7
      read(10,167) (fv(k),k=j,j+6)
```

```
c      write(6,167) (fv(k),k=j,j+6)
  901  continue
       do 902 j=1,icc,7
         read(10,167) (fm(k),k=j,j+6)
c      write(6,167) (fm(k),k=j,j+6)
  902  continue
c        calc. f7*density
       do 907 j=1,icells
         f7pw(j)=f7(j)*fm(j)/fv(j)
  907  continue
       do 909 j=1,icc,7
c      write(6,167) (f7pw(k),k=j,j+6)
  909   continue
  167   format(23x,7(1pe13.5))
        if (isubr.gt.0) then
       do 811 i=1,isubr
        af7s(i)=0.0
         k=(i-1)*isrcel
       do 811 j=1,isrcel
         k=k+1
       af7s(i)=f7pw(k)/isrcel+af7s(i)
  811    continue
        k=isubr*isrcel
       do 812 i=isubr+1,ncells
         k=K+1
       af7s(i)=f7pw(k)
  812    continue
c      write(6,166) (af7s(i),i=1,ncells)
        avgf7=0.0
       do 813 i=1,ncells
        avgf7=avgf7+af7s(i)/ncells
  813    continue
        if (ieven.eq.0) then
c         un-even power distribution
       do 814 i=1,isubr
         k=(i-1)*isrcel
        do 814 j=1,isrcel
           k=K+1
        f7pa(k)=f7pw(k)/avgf7*rmwpcc
  814    continue
        do 815 i=isubr*isrcel+1,icells
        f7pa(i)=f7pw(i)/avgf7*rmwpcc
  815   continue
c      write(6,167) (f7pa(i),i=1,icells)
       do 805 j=1,icells
       do 804 i=1,5
       write(13,701) hirp,day(i),f7pa(j),hhint(i)
  804   continue
       write(13,702) hhmov
       write(13,703) decid, day(6), hhint(6)
  805   continue
       write(15,166) (f7pa(i), i=1,icells)
       else
c         even power distribution
c      write(6,167) f7(55),f7(60),rmwpcc,avg,tot
        do 824 i=1,isubr
```

```
        k=(i-1)*isrcel
       do 824 j=1,isrcel
         k=K+1
       f7pa(k)=f7pw(k)/af7s(i)*rmwpcc
 824    continue
       do 825 i=isubr*isrcel+1,icells
       f7pa(i)=rmwpcc
 825   continue
c      write(6,167) (f7pa(i),i=1,icells)
      do 827 j=1,icells
      do 826 i=1,5
      write(13,701) hirp,day(i),f7pa(j),hhint(i)
 826   continue
      write(13,702) hhmov
      write(13,703) decid, day(6), hhint(6)
 827   continue
      write(15,166) (f7pa(i), i=1,icells)
      endif
      else
      tot=0.0
      do 941 j=1,icells
      f7pw(j)=f7pw(j)*fm(j)
      tot=tot+f7pw(j)
 941   continue
      avg=tot/icells
c      write(6,167) f7pw(55),f7pw(60),rmwpcc,avg,tot
      do 951 j=1,icells
      f7pa(j)=0.0
 951   continue
      do 947 j=1,icells
c      f7pa(j)=f7pw(j)/avg*rmwpcc
      f7pa(j)=f7pw(j)/avg*rmwpcc
 947   continue
c      write(6,167) (f7pa(i),i=1,icells)
      do 949 j=1,icells
      do 943 i=1,5
      write(13,701) hirp,day(i),f7pa(j),hhint(i)
 943   continue
      write(13,702) hhmov
      write(13,703) decid, day(6), hhint(6)
 949   continue
      endif
      else
      write(15,166) (f7pa(i), i=1,icells)
      do 931 j=1,icells
      f4(j)=f4(j)*7.5816e+16*atrmw
      do 932 i=1,5
      write(13,701) hirf,day(i),f4(j),hhint(i)
 932   continue
      write(13,702) hhmov
      write(13,703) decid, day(6), hhint(6)
 931   continue
      endif
      write(15,166) (f4(i),i=1,icells)
 166   format(1pe12.3)
 701   format(a3,5x,f10.5,1pe12.4,3x,a8)
```

```
702   format(a23)
703   format(a3,5x,f10.5,3x,a8)
      stop
      end
```

ORIGEN-2 to MCNP data processing Fortran program rero2m.f

```
      program rero2m
      integer matn(200),nmat(200),nn,pt(40),atmid(200,50)
      dimension xtotal(200),xisop1(200,50)
      dimension total(200),matnum(200),b10c(40)
      dimension gatm(200,50),atm(200,50),sum(200)
      dimension atmo2(200),atmal(200),atm03(200)
      character*56 hsurf(200)
      character*72 hhline(200)
      character*5  cella(200)
      character*9 mid1(50),midf,matf,celf,celfile,matfile,atmfile
      read(5,10)atmfile
      read(5,10)midf
      read(5,10)matf
      read(5,10)celf
      read(5,10)celfile
      read(5,10)matfile
      iid=3
c      ir=0 IRF, ir=1 IRP
      read(5,16) ir,icells,igotat,nnm
        igotat11=igotat+iid
      open(unit=10,file=midf,form='formatted',status='old')
      open(unit=11,file=matf,form='formatted',status='old')
      open(unit=12,file=celf,form='formatted',status='old')
      open(unit=15,file=atmfile,form='formatted',status='old')
      open(unit=13,file=matfile,status='new')
      open(unit=14,file=celfile,status='new')
   10 format(a8)
      read(10,11) (mid1(i),i=1,igotat11)
      do 901 j=1,icells
      do 901 i=1,igotat
      read(11,12) atmid(j,i),gatm(j,i)
  901  continue
      do 907 j=1,icells
      read(15,19) atmo2(j),atmal(j),atm03(j)
  907  continue
   27 format(a72)
   11 format(a9)
   16 format(4i5)
   12 format(i5,e10.3)
   19 format(3e10.3)
   13 format(2f10.6)
       nmat(1)=nnm
       do 509 j=2,icells
       nmat(j)=nmat(j-1)+1
  509  continue
      do 502 i=1,igotat
      do 502 j=1,icells
      atm(j,i)=gatm(j,i)*0.60225
  502 continue
       do 501 j=1,icells
      sum(j)=atmo2(j)+atmal(j)+atm03(j)
  501 continue
      do 503 j=1,icells
      do 503  i=1,igotat
```

```
      sum(j)=sum(j)+atm(j,i)
  503 continue
       igotat1=igotat-1
c      write(6,788) igotat, atm(30,9),atm(50,10),sum(60)
  788 format(i10,3(1pe12.3))
      do 376 j=1,icells
       write(13,120)nmat(j),sum(j)
       write(13,130)nmat(j)
       write(13,133) mid1(igotat+1),atmo2(j)
       write(13,133) mid1(igotat+2),atmal(j)
       write(13,133) mid1(igotat+3),atm03(j)
      do 376 i=1,igotat1,2
       write(13,131) mid1(i),atm(j,i),mid1(i+1),atm(j,i+1)
  376   continue
  120   format('c',5x,'material number ',i4,' total atom density =',
     1 f10.6)
  130   format('m',i4)
  131   format(10x,a9,2x,1pe15.4,5x,a9,2x,1pe15.4)
  133   format(10x,a9,2x,1pe15.4)
c    19x,"13027.60c",2x,1pe20.5)
      do 381  i=1,icells
        read(12,625)hhline(i)
        hsurf(i)=hhline(i)(24:72)
        cella(i)=hhline(i)(1:5)
  381 continue
  625 format(a72)
       do 902  j=1,icells
      write(14,630)cella(j),nmat(j),sum(j),hsurf(j)
  902   continue
  610 format(i5)
  620 format(i5,a75)
  615 format(i5)
  630 format(a5,1x,i4,1x,1pe11.4,1x,a56)
  635 format(a5)
      stop
      end
```

APPENDIX B

Intial RERTR-1 and -2 micro-plate fuel loading (atoms/barn-cm)

RERTR-1: m1501 to m1532.
RERTR-2: m1533 to m1564.

```
c     material number 1501 total atom density =  0.052949
m1501
        14000.37c      4.0240E-03
        13027.37c      4.2890E-02
        42000.37c      1.0000E-17
        92234.37c      7.7630E-13    92235.37c      1.2069E-03
        92238.37c      4.8282E-03    94238.37c      6.0345E-17
c     material number 1502 total atom density =  0.053314
m1502
        14000.37c      1.0000E-18
        13027.37c      4.2890E-02
        42000.37c      3.4745E-03
        92234.37c      2.1169E-13    92235.37c      1.3900E-03
        92238.37c      5.5594E-03    94238.37c      6.0225E-17
c     material number 1503 total atom density =  0.054980
m1503
        14000.37c      1.0000E-18
        13027.37c      4.2890E-02
        42000.37c      2.6120E-03
        92234.37c      4.1411E-13    92235.37c      1.8959E-03
        92238.37c      7.5823E-03    94238.37c      6.0285E-17
c     material number 1504 total atom density =  0.054458
m1504
        14000.37c      1.0000E-18
        13027.37c      4.2890E-02
        42000.37c      2.0520E-03
        92234.37c      1.1136E-13    92235.37c      1.9031E-03
        92238.37c      7.6124E-03    94238.37c      6.0225E-17
c     material number 1505 total atom density =  0.053954
m1505
        14000.37c      1.0000E-17
        13027.37c      4.2890E-02
        42000.37c      1.5120E-03
        92234.37c      3.0305E-13    92235.37c      1.9097E-03
        92238.37c      7.6426E-03    94238.37c      6.0285E-17
c     material number 1506 total atom density =  0.053954
m1506
        14000.37c      1.0000E-18
        13027.37c      4.2890E-02
        42000.37c      1.5120E-03
        92234.37c      1.9055E-13    92235.37c      1.9097E-03
        92238.37c      7.6426E-03    94238.37c      6.0225E-17
c     material number 1507 total atom density =  0.054980
m1507
        14000.37c      1.0000E-18
        13027.37c      4.2890E-02
        42000.37c      2.6120E-03
```

```
        92234.37c       1.0256E-12      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0406E-17
c     material number 1508 total atom density =  0.053954
m1508
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       1.5120E-03
        92234.37c       1.9543E-13      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0225E-17
c     material number 1509 total atom density =  0.052949
m1509
        14000.37c       4.0240E-03
        13027.37c       4.2890E-02
        42000.37c       1.0000E-17
        92234.37c       1.6743E-13      92235.37c       1.2069E-03
        92238.37c       4.8282E-03      94238.37c       6.0225E-17
c     material number 1510 total atom density =  0.052949
m1510
        14000.37c       4.0240E-03
        13027.37c       4.2890E-02
        42000.37c       1.0000E-17
        92234.37c       1.1009E-13      92235.37c       1.2069E-03
        92238.37c       4.8282E-03      94238.37c       6.0225E-17
c     material number 1511 total atom density =  0.053463
m1511
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       9.9020E-04
        92234.37c       3.1251E-13      92235.37c       1.9164E-03
        92238.37c       7.6666E-03      94238.37c       6.0285E-17
c     material number 1512 total atom density =  0.054980
m1512
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       1.2816E-12      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0466E-17
c     material number 1513 total atom density =  0.054980
m1513
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       6.1128E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0285E-17
c     material number 1514 total atom density =  0.054980
m1514
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       2.9372E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0285E-17
c     material number 1515 total atom density =  0.054980
m1515
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
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        92234.37c       1.3749E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
c     material number 1516 total atom density =  0.054458
m1516
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.0520E-03
        92234.37c       2.9059E-13      92235.37c       1.9031E-03
        92238.37c       7.6124E-03      94238.37c       6.0285E-17
c     material number 1517 total atom density =  0.053954
m1517
        14000.37c       1.0000E-17
        13027.37c       4.2890E-02
        42000.37c       1.5120E-03
        92234.37c       2.5650E-13      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0225E-17
c     material number 1518 total atom density =  0.053954
m1518
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       1.5120E-03
        92234.37c       7.4077E-13      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0345E-17
c     material number 1519 total atom density =  0.054980
m1519
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       8.7386E-14      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
c     material number 1520 total atom density =  0.054458
m1520
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.0520E-03
        92234.37c       5.8346E-13      92235.37c       1.9031E-03
        92238.37c       7.6124E-03      94238.37c       6.0285E-17
c     material number 1521 total atom density =  0.054980
m1521
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       7.1547E-14      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
c     material number 1522 total atom density =  0.054980
m1522
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       4.4651E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
c     material number 1523 total atom density =  0.054980
m1523
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
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        92234.37c       1.3767E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
c     material number 1524 total atom density =  0.053954
m1524
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       1.5120E-03
        92234.37c       1.1009E-12      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0586E-17
c     material number 1525 total atom density =  0.054420
m1525
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.0520E-03
        92234.37c       1.9862E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
c     material number 1526 total atom density =  0.055018
m1526
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       1.3460E-13      92235.37c       1.9031E-03
        92238.37c       7.6124E-03      94238.37c       6.0225E-17
c     material number 1527 total atom density =  0.053314
m1527
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       3.4745E-03
        92234.37c       8.3532E-14      92235.37c       1.3900E-03
        92238.37c       5.5594E-03      94238.37c       6.0225E-17
c     material number 1528 total atom density =  0.054980
m1528
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       5.4612E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0285E-17
c     material number 1529 total atom density =  0.053463
m1529
        14000.37c       1.0000E-17
        13027.37c       4.2890E-02
        42000.37c       9.9020E-04
        92234.37c       2.8565E-13      92235.37c       1.9164E-03
        92238.37c       7.6666E-03      94238.37c       6.0285E-17
c     material number 1530 total atom density =  0.052949
m1530
        14000.37c       4.0240E-03
        13027.37c       4.2890E-02
        42000.37c       1.0000E-17
        92234.37c       2.7896E-13      92235.37c       1.2069E-03
        92238.37c       4.8282E-03      94238.37c       6.0225E-17
c     material number 1531 total atom density =  0.054980
m1531
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
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      92234.37c   7.3655E-14   92235.37c   1.8959E-03
      92238.37c   7.5823E-03   94238.37c   6.0225E-17
c   material number 1532 total atom density =  0.054980
m1532
      14000.37c   1.0000E-18
      13027.37c   4.2890E-02
      42000.37c   2.6120E-03
      92234.37c   5.0029E-13   92235.37c   1.8959E-03
      92238.37c   7.5823E-03   94238.37c   6.0285E-17
c   material number 1533 total atom density =  0.052949
m1533
      14000.37c   4.0240E-03
      13027.37c   4.2890E-02
      42000.37c   1.0000E-17
      92234.37c   2.6493E-13   92235.37c   1.2069E-03
      92238.37c   4.8282E-03   94238.37c   6.0285E-17
c   material number 1534 total atom density =  0.053314
m1534
      14000.37c   1.0000E-18
      13027.37c   4.2890E-02
      42000.37c   3.4745E-03
      92234.37c   4.9571E-14   92235.37c   1.3900E-03
      92238.37c   5.5594E-03   94238.37c   6.0225E-17
c   material number 1535 total atom density =  0.054980
m1535
      14000.37c   1.0000E-18
      13027.37c   4.2890E-02
      42000.37c   2.6120E-03
      92234.37c   1.1238E-13   92235.37c   1.8959E-03
      92238.37c   7.5823E-03   94238.37c   6.0225E-17
c   material number 1536 total atom density =  0.054458
m1536
      14000.37c   1.0000E-18
      13027.37c   4.2890E-02
      42000.37c   2.0520E-03
      92234.37c   2.0531E-13   92235.37c   1.9031E-03
      92238.37c   7.6124E-03   94238.37c   6.0285E-17
c   material number 1537 total atom density =  0.053954
m1537
      14000.37c   1.0000E-17
      13027.37c   4.2890E-02
      42000.37c   1.5120E-03
      92234.37c   1.9868E-13   92235.37c   1.9097E-03
      92238.37c   7.6426E-03   94238.37c   6.0225E-17
c   material number 1538 total atom density =  0.053954
m1538
      14000.37c   1.0000E-18
      13027.37c   4.2890E-02
      42000.37c   1.5120E-03
      92234.37c   3.0859E-13   92235.37c   1.9097E-03
      92238.37c   7.6426E-03   94238.37c   6.0285E-17
c   material number 1539 total atom density =  0.054980
m1539
      14000.37c   1.0000E-18
      13027.37c   4.2890E-02
      42000.37c   2.6120E-03
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        92234.37c       8.5580E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0345E-17
c     material number 1540 total atom density =  0.053954
m1540
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       1.5120E-03
        92234.37c       1.3087E-13      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0225E-17
c     material number 1541 total atom density =  0.052949
m1541
        14000.37c       4.0240E-03
        13027.37c       4.2890E-02
        42000.37c       1.0000E-17
        92234.37c       3.2817E-13      92235.37c       1.2069E-03
        92238.37c       4.8282E-03      94238.37c       6.0285E-17
c     material number 1542 total atom density =  0.052949
m1542
        14000.37c       4.0240E-03
        13027.37c       4.2890E-02
        42000.37c       1.0000E-17
        92234.37c       2.5505E-13      92235.37c       1.2069E-03
        92238.37c       4.8282E-03      94238.37c       6.0285E-17
c     material number 1543 total atom density =  0.053358
m1543
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       9.9020E-04
        92234.37c       2.7764E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
c     material number 1544 total atom density =  0.055054
m1544
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       2.8721E-13      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0285E-17
c     material number 1545 total atom density =  0.054980
m1545
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       2.8504E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0285E-17
c     material number 1546 total atom density =  0.054980
m1546
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       1.5345E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
c     material number 1547 total atom density =  0.054980
m1547
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
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        92234.37c       2.3355E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0285E-17
c     material number 1548 total atom density =  0.054458
m1548
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.0520E-03
        92234.37c       1.2358E-13      92235.37c       1.9031E-03
        92238.37c       7.6124E-03      94238.37c       6.0225E-17
c     material number 1549 total atom density =  0.053954
m1549
        14000.37c       1.0000E-17
        13027.37c       4.2890E-02
        42000.37c       1.5120E-03
        92234.37c       2.0187E-13      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0285E-17
c     material number 1550 total atom density =  0.053954
m1550
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       1.5120E-03
        92234.37c       3.0733E-13      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0285E-17
c     material number 1551 total atom density =  0.054980
m1551
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       1.4454E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
c     material number 1552 total atom density =  0.054458
m1552
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.0520E-03
        92234.37c       2.4825E-13      92235.37c       1.9031E-03
        92238.37c       7.6124E-03      94238.37c       6.0225E-17
c     material number 1553 total atom density =  0.054980
m1553
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       8.3713E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0406E-17
c     material number 1554 total atom density =  0.054980
m1554
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       3.6159E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0285E-17
c     material number 1555 total atom density =  0.054980
m1555
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
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        92234.37c       4.2501E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0285E-17
c     material number 1556 total atom density =  0.053954
m1556
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       1.5120E-03
        92234.37c       1.4906E-13      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0225E-17
c     material number 1557 total atom density =  0.054420
m1557
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.0520E-03
        92234.37c       3.6099E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0285E-17
c     material number 1558 total atom density =  0.055054
m1558
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       2.9962E-13      92235.37c       1.9097E-03
        92238.37c       7.6426E-03      94238.37c       6.0285E-17
c     material number 1559 total atom density =  0.053314
m1559
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       3.4745E-03
        92234.37c       6.3477E-13      92235.37c       1.3900E-03
        92238.37c       5.5594E-03      94238.37c       6.0285E-17
c     material number 1560 total atom density =  0.055018
m1560
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       3.8984E-13      92235.37c       1.9031E-03
        92238.37c       7.6124E-03      94238.37c       6.0285E-17
c     material number 1561 total atom density =  0.053463
m1561
        14000.37c       1.0000E-17
        13027.37c       4.2890E-02
        42000.37c       9.9020E-04
        92234.37c       7.6907E-13      92235.37c       1.9164E-03
        92238.37c       7.6666E-03      94238.37c       6.0406E-17
c     material number 1562 total atom density =  0.052949
m1562
        14000.37c       4.0240E-03
        13027.37c       4.2890E-02
        42000.37c       1.0000E-17
        92234.37c       3.6063E-13      92235.37c       1.2069E-03
        92238.37c       4.8282E-03      94238.37c       6.0285E-17
c     material number 1563 total atom density =  0.054980
m1563
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
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        92234.37c       2.1127E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0285E-17
c     material number 1564 total atom density =  0.054980
m1564
        14000.37c       1.0000E-18
        13027.37c       4.2890E-02
        42000.37c       2.6120E-03
        92234.37c       3.4545E-13      92235.37c       1.8959E-03
        92238.37c       7.5823E-03      94238.37c       6.0225E-17
```