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MCWO - LINKING MCNP AND ORIGEN2 FOR FUEL BURNUP ANALYSIS

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ABSTRACT

The UNIX BASH (Bourne Again Shell) script MCWO has been developed at the Idaho National Engineering and Environment Laboratory (INEEL) to couple the Monte Carlo transport code MCNP with the depletion and buildup code ORIGEN2. MCWO is a fully automated tool that links the Monte Carlo transport code MCNP with the radioactive decay and burnup code ORIGEN2. MCWO can handle a large number of fuel burnup and material loading specifications, Advanced Test Reactor (ATR) powers, and irradiation time intervals. The program processes input from the user that specifies the system geometry, initial material compositions, feed/removal specifications, and other code-specific parameters. Calculated results from MCNP, ORIGEN2, and data process module calculations are then output successively as the code runs. The principal function of MCWO is to transfer one-group cross-section and flux values from MCNP to ORIGEN2, and then transfer the resulting material compositions (after irradiation and/or decay) from ORIGEN2 back to MCNP in a repeated, cyclic fashion. The basic requirement of the code is that the user has a working MCNP input file and other input parameters; all interaction with ORIGEN2 and other calculations are performed by *UNIX BASH script* MCWO. This paper presents the MCWO-calculated results of the RERTR-1 and -2, and Weapons-Grade Mixed Oxide (WG-MOX) fuel experiments in Advanced Test Reactor (ATR) and compares the MCWO-calculated results with the measured data.

Key words: Monte-Carlo, Fuel Burnup, MCNP, ORIGEN2, MCWO

1 INTRODUCTION

As computational power continues to increase, it becomes more practical to utilize Monte Carlo methods to perform fuel burnup calculations. The UNIX BASH (Bourne Again Shell) script MCWO[1] was developed at the Idaho National Engineering and Environment Laboratory (INEEL) to link the Monte Carlo transport code MCNP[2] with the depletion and buildup code ORIGEN2.[3] The primary functions of MCNP are to calculate one-group cross-sections and neutron fluxes that are used by ORIGEN2 in fuel burnup calculations and to provide criticality and neutron economy information if requested. After depletion and buildup calculations are performed by ORIGEN2, MCWO passes isotopic compositions of materials back to MCNP to begin another burnup calculation cycle.

MCWO consists of a UNIX BASH (Bourne Again SHell) script file that executes MCNP, ORIGEN2, and the written FORTRAN77 data processing codes to manipulate the input and output from MCNP and ORIGEN2 to form a completely automated nuclear fuel burnup and material depletion tool. MCWO consists of a LINUX BASH script file that frequently interacts with two data processing FORTRAN77 programs. The input to MCWO begins with a working MCNP input file. Other input includes material feed information and other code-specific variables used to perform burnup calculations in ORIGEN2 concurrently with flux/cross-section calculations in MCNP. The name MCWO was chosen because it couples the Monte-Carlo code MCNP with the isotope depletion and buildup code, ORIGEN2.

2 DESCRIPTION OF MCWO

In the last few years, interest in burnup calculations using Monte Carlo methods has increased. Previous burnup codes have used diffusion theory for the neutronics portion of the codes. The diffusion theory code PDQ works well for the INEEL's Advanced Test Reactor (ATR) 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 resort to energy and spatial homogenization of neutron cross sections.

MCWO consists of a LINUX BASH script file that repetitively interacts with two data processing FORTRAN77 programs, *m2o.f*[4] *and o2m.f.*[4] it is designed to link the Monte Carlo transport code MCNP with the radioactive decay and burnup code ORIGEN2. 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 input from the user that specifies the system geometry, initial material compositions, feed/removal specifications, and other code-specific parameters. The primary way in which MCNP and ORIGEN2 interact through MCWO is that MCNP provides one-group microscopic cross sections and fluxes to ORIGEN2 for burnup calculations, and ORIGEN2 provides material compositions for MCNP. After ORIGEN2 and MCNP have completed a depletion step, results are written into the ORIGEN2 input file first, and the isotopic compositions obtained from ORIGEN2 are used to generate a new MCNP input file for the next burn step. Various results from MCNP, ORIGEN2, and other calculations are then output successively as the code runs.

MCWO performs one or more MCNP and ORIGEN2 runs for each user-specified time step. The results obtained from MCWO are more accurate if long irradiation periods are broken up into smaller lengths of time, because the physics and composition of materials in the system may change significantly over time. In addition, there is no penalty on execution time by using smaller time steps in ORIGEN2 because almost all of the execution time lies with MCNP.

For each MCNP calculation step, MCNP can update fission power distribution and burnup-dependent cross sections for each fuel pin, then transfer the data to ORIGEN2 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 in the MCNP model can be depleted (on average) with reaction rate data that can be more accurate 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 ORIGEN2 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 ORIGEN2 CODE

ORIGEN2 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.

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The ORIGEN2 input must specify the location of the ORIGEN2 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 ORIGEN2 are listed in Table 1, which was chosen as the reference library in the following MCWO calculations. The cross sections of ^{149}Sm and ^{135}Xe chains and 24 chosen fission products from fuel irradiation are updated by MCWO. In addition, we also chose 18 actinides (U, Pu, Am, Cm) whose reactions are important to criticality for reactors under study to update their burnup dependent one-group cross section[5] of nuclides for ORIGEN2 calculation in MCWO fuel burnup analysis.

TABLE 1: Initial cross-section libraries provided by ORIGEN2

Library	**Character Identifier**	**Number Identifier**		
		Activation product	**Actinide**	**Fission product**
PWR: 235U-enriched UO2 with a burnup of 33,000 MWd/MTU	PWRU	204	205	206
PWR: 235U-enriched UO2 in a self-generated Pu recycle reactor	PWRPUU	207	208	209
PWR: Pu-enriched UO2 in a self-generated Pu recycle reactor	PWRPUPU	210	211	212
BWR: 235U-enriched UO2	BWRU	251	252	253
BWR: 235U-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

3 RESULTS AND DISCUSSIONS

The MCWO methodology was used to analyze the Reduced Enrichment for Research and Test Reactors (RERTR) and Weapons-Grade Mixed-Oxide (WG-MOX) fuel 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 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 = (fission neutron / fission) x (fission /MeV) x (W per MW)

$$= (2.42) \times (1/201.09) \times 1.0\times10^{6}$$
$$= 12034 \text{ per total core MW.}$$

The MeV per fission used in the above normalization is 201.09 MeV/fission.[6] All the MCNP-calculated fission and total heat rate distributions in this report are based on a typical middle of cycle condition. MCNP-calculated tallies were normalized for a NW-lobe power of 18.0 MW, SE-lobe and SW-lobe power of 23 MW.

3.1 RERTR-1 and -2 Experiments in ATR

The RERTR Experiments containing low-enriched uranium (LEU, < 20%) fuel, which are being developed by the Reduced Enrichment Research and Test Reactor (RERTR) program, have been designed and were irradiated in the Advanced Test Reactor (ATR) The irradiation vehicles were irradiated in the small SE and SW I-positions (see Fig. 1). The 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 basket.

MCWO provides the important fuel test parameters, linear heat generation rates and burnups, as demonstrated during the completed irradiation for RERTR-1 (from ATR 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[7] 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 in ATR small I-irradiation positions, MCNP (Fixed-Source mode with 3 tasks, nps = 2.5×10^{8}) calculations require 1500 minutes of DELL-650 XEON-2-CPU 3.06 GHz workstation computer time to achieve one standard deviation (1σ, about 3.5 %) in the cell fission tallies, for each time step run . The MCWO-calculated tallies are normalized to the corresponding test assembly located SW- and SE-lobe powers of 23 MW.

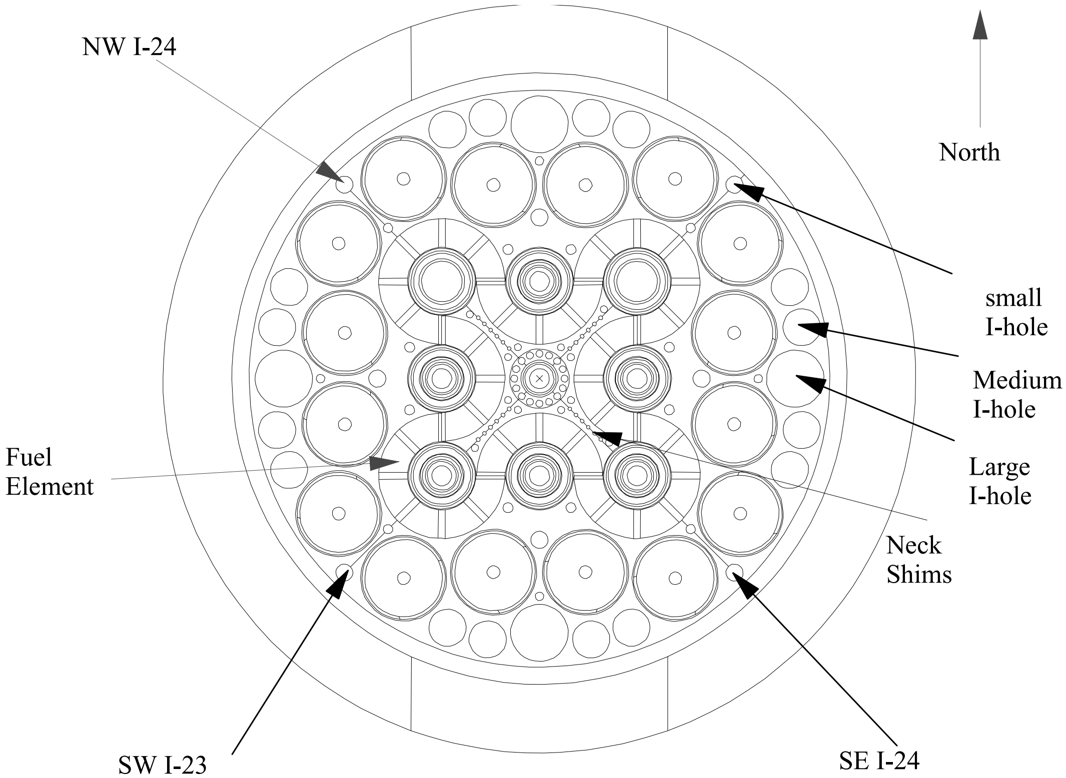

Fig. 1. ATR MCNP core model cross-section view.

MCWO was used to track the fuel stack power and neutron flux distributions in the RERTR fuel micro-plates. In irradiation of RERTR-1, the effective full power days (EFPDs) for Cycles 114B and 114C were51.1 and 43.3, respectively, at the SE I-22 position. To achieve higher burnup, the EFPDs of RERTR-2 for Cycles 114B, 114C, 115B, 115C, 116A, and 116B were 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 tabulated in Table 2, Reference 4.

The MCWO-calculated burnup distributions are also tabulated in Table 2 for comparison. Some of the microplates measured burnups at Argonne National Laboratory – East (ANL-E) are also tabulated in Table 2. 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. MCWO was used to perform the neutronics analysis of the RERTR fuel micro-plates in ATR. It is remarkable that the results matched well considering the complicated ATR geometry and the uncertainty ($1\sigma = 8.5\%$) of the power measurement in each lobe.

Table 2: MCWO-calculated and measured ^{235}U burnup distributions in the RERTR-1 and RERTR-2 fuel microplates

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 $1\sigma = 5.0\%$.

3.2 WG-MOX Fuel Experiment 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 were all included in the ATR MCNP Core Model (ATRM) as shown in Fig. 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 Fig. 2.

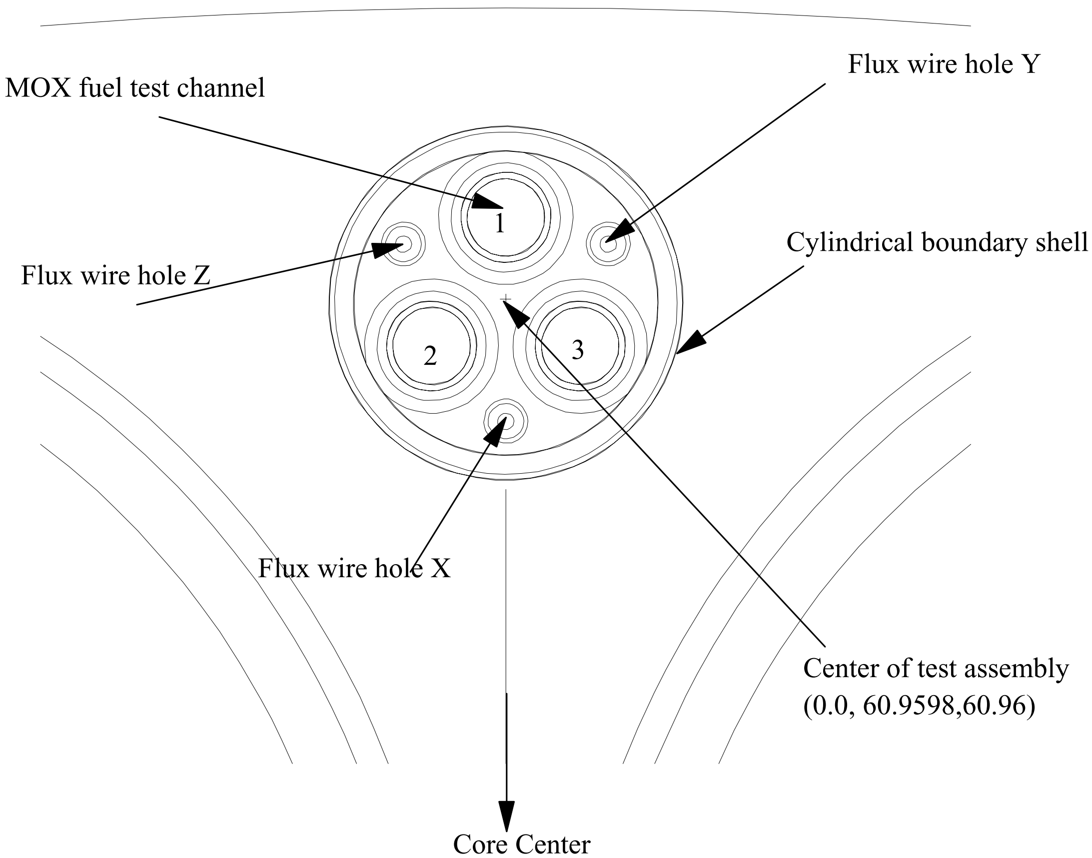

Figure 2: Detailed radial cross-sectional view of the WG-MOX fuel test assembly

The initial experiment phase (Phase-I irradiation), which contained nine MOX fuel capsules, was loaded into the NW I-24 position (see Fig. 1) in January 1998. After 153.5 effective full power days (EFPDs) of irradiation in Phase-I,[8] 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[9] 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[10] 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-1[11] 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 ORNL. Because of the ^{239}Pu depletion, the fuel pellet Linear Heat Generation Rate (LHGR) is quite low in the final Phase-IV-2 irradiation. 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 MW. The current PIEs involve three capsules withdrawn at the end of Phase-IV-2 in October 2003 with an average burnup of 50 GWd/t.

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[12] 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[12] 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.[14] FIMA MCWO-calculated ratios of ^{239}Pu/Pu are shown versus burnup in Fig. 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 Fig. 3. The MCWO-MS estimated and ^{148}Nd corrected burnups agreed well within a one uncertainty band ($1\sigma = \pm 5\%$). The MCWO-calculated ^{239}Pu/Pu ratio profile in Fig.3 shows that the buildup of ^{239}Pu from ^{238}U almost equal to the ^{239}Pu depletion when the ^{239}Pu/Pu ratio reaches 20.6%.

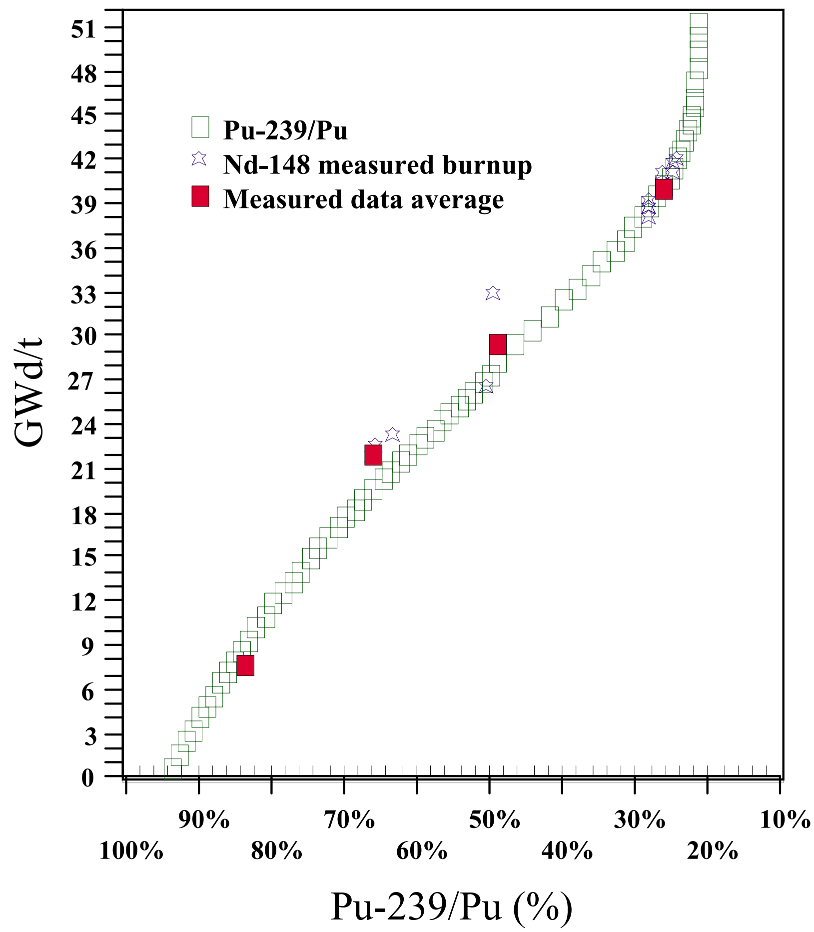

Fig 3: FIMA MCWO-calculated ^{239}Pu/Pu ratio profile and Mass-Spectrometer-measured ^{239}Pu/Pu ratio versus burnup.

4.0. CONCLUSIONS

MCWO 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 ORIGEN2 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). 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 in the WG-MOX testing in the ATR capsule neutronics design and irradiation as-run physics analyses. The comparison of the results shows that the MCWO-calculated and measured data have very good agreement. However, more detailed benchmarking efforts also need to be performed. Work is ongoing to make the input/output of MCWO more user-friendly. Also, work is continuing in the benchmarking of MCWO to experimental and analytical burnup results, as well as for a wide range of inputs.

Because of the lack of high-energy capability (Neutron E > 20.0 MeV) in MCNP, MCWO does not handle spallation products and accelerator-driven systems. Work is being planned to develop Monte-Carlo Lahet Code System (LCS) or MCNP-X,[15] which can handle all the high-energy particles interaction, coupled with the isotope depletion and buildup code ORIGEN2 via a coupling UNIX BASH script, MPXWO. The developed MPXWO will have the capability to analyze the (n,t) reaction in Li-6 in fusion reactor blanket tritium breeder and shielding design.

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