

Benchmark Comparisons of Deterministic and Monte Carlo Codes for a PWR Heterogeneous Assembly Design

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Abstract

Numerical benchmark calculations for a heterogeneous CORAIL assembly have been performed using deterministic transport codes (WIMS8 and APOLLO2) and Monte Carlo codes (MCNP4C and TRIPOLI4). For this benchmark, the eigenvalues, normalized pin power distributions, and the fuel inventory calculated using several nuclear data files such as ENDF/B-V, -VI, and JEF2.2, were compared.

Regarding the assembly eigenvalue, the differences between the APOLLO2, TRIPOLI4 and MCNP4C results are satisfactory when cross sections based on the same nuclear data file are used (deviation less than 200 pcm (Δk)). A significantly higher difference in the k_{∞} value (up to 500 pcm) is observed between the Monte Carlo cases using cross sections based on different evaluated nuclear data files (particularly JEF2.2 versus ENDF/B-V or -VI). Although the heterogeneous fuel pin configuration results in a sharp flux gradient in the assembly, there is good agreement between the normalized power distributions calculated by the codes.

A good agreement in the fuel inventory calculated by the two deterministic codes is also observed.

KEYWORDS: *CORAIL Heterogeneous PWR Assembly, Numerical Benchmark, MCNP4C, TRIPOLI4, WIMS8, APOLLO2*

1. Introduction

In the French nuclear program, a single recycle (mono-recycling) of the plutonium recovered from spent UO_2 assemblies is currently practiced in 20 of 58 pressurized water reactors (PWR). In this approach, mixed-oxide (MOX) fuel assemblies comprise roughly one-third of the core loading; it has been shown that a LWR core loading of 20-50% typical MOX fuel assemblies can be tolerated without strong modifications to reactor systems (e.g., control rods) to maintain safety criteria, depending on the PWR reactor type.[1] The mono-recycling approach consumes ~25% of the Pu loaded in the MOX assembly, providing a commensurate reduction of the long-term (i.e., at 100,000 years after disposal) waste radiotoxicity and slowing the growth rate of transuranics (TRU) in the spent fuel stockpile.

Multiple recycles would keep the plutonium (Pu) in the reactor fuel cycle and practically eliminate it from the disposed nuclear waste (limited to partitioning losses). However,

because the Pu isotopic vector is “degraded” with irradiation (e.g., consumption of Pu-239 and buildup of Pu-240), multi-recycling requires an increase of the Pu loading to meet the operating cycle length requirements. After a few recycles, the Pu loading in a MOX assembly can exceed a known point (~12% Pu/HM) at which the coolant void coefficient turns positive.[2]

To mitigate this problem, the French CEA has investigated the feasibility and the performances of the so-called CORAIL concept and MOX-UE concept.[3,4] The USDOE has also studied the CORAIL assembly concept.[5] The CORAIL assembly uses a heterogeneous fuel pin layout (UO₂ pins in the interior and MOX pins on the periphery) in a design that is “retrofittable” to a typical PWR core. After discharge, the plutonium from the irradiated MOX and UO₂ pins is recycled to a newly fabricated assembly, while the uranium enrichment of the UO₂ pins is adjusted in order to meet the operating requirements on cycle length. It has been found that even with multi-recycling the reactivity coefficients for a full-core loading of CORAIL assemblies are comparable to those of a reference UO₂-fueled core.[5]

However, the heterogeneous fuel pin configuration of the CORAIL assembly causes sharp flux gradients within the assembly, yielding a power peaking factor that is much larger than that observed in a typical UO₂ fuel assembly. As such, the power peaking factor is one of the primary constraints in the design and utilization of the CORAIL assembly. The pin power distribution in the CORAIL assembly was previously calculated with the WIMS8[6] code at Argonne National Laboratory (ANL) and compared with the results of calculations performed by CEA-Cadarache with the APOLLO2[7] code. Differences of several percent were initially observed and a numerical benchmark problem was proposed in order to resolve these differences.

The purpose of the benchmark is to compare the eigenvalue (or infinite multiplication factor) and two dimensional pin power distribution in the CORAIL assembly as calculated by the deterministic neutron transport codes WIMS8 and APOLLO2, and the Monte Carlo codes MCNP4C[8] and TRIPOLI4[9]. In addition, the fuel inventory of the CORAIL assembly is compared at different burnup states in the assembly depletion.

2. Benchmark Problem

The assembly configuration for this benchmark is the CORAIL assembly design originally proposed by CEA for plutonium stabilization in a PWR fuel cycle.[3] The heterogeneous pin layout is shown in Figure 1. The assembly contains 180 UO₂ fuel pins in the interior and 84 MOX fuel pins in the peripheral region.

Tables 1 and 2 contain the detailed design data specified for the benchmark, where cases with 8% and 12% plutonium content in the MOX pins are considered. Static benchmark calculations were performed with both deterministic and Monte Carlo codes. Because of limited cross section evaluations at operating temperatures in the available MCNP4C libraries, cold state data at 294 K are provided for the Monte Carlo calculations; however, the coolant number densities for the static benchmark are those of the hot coolant condition (i.e., densities at 583 K) to represent realistic operating conditions. Therefore, the differences between the static benchmark and normal operating conditions are the temperatures of fuel, cladding and coolant. The depletion benchmark calculations were performed with the deterministic codes only (WIMS8 and APOLLO2). For these calculations, realistic hot state conditions (densities and temperatures) were specified with a specific power density of 37 W/g initial heavy metal. In this benchmark problem, the gap between fuel pellet and cladding is ignored and reflective boundary conditions are assumed at the assembly surfaces.

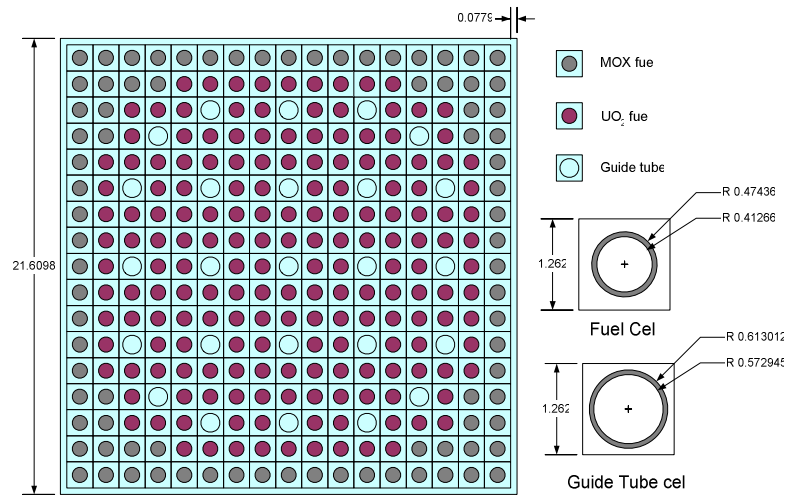


Figure 1. Heterogeneous Pin Loading Pattern in CORAIL Assembly

Table 1. Composition Data for CORAIL Assembly Benchmark*

	Isotope	8% Pu	12% Pu
UO ₂ pin	U-235		1.1315E-03
	U-238		2.1226E-02
	O-16		4.4716E-02
MOX pin	U-235	5.2055E-05	4.9794E-05
	U-238	2.0508E-02	1.9617E-02
	Pu-238	6.9723E-05	1.0459E-04
	Pu-239	7.2243E-04	1.0837E-03
	Pu-240	5.3327E-04	7.9993E-04
	Pu-241	2.1750E-04	3.2627E-04
	Pu-242	2.0904E-04	3.1358E-04
	Am-241	2.1892E-05	3.2839E-05
O	4.4667E-02	4.4655E-02	
Cladding	Fe-54		8.0198E-6
	Fe-56		1.2682E-4
	Fe-57		3.0420E-6
	Fe-58		3.8716E-7
	Cr-50		3.0764E-6
	Cr-52		5.9257E-5
	Cr-53		6.7185E-6
	Cr-54		1.6690E-6
	O		2.8737E-04
	Zr		3.9550E-02

*Number densities are in #/barn-cm.

Table 2. Coolant Composition Data for CORAIL Assembly Benchmark

State		Soluble boron concentration, ppm	Temperature, K (fuel/clad/coolant)	Coolant number density	
				isotope	#/barn-cm
Static benchmark	Normal	600	294 / 294 / 294	H ₂ O	2.3399E-02
				B-10	4.6584E-06
				B-11	1.8751E-05
Depletion benchmark	Normal	600	900 / 630 / 583	H ₂ O	2.3399E-02
				B-10	4.6584E-06
				B-11	1.8751E-05

3. Descriptions of Computation Codes

The benchmark calculations were performed with the WIMS8 and MCNP4C codes at ANL and the APOLLO2 and TRIPOLI4 codes at CEA-Cadarache.[10] The WIMS8 code is a deterministic neutron transport code utilized for calculating neutron fluxes, reaction rates, and the eigenvalue for a lattice problem. A 172-group neutron cross section library based on JEF2.2 is available to account accurately for the self-shielding of resonances (particularly the low-energy lying resonances). The code is also capable of estimating the time-dependent heavy metal composition based on a pin-by-pin depletion. In the WIMS8 calculations, a characteristics method (i.e., CACTUS module) was selected to solve the neutron transport equations; this is one of many transport solution techniques available in the WIMS8 code. After evaluating the resonance self-shielding at the 172-group level, the transport equation for the lattice is solved using 172, 28, or 6 energy groups.

The MCNP4C code is a continuous-energy Monte-Carlo particle transport code. Tabulated cross section data derived from ENDF/B-V, ENDF/B-VI and JEF-2.2 were utilized in this benchmark. Several versions of ENDF/B-VI have been released. The results calculated using data from release versions 2 and 5 of ENDF/B-VI are reported in this benchmark. The MCNP4C calculations tracked 5,000,000 neutron histories. The first 250,000 histories were ignored to allow convergence of the fission source before averaging k_{∞} or accumulating the fission energy deposition (including gamma heating) tallies from which the pin power distribution was derived. Reflective boundary conditions were applied in the MCNP4C and WIMS8 calculations.

The CEA calculations of this benchmark problem were performed with the deterministic code APOLLO2 and the continuous-energy Monte-Carlo code TRIPOLI4. Pin cell and assembly calculation schemes were defined to avoid significant biases. Both the CEA93 library of APOLLO2 and point-wise nuclear data of TRIPOLI4 are based on the JEF2.2 data file. The processing was carried out by the NJOY code. TRIPOLI4 automatically handles its point-wise cross-section set in the PENDF format coming from the NJOY processing. The X-MAS 172 group structure of the APOLLO2 code is sufficiently refined to account for the flux depression in the thermal resonances of Pu-239 and Pu-240 at 0.3eV and 1eV respectively. The resonance absorption during neutron slowing-down is described by an accurate space- dependent self-shielding formalism. The integral transport equation is solved by a collision probability method (P_{ij}). The spatial calculation is achieved using a UP_1 model (interface currents are linearly anisotropic). In order to calculate correctly the power distribution, the S_n nodal method must also be used. Common optimized options are summarized: S_4 quadrature, P_1 anisotropic scattering, 20 energy groups (12 fast and 8 thermal). The Monte-Carlo calculations were performed using the TRIPOLI4 code with the JEF2.2 library. The TRIPOLI4 calculations tracked 4,000,000 neutron histories. However, the water gap between the fuel assemblies (the gap thickness is 0.1588 cm) was not modeled explicitly in the APOLLO2 and TRIPOLI4 calculations; the gap was integrated into the peripheral MOX fuel cells.

4. Benchmark Results

4.1 Results of Static Benchmark

Comparisons of the k_{∞} values are provided in Table 3 with calculations performed using the indicated codes and data libraries. The ENDF/B-VI release 5 calculations denote that the data

for U-235, U-238 and Pu-239 are taken from ENDF/B-VI release version 5, while ENDF/B-VI release 2 library data are used for all other nuclides. For the WIMS8 calculations, the number in parenthesis next to the library indicates the number of collapsed neutron energy groups utilized in the transport solution.

In the MCNP4C calculations, the k_{∞} values are comparable to each other regardless of the ENDF library or release versions: the maximum difference is 76 pcm (Δk) between ENDF/B-V and ENDF/B-VI release 2 libraries. However, a significant difference in k_{∞} value is observed between calculations using different evaluated nuclear data files; the k_{∞} value for the 8% Pu case calculated with the JEF2.2 is 548 pcm greater than the result calculated with the ENDF/B-VI release 2. Note that the result between TRIPOLI4-JEF2.2 and MCNP4C-JEF2.2 is about half as large; the discrepancies are 228 pcm and 195 pcm for 8% and 12% Pu cases, respectively.

The WIMS8 calculations (JEF2.2 library) consistently predict a lower k_{∞} than MCNP4C. When the ENDF libraries are used in MCNP4C, the differences range from 160 to 420 pcm; when the JEF2.2 library data are used in MCNP4C, the difference compared to WIMS8 is about 700 pcm. The results of the APOLLO2 calculations agree well with the results of the TRIPOLI4 or the MCNP4C calculations using the JEF2.2 library.

Figure 2 provides the comparisons of the normalized pin power distribution for the static benchmark. The WIMS8 power distributions presented in this figure were calculated with a 28-group transport solution, which is the group structure that has been adopted at ANL for calculations involving Pu (or TRU) containing fuels. The power distributions calculated by MCNP4C with ENDF/B-VI release 2 library were considered as the reference power distributions for the sake of this comparison. The normalized pin powers of the 28-group WIMS8 calculation are generally within $\pm 1\sigma$ of the MCNP4C result and the root mean square (RMS) of the power difference between WIMS8 and MCNP4C are very similar to the RMS of the standard deviation of the MCNP4C calculation. Some differences in the normalized pin power (e.g., 2.8% in 12% Pu case for the peripheral MOX fuel cells) are found between the results of TRIPOLI4 and MCNP4C calculations, which are caused by the different modeling of the water gap between the assemblies. Note that the water gap was modeled explicitly in the MCNP4C and WIMS8 calculations, but the water gap was integrated into the peripheral MOX fuel cells in the TRIPOLI4 and the APOLLO2 calculations. However, the results between APOLLO2 and TRIPOLI4 concerning the power distribution assembly calculation are very satisfactory.

Table 3. Comparison of k_{∞} for Static Benchmark

Methodology	Code	Library	k_{∞}	
			8% Pu	12% Pu
Monte-Carlo	MCNP4C	ENDF/B-VI release 2	1.28861 \pm 0.00031	1.29541 \pm 0.00031
		ENDF/B-VI release 5	1.28906 \pm 0.00031	1.29609 \pm 0.00031
		ENDF/B-V	1.28937 \pm 0.00032	1.29505 \pm 0.00029
		JEF-2.2	1.29409 \pm 0.00031	1.29992 \pm 0.00031
	TRIPOLI 4	JEF-2.2	1.29637 \pm 0.00038	1.30187 \pm 0.00039
Deterministic transport	WIMS8	JEF-2.2 (6)	1.28645	1.29185
		JEF-2.2 (28)	1.28633	1.29217
		JEF-2.2 (172)	1.28706	1.29263
	APOLLO2	JEF-2.2	1.29649	1.30212

Table 4. Eigenvalue Comparison for Depletion Benchmark

Burnup (MWd/t)	8% Pu case		12% Pu case	
	WIMS8	APOLLO2	WIMS8	APOLLO2
0 (no Xe)	1.25861	1.26630	1.26428	1.27211
15,000	1.10731	1.11470	1.11989	1.12769
30,000	1.02068	1.02550	1.03676	1.04258
45,000	0.94718	0.94848	0.96656	0.96970

Table 5. Comparison of Heavy Metal Number Densities

	8% Pu case					
	15,000 MWD/t		30,000 MWD/t		45,000 MWD/t	
	WIMS8 ^{a)}	APOLLO2 ^{b)}	WIMS8	APOLLO2	WIMS8	APOLLO2
U-234	5.967E-08	-0.1	1.074E-07	-1.0	1.474E-07	-1.4
U-235	1.650E-04	-0.1	1.113E-04	-0.1	7.188E-05	-0.3
U-236	1.366E-05	0.2	2.287E-05	-1.0	2.877E-05	-2.4
U-237	3.372E-08	15.0	4.361E-08	22.5	5.405E-08	25.2
U-238	6.289E-03	0.0	6.222E-03	0.0	6.149E-03	0.0
Np237	7.677E-07	11.6	1.818E-06	18.0	3.001E-06	21.9
Np239	4.676E-07	-1.4	5.187E-07	-2.2	5.663E-07	-3.2
Pu-238	6.278E-06	-0.3	6.447E-06	0.2	6.987E-06	1.6
Pu-239	7.579E-05	-2.0	7.520E-05	-3.7	7.015E-05	-5.5
Pu-240	5.134E-05	0.1	5.132E-05	-0.2	5.003E-05	-0.8
Pu-241	2.413E-05	-0.5	2.762E-05	-1.4	2.911E-05	-2.5
Pu-242	2.082E-05	-0.4	2.263E-05	-0.5	2.522E-05	-0.7
Am-241	2.238E-06	-0.9	2.366E-06	-2.0	2.348E-06	-3.4
Am-242m	4.412E-08	13.2	4.392E-08	11.0	4.275E-08	9.0
Am-243	1.967E-06	5.5	3.467E-06	4.9	5.015E-06	4.3
Cm-242	3.726E-07	1.1	5.153E-07	0.5	6.258E-07	-0.3
Cm-243	6.658E-09	1.9	1.673E-08	0.8	2.640E-08	-0.3
Cm-244	3.668E-07	6.2	1.255E-06	5.8	2.652E-06	5.1
Cm-245	1.614E-08	5.5	1.017E-07	4.8	2.841E-07	2.9
	12% Pu case					
	15,000 MWD/t		30,000 MWD/t		45,000 MWD/t	
	WIMS8	APOLLO2	WIMS8	APOLLO2	WIMS8	APOLLO2
U-234	8.913E-08	-2.6	1.626E-07	-3.5	2.257E-07	-4.1
U-235	1.677E-04	0.1	1.157E-04	0.3	7.722E-05	0.3
U-236	1.320E-05	0.0	2.225E-05	-1.1	2.815E-05	-2.4
U-237	2.740E-08	17.5	4.066E-08	25.1	5.026E-08	28.1
U-238	6.206E-03	0.0	6.141E-03	0.0	6.072E-03	0.0
Np237	6.658E-07	11.5	1.762E-06	17.7	2.923E-06	21.6
Np239	4.434E-07	1.1	4.821E-07	0.3	5.226E-07	-0.7
Pu-238	9.557E-06	-0.3	9.698E-06	-0.2	1.027E-05	0.4
Pu-239	1.083E-04	-1.6	1.023E-04	-3.1	9.331E-05	-4.6
Pu-240	7.623E-05	0.1	7.549E-05	-0.1	7.327E-05	-0.4
Pu-241	3.426E-05	-0.2	3.756E-05	-0.8	3.926E-05	-1.6
Pu-242	3.080E-05	-0.2	3.225E-05	-0.3	3.454E-05	-0.3
Am-241	3.667E-06	-1.7	4.003E-06	-3.0	4.112E-06	-4.2
Am-242m	6.164E-08	12.5	7.989E-08	10.0	8.344E-08	8.0
Am-243	2.227E-06	3.5	4.157E-06	3.0	5.976E-06	2.5
Cm-242	4.477E-07	1.9	6.415E-07	1.3	7.946E-07	0.6
Cm-243	7.465E-09	2.4	1.994E-08	1.7	3.271E-08	0.6
Cm-244	3.612E-07	4.4	1.317E-06	4.2	2.778E-06	3.6
Cm-245	1.498E-08	3.7	1.033E-07	3.3	3.003E-07	1.6

- a) Number density in #/barn-cm
b) Difference in %

This latter difference is the cause of the difference observed for the higher actinides, such as Am-243 and the Cm isotopes. However, these differences do not much affect the k_{∞} value because the concentrations of these nuclides are much smaller than that for U or Pu. It can be seen in Table 5 that the number densities of the fissile Pu isotopes (i.e., Pu-239 and Pu-241) calculated by the APOLLO2 code are increasingly smaller with burnup than those of the WIMS8 results. This is the primary reason why the k_{∞} values reported in Table 4 draw closer with burnup .

Table 6 and Figures 3 and 4 provide comparisons of the normalized pin power distribution during depletion of the CORAIL assembly. Generally, the power distributions calculated by the two codes agree well within 1% difference. But, similar to the static benchmark results, slightly larger differences in the normalized pin power are found due to the different modeling of the water gap between the assemblies in the WIMS8 and the APOLLO2 calculations.

Table 6. Comparison of Normalized Peak Pin Power

Burnup (MWd/t)	8% Case		12% Case	
	WIMS8	APOLLO2 ^{a)} S_n / P_{ij}	WIMS8	APOLLO2 S_n / P_{ij}
0 (no Xe)	1.152	1.149 / 1.143	1.230	1.220 / 1.262
15,000	1.093	1.091 / 1.083	1.208	1.194 / 1.229
30,000	1.086	1.071 / 1.094	1.210	1.190 / 1.223
45,000	1.090	1.073 / 1.091	1.215	1.192 / 1.221

a) APOLLO2 used two schemes. The first uses the $P_{ij}+S_n$ method, the second uses only a P_{ij} method

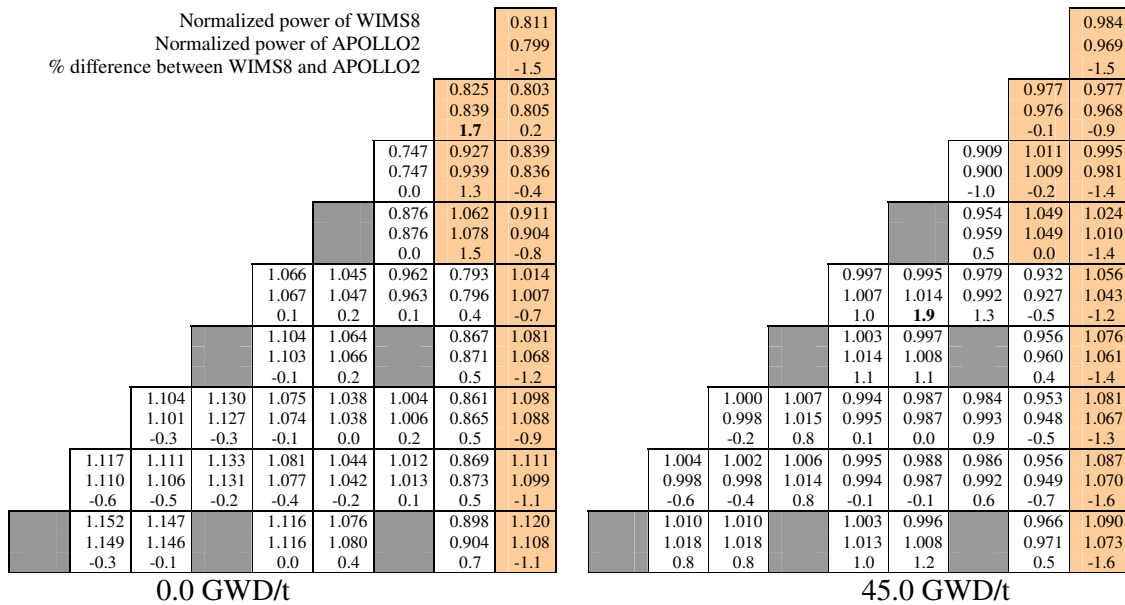


Figure 3. Normalized Pin Power Distributions for 8% Pu Depletion Benchmark

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