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Full Core 3-D Simulation of a Partial MOX LWR Core

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May 2009

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Approved by

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ABSTRACT

A comparative analysis and comparison of results obtained between 2-D lattice calculations and 3-D full core nodal calculations, in the frame of MOX fuel design, was conducted. This study revealed a set of advantages and disadvantages, with respect to each method, which can be used to guide the level of accuracy desired for future fuel and fuel cycle calculations. For the purpose of isotopic generation for fuel cycle analyses, the approach of using a 2-D lattice code (i.e., fuel assembly in infinite lattice) gave reasonable predictions of uranium and plutonium isotope concentrations at the predicted 3-D core simulation batch average discharge burnup. However, it was found that the 2-D lattice calculation can under-predict the power of pins located along a shared edge between MOX and UO2 by as much as 20%. In this analysis, this error did not occur in the peak pin. However, this was a coincidence and does not rule out the possibility that the peak pin could occur in a lattice position with high calculation uncertainty in future un-optimized studies. Another important consideration in realistic fuel design is the prediction of the peak axial burnup and neutron fluence. The use of 3-D core simulation gave peak burnup conditions, at the pellet level, to be approximately 1.4 times greater than what can be predicted using back-of-the-envelope assumptions of average specific power and irradiation time.

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ACRONYMS

AFCI	Advanced Fuel Cycle Initiative
BOC	Beginning of Cycle
BU	Burnup
CMS	Core Management Software
CRTG	Control Rod Guide Tube
EOC	End of Cycle
IBA	Integral Burable Absorber
INL	Idaho National Laboratory
IT	Instrument Tube
LHGR	Linear Heat Generation Rate
LWR	Light Water Reactor
MA	Minor Actinides
MOX	Mixed Oxide fuel
PF	Peaking Factor
PWR	Pressurized Water Reactor
SNF	Spent Nuclear Fuel
UOX, UO2	Uranium Oxide fuel
US	United States

Full Core 3-D Simulation of a Partial MOX LWR Core

1. Introduction

Many previous studies have explored the viability of thermal recycling strategies by loading Light Water Reactor (LWR) cores with Mixed Oxide (MOX) fuels. However, most of these studies were based on 2-D lattice calculations of a generalized Pressurized Water Reactor (PWR) fuel assembly. The deployment of a recycled MOX strategy in one or more of the currently operating LWRs would involve replacement of a certain fraction of the Uranium Oxide (UOX) fuel in the core with MOX fuel reprocessed from LWR Spent Nuclear Fuel (SNF). To successfully deploy such strategies, many questions need to be identified and evaluated such as the characteristics of fuel assembly design, core loading patterns and operational management and licensing issues. To date, none of the Advanced Fuel Cycle Initiative (AFCI) past studies have investigated such issues. Though much experience has been gained by Europe, Russia and Japan with plutonium-only MOX fuels, little attention has been given to the detailed reactor physics characteristics of a MOX assembly, its subsequent influence on surrounding UO2 fuel and how MOX could be introduced in the United States' reactor fleet. In this regard, the MOX composition resulting from the reprocessing of spent LWR fuel in the US will have several significant differences from that of the European MOX and that of the on-going weapons-grade-plutonium disposition program in the US. In particular, the isotopic composition of the MOX may vary because of the longer cooling time of the US spent fuel inventory resulting in a lower Pu-241 content than the MOX used in Europe. In comparison to the MOX used for the US disposition program, the fissile content of plutonium is significantly lower, leading to higher plutonium cocentration requirements (i.e., transuranic-enrichment) in this MOX fuel.

In order to meet non-proliferations objectives, one of the driving principles of AFCI is to ensure that the technologies used would not separate plutonium by itself during recycling. Therefore, such an advanced MOX fuel cycle would require that plutonium be co-separated from spent fuel along with Minor Actinides (MAs) or with spent fuel uranium. The experience base for fuels denatured with MAs is minimal in the international community and there is also very little understanding of refueling reactors with this fuel composition.

The following scoping study follows the core reload transitional cycles to an equilibrium configuration assuming modern day operational and licensing practices and provides perspective on the information gains from using 3-D core design and analysis versus 2-D infinite lattice calculations. This analysis is the product of a short training and collaboration between the Idaho National Laboratory (INL) fuel cycle analysis group with Studsvik Scandpower in Idaho Falls, Idaho. Using the Studsvik Core Management Software (CMS), INL staff analyzed a 2800 MWth 3-Loop PWR (157 assembly core) design, representative of the PWRs in the US fleet. Starting from an all-UO2 reference core in an equilibrium cycle having a 3-batch reload strategy and a 12 month refueling interval, the core was transitioned to a new equilibrium core having 1/3 MOX fuel assemblies. This new equilibrium core had an 18-month refueling interval. Both MOX and UO2 assemblies were irradiated for three cycles (i.e., 3-batch scheme). The final equilibrium core design was not intended to be a final core design in a sense that many of the licensing constraints were not considered in its development. However the equilibrium core design produced and used in this scoping study was realistic enough to perform a reasonable 2-D versus 3-D reactor physics comparison.

2. Model Description

2.1 Methodology

Core physics analysis of the designs were performed with Studsvik Core Management Software (CMS) - an industry standard and NRC approved computer code package for comprehensive neutronic simulation of LWRs. The primary applications of the CMS code package are fuel bundle design (e.g., enrichment zoning and burnable poison design), in-core fuel management and loading pattern optimization, evaluation of fuel cycle energy, various fuel and core licensing calculations (e.g. reactivity coefficients and shutdown margin). The CMS package consists of the 2-D transport code CASMO-5 [1] used to generate homogenized cross section data and heterogeneous pin-by-pin form functions, which are subsequently used in the two-group 3-D nodal diffusion code SIMULATE-3 [2] for the whole core coupled neutronic-thermal hydraulic analysis. The link between CASMO-5 and SIMULATE-3 is realized via the auxiliary utility code CMS-link, which generates a binary macroscopic cross-section library accessible to SIMULATE from the data generated by CASMO-5 [3]. Because SIMULATE-3 is a full core 3-D code with pin-power reconstruction, it has the capability to model the flux interface effects between MOX and UOX assemblies.

The reference core design and follow-on cycles were depleted in 3-D (24 axial nodes and 4 radial nodes per fuel assembly) at: hot full power, with equilibrium xenon concentrations, all rods out, maintaining criticality with soluble boron. In CASMO-5, the depletion steps are carried out at various burnup steps at the assembly level depending on the rate at which the lattice reactivity is changing. In SIMULATE-3, the burnup steps are a constant 1.0 MWD/kg.

Sufficient core reloads were carried out to ensure that an equilibrium cycle exposure of 18.0 MWD/kg (i.e., 18 months, CF=0.85) was converged to within 0.01 MWD/kg. The core loading pattern for each transition cycle was carried out using a reactivity ranking (Assembly k_∞) scheme as opposed to a fixed pattern. The reactivity ranking assigns a core loading pattern by order of assembly beginning-of-cycle k_∞ as opposed to specified locations for fresh, once and twice-burned fuel. The reactivity ranking scheme was used to create a reactivity based "ring-of-fire" loading pattern, discussed in the following core design section. Once the equilibrium cycle was found, the exact loading pattern of the equilibrium core was optimized using a simulated annealing algorithm, ensuring that peaking factors ($F_{\Delta h}$) for this core design were held below 1.75. The simulated annealing algorithm was constrained such that the core locations of fresh assemblies, established in a ring-of-fire pattern, were left unchanged. The equilibrium cycle search, reactivity ranking based shuffling and simulated annealing were all performed using the CMS graphical user interface tool, XIMAGE [4]. Once the equilibrium core design was established using the nodal core simulator, pin-power reconstruction was performed on each assembly and for multiple axial slices of each assembly. This information was used in this analysis to determine the maximum 3-D peak power and exposure of any assembly in the core.

2.2 Core Design

A static fuel management or shuffling strategy was *not* used in this analysis. Instead, fuel shuffling was carried out based on a reactivity ranking pattern. Using the reactivity ranking pattern, the most reactive fuel (i.e., fresh) was shuffled into a *ring-of-fire* pattern. A ring-of-fire pattern is currently a common type of loading pattern whereby the most reactive fuel is located in the outer core but constrained to not be adjacent to the reactor vessel walls (Figure 1). This ensures optimal power

flattening across the core while at the same time minimizing neutron damage to the reactor pressure vessel.

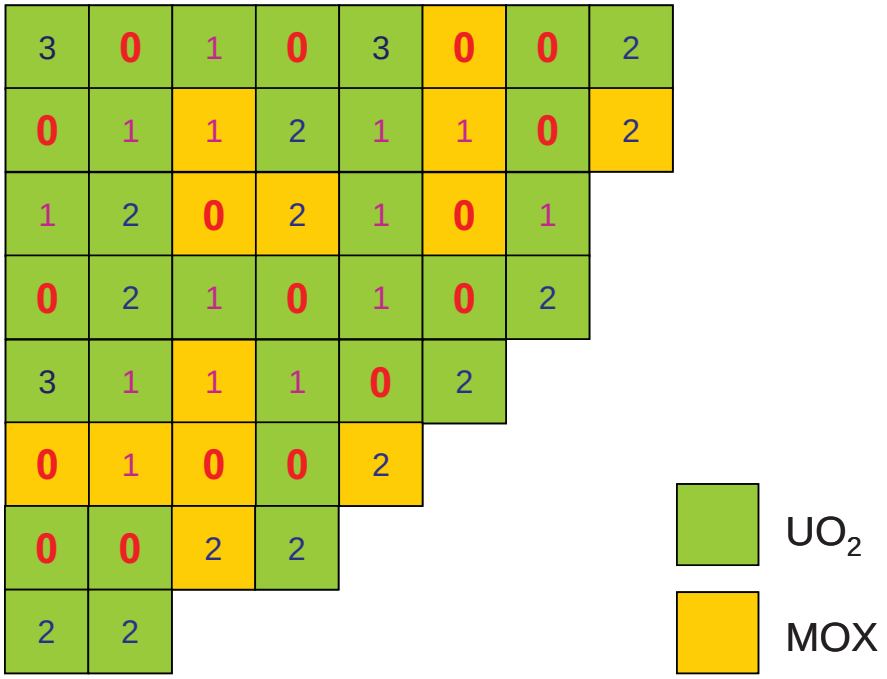

Figure 1: Quarter core symmetric representation of the equilibrium core with a 1/3 MOX (yellow), 2/3 UO2 (green) loading. Numbers represent: Fresh (0), Once Burned (1), Twice burned (2), Thrice burned (3).

No special rule was made to ensure that MOX assemblies were *not* placed beneath control rod cluster assemblies as might be done in a more rigorous investigation [5]. This is generally assumed to be a necessary requirement due to the reduction in control rod worth when inserted into the harder neutron spectrum characteristic of MOX. Also, no special rule was made to ensure that MOX assemblies are surrounded on all sides by UO2 assemblies. This is done to ensure that asymmetric power peaking does not occur in any MOX assemblies' peripheral pins [5]. This asymmetric edge effect was thoroughly analyzed in the MOX equilibrium core model and will be discussed in the peak power section. It should also be noted that the final core loading pattern was not $1/8^{th}$ core symmetric, typical of most core designs in operating PWRs, due to the time constraints and scope of analysis.

2.3 Assembly Design

The fuel assembly design was a standard 17x17 lattice with 24 Control Rod Guide Tubes (CRGT) and one Instrument Tube (IT). The detailed specifications of the fuel assembly design are listed in Table 1. The U-235 enrichment of the UO2 pins was 4.8%. The average Pu enrichment of the MOX assembly was 6.3% plutonium having a fissile content (i.e., Pu-239,Pu-241) of 4.7%. Depleted uranium was used for the uranium component of the MOX assembly. No MAs were incorporated into the MOX composition. Both UO2 and MOX assemblies incorporated 16 integral burnable absorber (IBA) poison rods containing Gd2O3. In both the UO2 assemblies and the MOX assemblies, the IBA pins were UO2-only. A MOX IBA pin design containing Gd2O3 was not considered at this time. The location of these IBA pins for both the UO2 and MOX assembly are shown in Figure 2.

The U-235 enrichment and Gd2O3 concentration of the UO2 IBA (Gd rod) were 3.0% and 6.0%, respectively. The U-235 enrichment and Gd2O3 concentration of the MOX IBA (Gd rod) were 4.4% and 4.0%, respectively.

As seen in Figure 2, the plutonium content of the MOX assembly is graduated, with the lowest concentration of plutonium in the peripheral pins. This is a typical method of reducing the power peaking in the peripheral pins of the MOX assembly when it is located adjacent to UO2 assemblies.

Table 1: Fuel assembly design specifics

Assembly Type	UO2	MOX
Lattice Type	17x17	17x17
Number of Fuel Pins	264	264
U-235 Enrichment (% by weight)	4.8	0.23
Plutonium Enrichment (Tot-Pu/Fiss-Pu) (%)	n/a	6.3/4.7
Inner Enrichment Zone		8.4/6.3
Middle Enrichment Zone		6.6/5.0
Outer Enrichment Zone		4.3/3.2
Number of Control Rod Guide Tubes (CRGT)	24	24
Number of Instrument Tubes (IT)	1	1
Number of IBA Pins (UO2+GO2)	16	16
Gd2O3 Concentration (%) in IBA Rods	6.0	4.0
UO2 Enrichment in IBA Rods (%)	3.0	4.4
Assembly Pitch (cm)	21.50	21.50
Pin Pitch (cm)	1.26	1.26
Fuel Pellet Radius (cm)	0.410	0.410
Clad Inner Radius (cm)	0.417	0.417
Clad Outer Radius (cm)	0.475	0.475
Fuel Density (g/cc)	10.29	10.24
CRGT/IT Inner Radius (cm)	0.573	0.573
CRGT/IT Outer Radius (cm)	0.613	0.613
Max. Discharge Burnup (MWD/kg)	63	65
Fuel Temperature* (K)	820.5	820.5
Bulk Coolant Temperature* (K)	579.5	579.5
Nominal Coolant Pressure* (bar)	155	155
Average Critical Boron Concentration* (ppm)	600	600
Rated Power Density (kW/liter)	104.5	104.5
Fuel Pellet Material	UO2	PuO2+UO2

*Nominal values adopted for single assembly depletion with CASMO-5

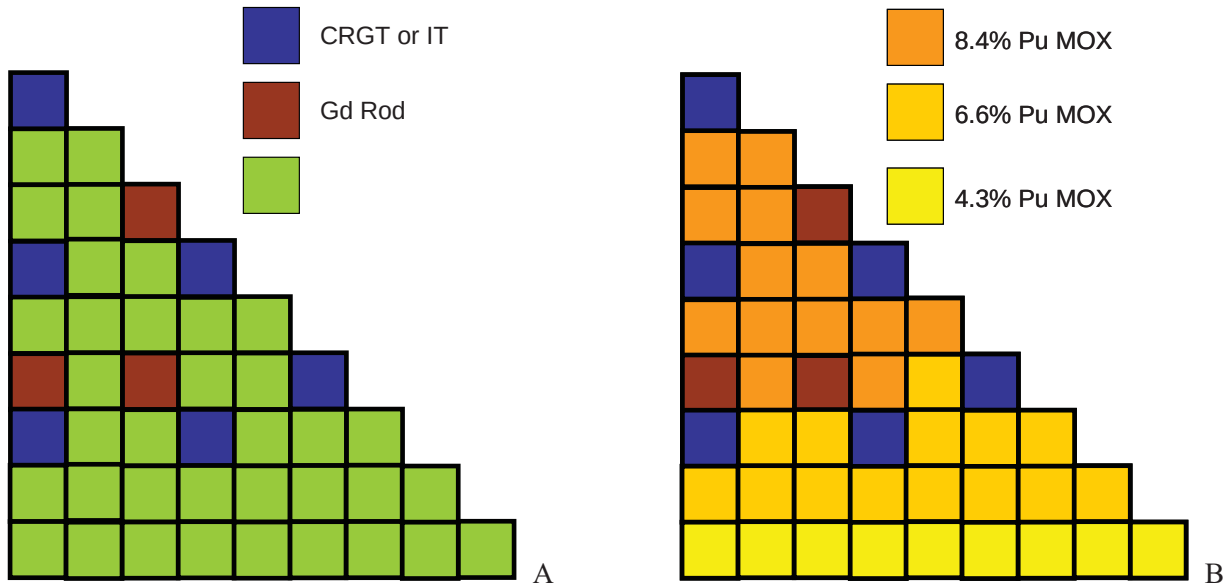

Figure 2: 1/8th assembly representation of the UO2 assembly (A) and MOX assembly (B)

3. Three Dimensional Simulation Results

The use of 3-D core simulation offers several enhancements to the quality of design data describing the MOX fuel. First, the enrichment zoning of MOX is principally dictated by power peaking throughout the irradiation life in the core. Therefore, the composition requirement of the fuel design is based on power peaking as well as the fuel's power history. Single assembly infinite lattice calculations must assume that all assemblies in the core are of identical composition, have an identical constant power history within the core and perform identically with regard to peak power, peak burnup, etc. In reality, this is not the case because the core power distribution is not flat and the evolution of power with burnup is not constant. Therefore, the average discharged batch composition of the spent fuel will be different to some degree from that predicted by a single assembly calculation. Second, the peak power performance of pins within the assembly is dictated by the neighbor effects of adjacent fuel assemblies. In a single assembly calculation, typically a reflective boundary condition is used which is equivalent to an assumption that all neighboring assemblies are identical in geometry, composition and burnup to the assembly being depleted. In reality, an assembly may be loaded in the core next to any combination of assemblies with different design (e.g., UO2 or MOX, IBA or no IBA, etc.) and level of depletion. The influence of these neighbor assemblies will have a significant effect on the power peaking. Finally, the peak exposure (i.e., burnup) of the any given fuel pellet is a function of the 3-D power distribution within the assembly and the cycle-by-cycle fuel management trajectory as a result of shuffling. In a single assembly calculation, there is no provision for capturing the true magnitude and distribution of power within the assembly as a function of cycle number and depletion.

Furthermore, single assembly 2-D calculations have no provision for representing axial power shape, axial composition zoning or axial thermal-hydraulic feedback to the depletion model. Therefore, it is a worthwhile exercise to capture these 3-D effects on the design of the fresh fuel composition as well as the 3-D effects on the ultimate discharged fuel compositions. Ideally, the single assembly calculation of discharge burnup and isotopic composition should match very closely the total batch averaged burnup and isotopic composition from 3-D core simulation. This is plausible because in an effort to make a core design as efficient as possible, a fuel manager would devote a large amount of effort to ensure that the

maximum amount of power is extracted per unit mass of fuel investment. In order to do this, it is optimal to flatten the discharged fuel exposure distribution.

The added information of 3-D core simulation is not strictly limited to improved charge and discharge composition data. It also provides insight into peak pin power and exposure performances. This kind of information is invaluable for determining the most limiting irradiation conditions that a MOX fuel and accompanying structural materials will be exposed.

3.1 Core Level Performances

At the core level, three performance indicators were evaluated in the equilibrium core: Assembly averaged beginning-of-cycle (BOC) and end-of-cycle (EOC) power peaking and assembly averaged discharge burnup (Figure 3). Based on the SIMULATE-3 results without pin power reconstruction (on a node averaged basis), the peak discharge burnup of MOX was 65 MWD/kg. The peak assembly power at BOC occured in a fresh MOX assembly and was 1.46 times that of the core average power. The peak EOC power also occured in a MOX assembly and was 1.37 times that of the core average power.

Another important peaking factor to consider is the peak enthalpy rise in any given fuel pin channel or $F_{\Delta h}$. $F_{\Delta h}$ is defined as the change in enthalpy along a thermal-hydraulic channel surrounding each pin divided by the average change in enthalpy for any given pin-channel in the core. $F_{\Delta h}$ is an integral quantity addressing total energy input to the coolant local to a fuel pin. The peak BOC and EOC $F_{\Delta h}$ was 1.73 and 1.66, respectively. Both occured next to the outermost ring of CRGT locations (Figure 4).

75 0.97 0.92	-- 1.43 1.30	-- 1.32 1.10	-- 1.24 1.23	63 0.92 0.90	-- 1.42 ***1.37***	-- 1.03 1.28	48 0.32 0.51
-- 1.43 1.30	-- 1.31 1.07	-- 1.39 1.15	57 0.99 0.90	-- 1.21 1.08	-- 1.31 1.24	-- 0.94 1.17	54 0.33 0.49
-- 1.32 1.10	57 1.03 0.91	-- ***1.46*** 1.24	***65*** 1.22 1.06	-- 1.17 1.05	-- 1.29 1.29	-- 0.65 0.79	
-- 1.24 1.23	60 0.93 0.87	-- 1.21 1.04	-- 1.40 1.33	-- 1.23 1.16	-- 0.91 1.12	43 0.32 0.46	
63 0.92 0.90	-- 1.18 1.05	-- 1.34 1.19	-- 1.25 1.16	-- 0.97 1.16	43 0.41 0.57		
-- 1.42 1.37	-- 1.28 1.22	-- 1.25 1.23	-- 0.91 1.09	55 0.47 0.61			
-- 1.03 1.28	-- 0.89 1.13	59 0.58 0.70	47 0.30 0.42				
48 0.32 0.51	51 0.24 0.40						

BU
BOC PF
EOC PF

Assembly Average Discharged Burnup (MWD/kg)
BOC Asmb Avg Peak Factor (Assembly/Core)
EOC Asmb Avg Peak Factor (Assembly/Core)

Figure 3: Assembly average core level performances. Bolded values represent performance peaks.

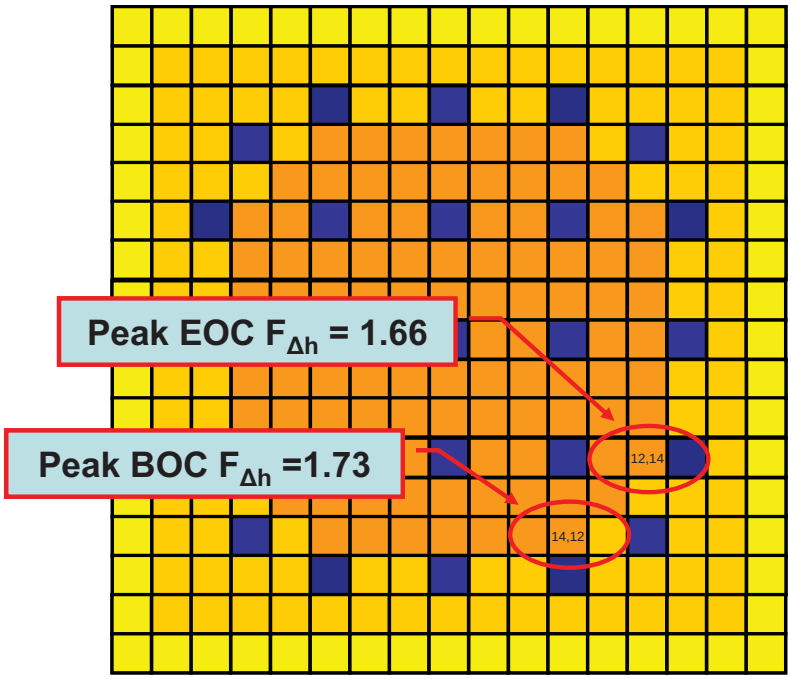

Figure 4: Peak enthalpy rise, $F_{\Delta h}$

The peak $F_{\Delta h}$ in this core design occured in the assembly having the peak assembly power. It should be noted that this is not always the case. It is conceivable for the peak $F_{\Delta h}$ pin to occur in a core location that is *not* in the average peak assembly. An example of this is a fuel assembly that is placed adjacent to significantly more reactive fuel assembly. In such a scenario, the incoming flux from the more reactive neighbor assembly causes localized power peaking along its own assembly edge. This point will be illuminated by the axial power peaking discussion and comparison between single assembly and full core simulation results in Section 3.4.

3.2 Axial Power Performances

Using $F_{\Delta h}$ is a useful value of power peaking primarily because of its affect on the thermodynamic condition and the flow regime of the water in that flow channel (i.e., liquid phase, sub-cooled nucleate boiling, etc.). However, to understand the location of the peak Linear Heat Generation Rate (LHGR) at the pellet level, it is necessary to evaluate pin power in each axial node along the entire length of each assembly in the core (i.e., a total 994,752 nodal pin powers at each depletion step). This information was generated using the pin power reconstruction methodology at every axial node (24 nodes per assembly) for every fuel assembly within the core. For this core design, the 3-D peak power also occurred within the peak $F_{\Delta h}$ pin of the peak assembly. It should be noted that as with $F_{\Delta h}$ and the assembly average peak, it is not always the case that the axial 3-D peak will occur in the same pin as the peak $F_{\Delta h}$. Figure 5 shows the peak LHGR along the length of the peak pin within the peak power assembly within the core, which was a fresh MOX. The average LHGR of this peak pin was 306.7 W/cm. The peak LHGR taking into account the axial power distribution of the pin was 369.2 W/cm. Therefore, the peak-to-average power of the pin was 1.20. Multiplying this value by the $F_{\Delta h}$ gives a 3-D localized power peaking factor of 2.08.

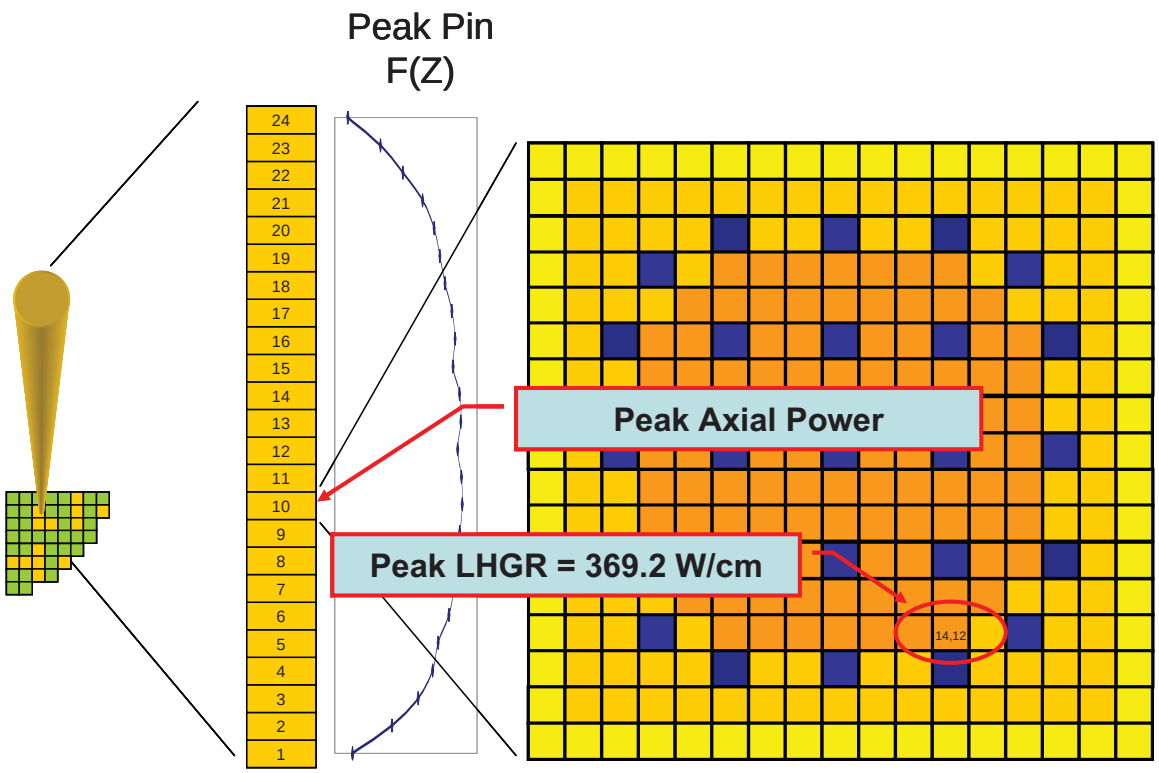

Figure 5: Peak 3-D LHGR. Pellets within this axial slice of this fuel pin have the highest power density of any in the core.

3.3 Axial Dependence of Burnup

The added detail of the axial pin power shape in a 3-D whole-core simulation also allows the analyst to capture the axial burnup distribution. Figure 6 shows the differences between the peak assembly averaged burnup, pin averaged burnup and peak burnup. Since the peak power assembly is a fresh MOX assembly, a thrice burned assembly was selected for the burnup comparison. However, instead of the peak exposure assembly, a median exposure assembly was selected to better represent the average assembly being discharged from the core. This assembly appears on the equilibrium core's periphery after being shuffled from the inner core where it was irradiated in the previous two cycles.

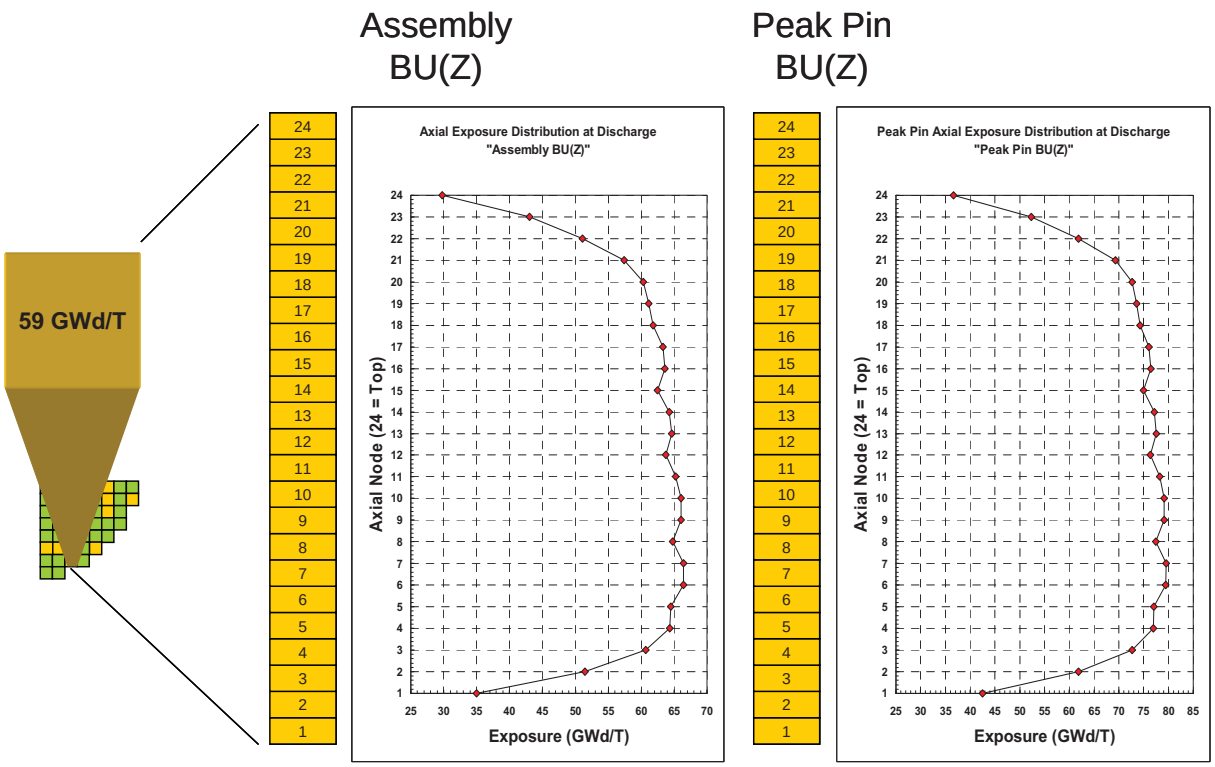

Figure 6: Prediction of burnup for: assembly average, axial nodal (slice), peak exposure pin

From the figure, it can be seen that for increasing level of detail, an increasing value of peak burnup is found. At the assembly-average level, the burnup is expected to be approximately 59 GWd/t. This roughly corresponds to the burnup that a zero-dimensional depletion might arrive at for three cycles, noting that three cycles at 18 GWd/t each gives a total average assembly irradiation of 54 GWd/t. The average burnup of the 16 MOX assemblies discharged every cycle is 58 GWd/t suggesting that the whole-core simulation result gives MOX a higher than average power density. Looking at the axial assembly level exposure distribution suggests that the peak burnup would be 66 GWd/t. This higher value is the added detail of the axial dimension of the nodal simulation. The peak pellet level exposure (i.e., z-nodal or 15.24 cm axial segment) of this assembly is 79 GWd/t. This highest value is the result of added detail of pin power reconstruction based on the nodal simulator results and is 1.46 times higher than what would be assumed if a zero-dimensional depletion was performed for the fuel assembly itself.

3.4 Lattice Code versus Whole-Core Calculations

Given the differences in power peaking that can be observed at the assembly, pin and pellet level, it is of interest to examine the predictive capability of single assembly calculations to identify this peak. The relative error between pin powers for the peak slice in Figure 5, generated by CASMO-5 versus SIMULATE-3, are shown in Figure 7. The relative error is calculated as follows:

$$\varepsilon = \frac{P_{s3} - P_{c5}}{\left(P_{s3} + P_{c5}\right)/2}$$

Notice that the relative error in pin power for the peak pin is only -1%. Therefore, the CASMO-5 code over predicts SIMULATE-3 for this pin by 1%. However, CASMO-5 underpredicted peak power in

the bottom-right corner pin by 20%. This corner pin has only 14 W/cm lower linear power than the peak pin. The large discrepancy between the CASMO-5 and SIMULATE-3 extends down both of the sides of the MOX assembly adjacent to two UO2 assemblies (Figure 8).

The reason for this large relative error is the spectral mismatch between the MOX assembly and the two UO2 assemblies. The thermal flux characteristic of UO2 is greater than that for MOX. Pu-239 and Pu-241 possess a very large fission resonance at approximately 0.3 eV. When the thermal flux leaving the UO2 assemblies enters the MOX pins it is readily absorbed by this resonance leading to a higher fission rate than the assembly average. This condition does not exist on the opposite side facing MOX assemblies because these sides are adjacent to other MOX assemblies. Thus, there is no significant spectral mismatch.

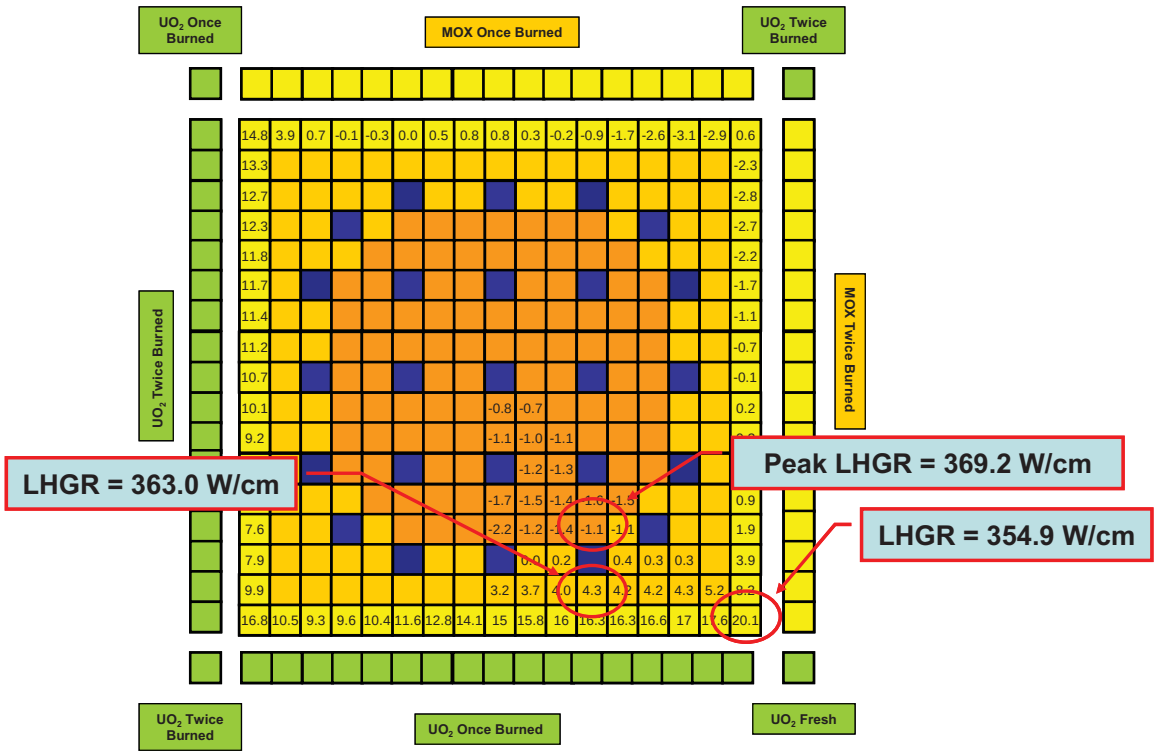

Figure 7: Relative error comparison of peak power for inner, middle and outer enrichment zones of the peak MOX assembly

Though the power peaking along the assembly edge has virtually zero impact on the certainty in CASMO-5 to represent *overall peak* power, it gives very little confidence in the peak power conditions of the outer two enrichment zones. Hence, single assembly calculations can accurately predict peak power conditions if they occur in the inner assembly fuel pins. However, lattice calculations can not accurately predict power conditions for fuel pins lying on the assembly periphery.

In addition, a level of enrichment zoning was adopted to adequately ensure that the peak power occurred in the inner enrichment zone, away from the edge. This arrangement was adopted from European MOX assembly designs and no iteration on this zoning was performed between the assembly and core calculations [6]. However, if for instance the enrichment in the outer zone was selected to be higher, the location of the power peak could likely have occurred on the edge where the relative error is the highest. Optimization of this enrichment zoning cannot be performed in an infinite lattice calculation.

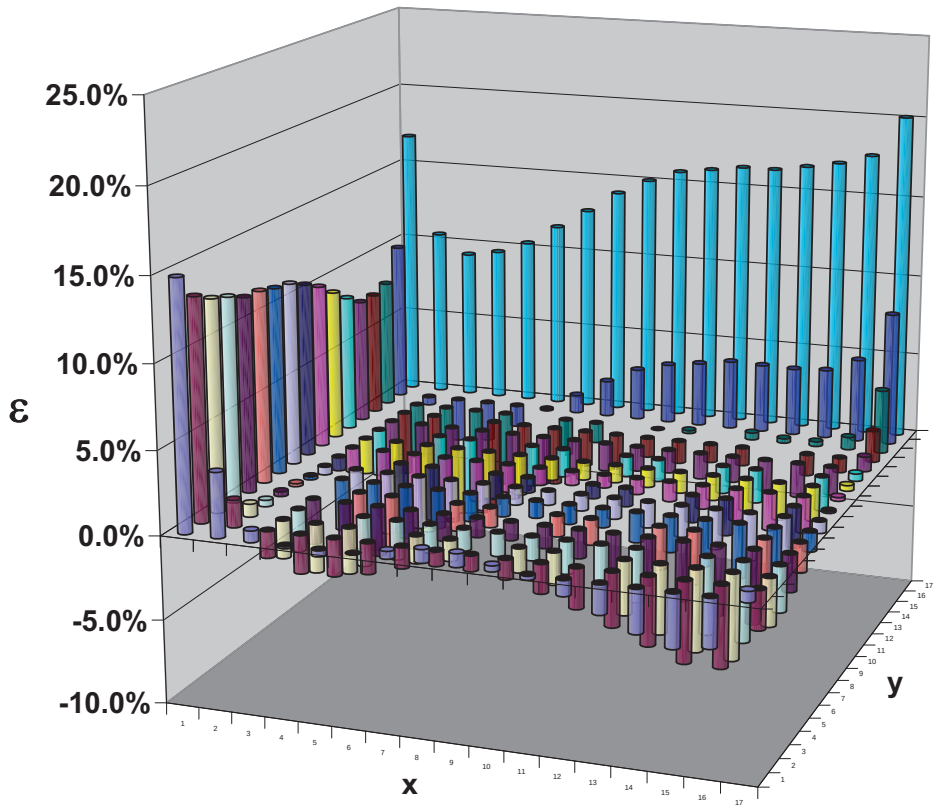

Figure 8: Relative error distribution between CASMO-5 and SIMULATE-3 for the peak MOX assembly

3.5 Isotopic Comparison

To evaluate the 3-D effect on spent fuel isotopics, the batch average burnup for discharged MOX was calculated based on the assembly average discharge burnup values for each assembly generated by SIMULATE-3. This batch average burnup value (58.5 GWd/T) was then used to interpolate isotopic information from the CASMO-5 output. The isotopics of each discharged assembly were then extracted from the SIMULATE-3 output file using the CMS post-processing and spent fuel decay utility, SNF [7] (Figure 9).

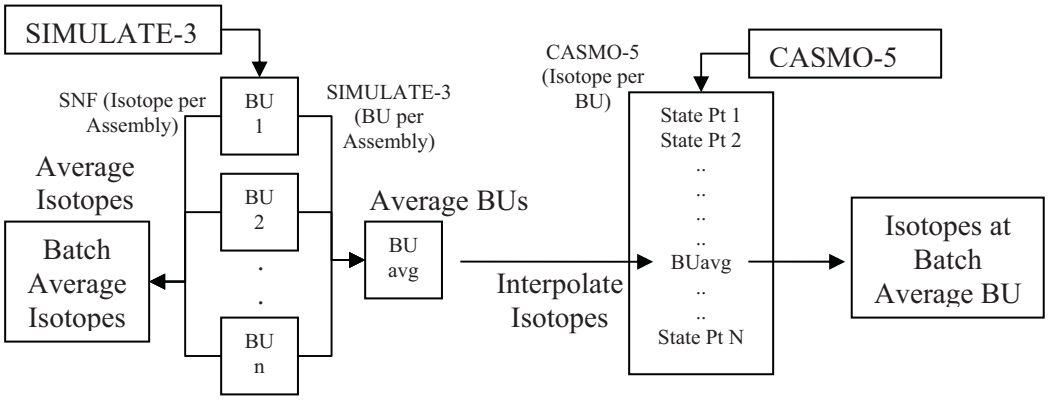

Figure 9: Istotopic comparison methodology

Thus, an equal comparison was made between the single assembly calculation at the average discharged batch burnup and the average isotopic makeup of the batch discharged by the core simulation. Table 2 shows the error between SIMULATE-3/SNF and CASMO-5. The relative error between the 3-D and 2-D calculations for most of the uranium and plutonium isotopes is only a few percent. However, the relative error in calculating the MA concentration at discharge is significantly higher. The reason for this is likely the 3-D effect of a few assemblies experiencing a higher than average exposure to a higher power density than the rest of the batch. MAs are produced from successive neutron captures in major actinides, and are thus accumulated as the result of neutron exposure or burnup. The MOX assembly with the highest concentration of MAs was irradiated for two cycles in peak (i.e., same peak assembly from Section 3.1 & 3.2) or near-peak power positions and then shuffled to the core periphery for the last cycle. This had the effect of building in Pu-241 more rapidly than predicted by CASMO-5 for the first two cycles. In the last cycle, the power in this assembly was less than that predicted by CASMO-5. Therefore, in the last cycle, the rate of Pu-241 creation was less than predicted by CASMO-5. Thus, the Pu-241 decay into Am-241 was greater than predicted by CASMO-5. The combined effect is a greater than average generation of Am-241's parent (first two cycles) and a greater than average allowance for the decay of this parent into Am-241 (last cycle).

Table 2: Isotopic comparison between SIMULATE-3 and CASMO-5 at the discharged MOX batch average burnup of 58.5 GWd/T.

Nuclide	SNF w% @ 58.5 GWd/T	C5 w% @ 58.5 GWd/t	%Error (SNF-C5)/SNF
U-234	4.76E-05	4.75E-05	0.2%
U-235	2.30E-03	2.28E-03	1.1%
U-236	6.19E-04	6.23E-04	-0.6%
U-238	9.97E-01	9.97E-01	0.0%
Np-237	3.80E-03	3.79E-03	0.4%
Pu-238	2.23E-02	2.26E-02	-1.2%
Pu-239	4.03E-01	3.95E-01	1.9%
Pu-240	2.81E-01	2.86E-01	-1.7%
Pu-241	1.59E-01	1.62E-01	-2.0%
Pu-242	7.04E-02	7.10E-02	-0.9%
Am-241	1.97E-02	1.76E-02	10.4%
Am-242m	4.13E-04	4.28E-04	-3.6%
Am-243	2.17E-02	2.18E-02	-0.3%
Cm-242	2.74E-03	3.69E-03	-34.8%
Cm-243	1.75E-04	1.87E-04	-6.7%
Cm-244	1.39E-02	1.38E-02	1.1%
Cm-245	1.93E-03	1.85E-03	4.5%
Cm-246	1.60E-04	1.47E-04	8.4%
Cm-248	3.18E-07	2.61E-07	18.1%
Cf-252	3.79E-10	2.72E-10	28.4%

The concentration of MAs at discharge was calculated to be less than 7% of total TRU for both 3-D and 2-D calculations. Therefore, small changes in MA production due to power history sensitivities can give large relative errors. Nevertheless, much of these errors should diminish with decay time outside the reactor. For example, the error in Am-241 at discharge is 10.4% higher than predicted by CASMO-5. However, the error in its parent, Pu-241, is only -2.0%. As the Pu-241 in the spent fuel batch decays into Am-241, the error associated with the Pu-241 at discharge will transfer into the error of Am-241. Thus, after a few half-lives the error in Am-241 should only be a few percent.

4. Summary

The comparison of fuel and fuel cycle analysis results between 2-D lattice calculations and 3-D full core nodal calculations has revealed a set of advantages and disadvantages which can guide the analyst with regard to when each modeling tool is more appropriate. For the purpose of isotopic generation for fuel cycle analyses, the approach of using a 2-D lattice code (i.e., fuel assembly in infinite lattice) gave reasonable predictions of uranium and plutonium isotope concentrations at the predicted batch average discharge burnup. Somewhat larger relative errors were calculated for the minor actinides. However, these errors were on very small quantities and would diminish with decay time. This representativeness of a single assembly calculation can be explained by the expected core design optimization to ensure that the power and burnup distribution in the fuel is as flat and with little deviation from the design margin as reasonably allowable.

Despite the affinity of a single assembly code to predict the batch average burnup and isotopics, single assembly approximations of local power peaking and local burnup distributions are somewhat lacking. This is especially true when dissimilar assemblies with dissimilar neutron spectra (i.e., UO2 and MOX) are adjacent to one another. In a single assembly calculation, usually an assumption is made, as was done here, that the sides of fuel assembly are perfectly reflective to neutrons. This physically implies that the calculation represents an infinite repeating array in all directions of the exact same assembly at the exact same level of burnup. Also, single assembly calculations are performed at the *2-D* level. This physically implies that the design and irradiation performance of the fuel assembly is constant in the axial direction. Both of these simplifications can be useful for obtaining accurate cross section information to be used in the core simulator, which is often the purpose of a fuel assembly level calculation. However, in reality a fuel assembly design and its in-core performance is highly three dimensional and cannot be fully understood in a 2-D infinite lattice calculation.

The core flux and power distribution dictates the assembly's average power based on its position in the core and its burnup. The axial power distribution as well as the thermal-hydraulic feedback of the moderator density dictates the assembly's axial power profile. The communication of neutron spectra between adjacent UO2 and MOX fuel assemblies influences the power distribution and peaking in the pins along their shared interface. The combination of all three of these influences on power distribution combined with the fuel shuffling path or power history that the assembly takes between its first and last cycles of irradiation dictates the peak local burnup performance.

The 3-D location of the peak MOX fuel assembly in addition to edge effects with neighboring UO2 assemblies caused a 20% error in the prediction of peak power in one of its corner pins by the infinite lattice code. The peak power for this assembly occurred in the fuel assembly interior where there was no edge effect and the error was 1%. However, the proper design of plutonium enrichment zoning and burnable poison placement requires accurate identification and magnitude of peak power pins. The infinite lattice calculation was not capable of predicting the peak power in the assembly's outer enrichment zone along the outer two rows of pins.

Another important consideration in realistic fuel design is the prediction of the peak axial burnup and neutron fluence. The core simulator predicted that the maximum assembly average burnup would be 65 GWd/t. A simple hand calculation based on average core power density and fuel assembly life-time, necessary to perform the lattice calculation gives 54 GWd/t. Selecting an assembly at the median discharge burnup of 59 GWd/t, using the core simulator and pin-power reconstruction gives a peak local (i.e., roughly at the pellet level) burnup of 79 GWd/t. Thus, the effect of local power distributions, thermal-hydraulics, spectral mismatch and power history gives a much higher prediction of peak irradiation conditions than can be estimated at the single assembly infinite lattice level.

5. References

1. J. Rhodes, D. Lee, K. Smith, T. Smed, "CASMO-5/5M User Manual," SSP-08/431 Rev 0, (2007)

2. D. Plannck, A. DiGiovine, J. Umbarger, "Simulate-3 User's Manual," SOA-96/12-Rev 0, (1996)

3. T. Bahadir, J. Umbarger, M. Edenius, "CMS-Link User's Manual," SOA-9704-Rev 2, (1999)

4. K. Rempe, J. Stevens, "XIMAGE BWR: Core Design Environment, User's Guide and Reference Manual," SSP-99/409-Rev 0 BWR, (1999)

5. T. Kozlowski, T. Downar, "PWR MOX/UO2 Core Transient Benchmark," Nuclear Energy Agency: Organization for Economic Co-operation and Development, NEA/NSC/DOC(2006)20, ISBN 92-64-02330-5, NEA No. 6048, (2007)

6. A. DiGiovine, H. Gheorghiu, "Generic CMS PWR Equilibrium Model, Revison 3," SSP-99/408 Rev 0, (1999)

7. G. Anton, J. Cronin, J. Umbarger, "SNF User's Manual," SSP-06/407-Rev 1, (2008)