Monte Carlo Depletion Analysis of BWR Fuel Assembly with Gadolinia Rods using MCS against LAGER Project

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1. Introduction

Accurate prediction of local power distribution and isotopic inventories in light water reactor (LWR) cores is essential for nuclear fuel management, reactivity control, and the evaluation of safety margins. In modern boiling water reactors (BWRs), gadolinia (Gd_2O_3) burnable poisons are widely incorporated into fuel rods to control initial excess reactivity and flatten the power distribution. However, due to the exceptionally large thermal neutron capture cross-sections of odd-mass gadolinium isotopes, severe spatial self-shielding occurs within the gadolinia-bearing fuel pins. This results in steep radial and azimuthal burnout gradients, leading to highly non-uniform local power and burnup profiles.

To properly resolve these localized phenomena, high-fidelity depletion modeling tools capable of fine spatial discretization are required. Traditional deterministic lattice physics codes often rely on spatial homogenization and geometric approximations, which may introduce non-negligible errors when capturing depletion gradients. To address these limitations, the continuous-energy Monte Carlo code MCS [1], developed at the Ulsan National Institute of Science and Technology, provides advanced capabilities for 3D multi-cycle depletion analysis, featuring detailed cell-wise burnup mesh capabilities, on-the-fly Doppler broadening, and multi-physics coupling options.

Validation of such high-fidelity tools requires high-resolution experimental benchmark data. The Laser Ablation of Gadolinium Evolution Radially (LAGER) project, conducted via post-irradiation examination (PIE) at the Studsvik hot cell laboratory, offers an unprecedented experimental database [2]. Utilizing laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS), the LAGER program provides high-resolution 2D isotopic concentration profiles across irradiated BWR fuel assembly samples from the Forsmark 2 reactor.

In this study, Monte Carlo depletion simulations of a 10×10 BWR fuel assembly irradiated in Forsmark 2 were performed using the MCS code. The local radial and azimuthal distributions of key actinides and fission products were validated against the LAGER experimental measurements. This paper presents the numerical modeling methodology, the azimuthal rotational alignment scheme, and the validation results of the MCS depletion framework for gadolinia-loaded fuel assemblies.

2. Methodology and Modeling

2.1 MCS Modeling and Operating Conditions

A 2D Monte Carlo depletion model for the 10×10 BWR fuel assembly was constructed using the MCS code, with geometry and material definitions established based on CASMO-5 [3] benchmark specifications. The assembly configuration features fuel rods with various enrichments, including gadolinia-loaded poison pins with an initial enrichment of 3.65 wt.% ^{235}U and 4.0 wt.% Gd_2O_3. The fuel operated over an 11-month cycle, achieving an assembly-average burnup of approximately 11 MWd/kgU. As illustrated in Fig. 1, most 2D structural components—including fuel pins, the assembly channel box, inner water boxes, wide/narrow water gaps—were explicitly represented, while the spacer grids were smeared into the coolant.

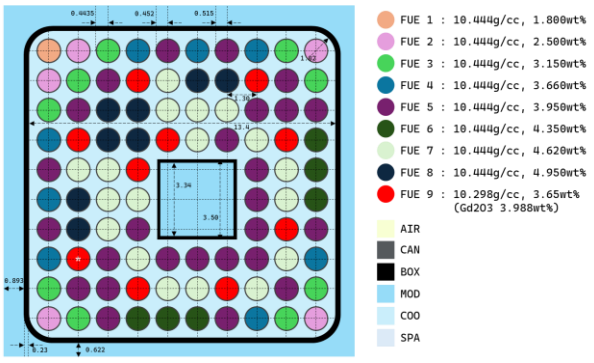


Fig. 1. Configuration of 10×10 BWR Assembly.

To capture the distinct axial void and moderation environments along the active fuel height, individual 2D slice depletion models were generated for four axial nodes corresponding to the PIE sample locations: LA1 in the lower non-boiling region (0% coolant void), LA2 at the mid-elevation (60% void), and LA3 through LA4

in the upper high-void region (80% void). Fig. 1 presents the 2D cross-sectional pin layouts for the axial slice at the LA1 location.

Node-specific operating parameters applied to each 2D slice model were derived from the irradiation history shown in Fig. 2. For each 2D calculation, operating parameters—including power density, fuel temperature, coolant temperature, and coolant void fraction—were assigned as explicit depletion conditions. Since the coolant void fraction is not used directly in Monte Carlo calculations, it was incorporated into the coolant density.

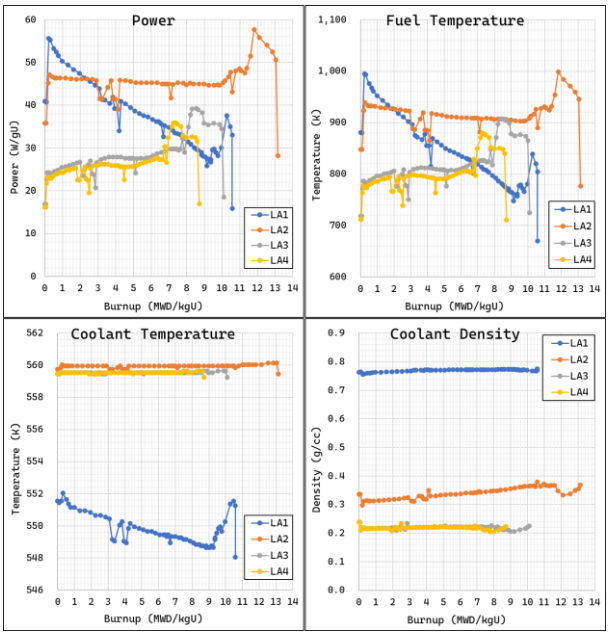


Fig. 2. Operation histories of BWR assemblies including LA1 to LA4 samples.

2.2 Spatial Discretization and Depletion Setup

To resolve the steep thermal neutron flux gradients and severe spatial self-shielding within the gadolinia pins, fine cell-wise depletion meshes were implemented across the 2D assembly domain. The standard UO_2 fuel pins and general gadolinia-bearing pins were divided into 10 and 20 concentric radial rings, respectively. The target gadolinia pins selected for direct comparison with LAGER experimental data were further refined into 22 to 27 radial rings and 8 azimuthal sectors, enabling high-resolution 2D tracking of non-uniform burnout.

Nuclear cross-sections were evaluated using the continuous-energy ENDF/B-VII.1 library. Thermal Doppler broadening was treated on-the-fly using the windowed multipole technology [4], as implemented via the OpenW framework to accurately account for local temperature gradients without requiring discrete temperature-interpolated ACE tables. Monte Carlo depletion calculations for each 2D assembly slice were executed with 100 million total neutron histories (10 inactive and 100 active cycles with 1 million histories per cycle), maintaining the standard deviation of the eigenvalue within 7 pcm.

3. Experimental Data and Numerical Result

3.1 Experimental Data Processing and Alignment Scheme

The LAGER experimental database from Studsvik PIE measurements includes high-resolution LA-ICP-MS data consisting of approximately 1.1 million data points across 98 radial zones and up to 1,126 azimuthal angles. The measurements cover 24 distinct nuclides, including major actinides ($^{234/235}$U), fission products (^{88}Sr, $^{135/137}$Ba, ^{138}La, $^{140/142}$Ce, ^{141}Pr, $^{143–148}$Nd, $^{147–152}$Sm), and burnable poison isotopes ($^{154–160}$Gd).

To compare the raw experimental measurements directly with MCS cell-wise tally outputs, data processing was executed in two steps. First, raw counts per second (CPS) were background-subtracted and converted to mass fractions normalized per unit mass of uranium (mg/gU). The fine radial and azimuthal coordinates were then averaged into an evaluation grid consisting of 22–27 radial rings and 8 azimuthal sectors, directly matching the MCS depletion tally mesh.

Because the absolute physical orientation of the hot-cell sample was not constrained during laser ablation scanning, an azimuthal rotational alignment scheme was applied. The experimental sector mesh was rotated using the peak ^{155}Gd depletion location as a reference marker to align with the north direction of the MCS assembly model.

3.2 Comparison of Isotopic Distributions

The reconstructed 2D radial and azimuthal isotopic concentration maps calculated by MCS were evaluated against the LAGER experimental distributions across different axial nodes (LA1 to LA4).

Fig. 3 shows the distribution of ^{235}U for LA1 to LA4 samples. As the primary fissile isotope, ^{235}U serves as a direct indicator of thermal neutron absorption and fuel depletion history. In terms of integrated total mass, the MCS calculations and experimental measurements demonstrate reasonable agreement. However, distinct differences appear in the spatial profile characteristics: while MCS captures pronounced spatial effects, such as steep radial depletion near the pellet periphery (rim effect) and azimuthal asymmetry induced by the neighboring water box, the experimental profile displays significantly muted spatial variation. Furthermore, the data integrity and signal quality of the ^{235}U mass appear to be affected by noise or normalization uncertainties.

Fig. 4 shows the distribution of ^{144}Nd for LA1 to LA4 samples. Because ^{144}Nd is a stable fission product with a low neutron capture cross-section and minimal radial migration, it acts as an ideal metric for accumulated

burnup and integrated local fission density. Similar to ^{235}U, the total inventory of ^{144}Nd calculated by MCS matches the experimental value well. However, while MCS predicts clear spatial gradients reflecting higher fission density near the outer rim, the experimental distribution shows a much flatter spatial variation. Unlike ^{235}U, the ^{144}Nd experimental data exhibits greater physical consistency, making it a more dependable benchmark for total burnup evaluation.

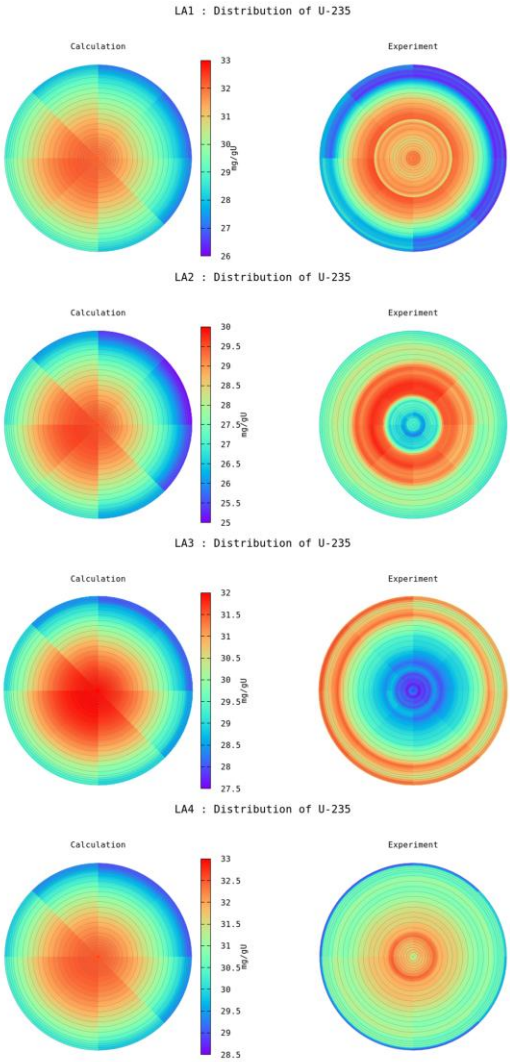


Fig. 3. Distribution of ^{235}U isotope for LA1 to LA4 samples.

Fig. 5 shows the distribution of ^{155}Gd for LA1 to LA4 samples. As a major burnable poison isotope with an exceptionally large thermal capture cross-section, ^{155}Gd is critical for evaluating reactivity control and steep flux depression within poison pins. The measured ^{155}Gd profiles do not exhibit the sharp spatial burnout gradients predicted by MCS. Furthermore, the total residual inventory comparison reveals a clear dependence on local burnup stages. In the high-burnup nodes (LA1 and LA2), a discrepancy in total inventory exists, with MCS calculations showing significantly greater burnout than the measurements. Conversely, in the relatively lower burnup nodes (LA3 and LA4), the calculated ^{155}Gd inventory agrees reasonably with the experimental data, although the fine local spatial variations predicted by MCS remain unobserved in the measured profiles.

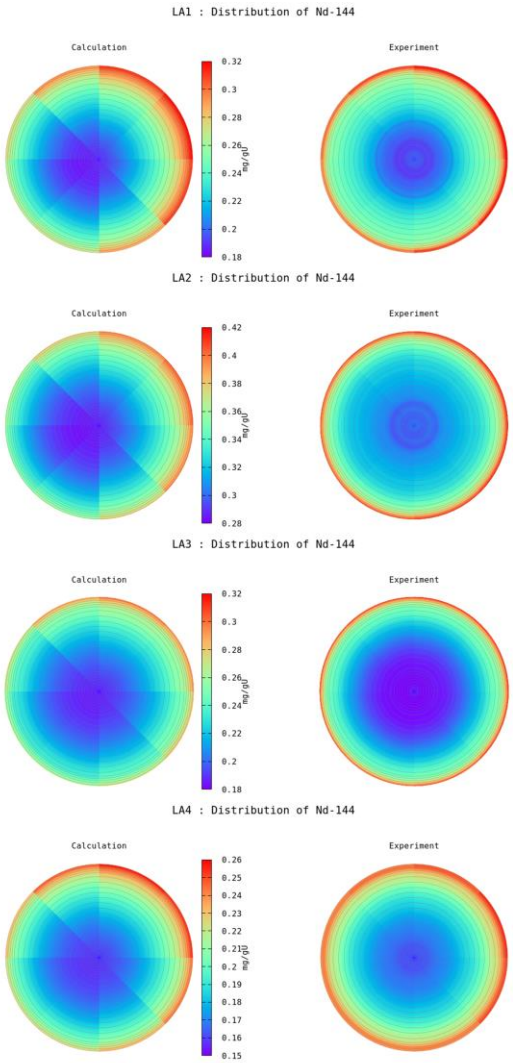


Fig. 4. Distribution of ^{144}Nd isotope for LA1 to LA4 samples.

3.3 Discussion on Measurement Uncertainties and Modeling Assumptions

The spatial and quantitative discrepancies observed between the MCS calculations and LAGER experimental data stem from a combination of measurement processing limitations and numerical modeling assumptions. Primary experimental uncertainties arise from the raw CPS signal processing, where background noise subtraction and mass conversion factors introduce potential systematic bias. These uncertainties are particularly pronounced in regions with low isotopic concentration or steep depletion gradients.

On the numerical simulation side, a fundamental limitation stems from the application of a 2D single-assembly model. The 2D single-assembly calculation inherently neglects 3D axial neutron transport, axial flux tilting, and spectral interference from surrounding assemblies with differing burnups and void conditions. Furthermore, critical spectrum correction was not accounted for in this MCS calculation. Because local depletion chains are highly sensitive to the energy spectrum, uncorrected 2D single-assembly spectra can introduce systematic bias in predicted reaction rates. Extending the calculation framework to multi-assembly coupled models, alongside incorporating thermal expansion and critical spectrum adjustments, will be essential to resolve these remaining physics discrepancies.

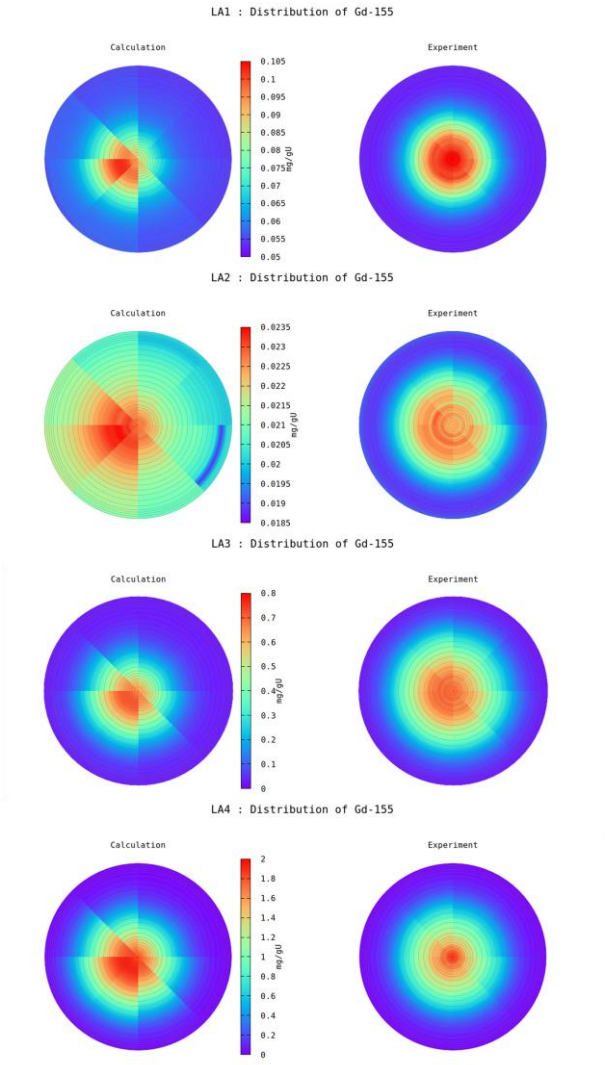


Fig. 5. Distribution of ^{155}Gd isotope for LA1 to LA4 samples.

4. Conclusions and Future Work

Monte Carlo depletion calculations for a BWR assembly were performed using the MCS code and validated against LAGER experimental data. By applying node-specific operating conditions and fine spatial discretization, combined with a ^{155}Gd-based rotational alignment scheme, MCS demonstrated robust capabilities in predicting complex 2D depletion environments and non-uniform isotopic distributions within gadolinia-bearing pins.

Despite the observed spatial profile deviations and differences in residual ^{155}Gd inventories at high burnup, the LAGER benchmark carries profound physical significance. Since gadolinia burnable poisons typically burn out completely early in commercial reactor operating cycles to control initial excess reactivity, experimental data evaluating the residual gadolinium distribution in irradiated fuel pins are globally scarce. The LAGER dataset uniquely captures this intermediate-burnup state, providing an unprecedented physical benchmark for the validation of high-fidelity depletion codes.

Future work will expand the calculation framework beyond the 2D single-assembly model to 3D multi-assembly or core-level transport simulations. This expansion will enable the explicit treatment of inter-assembly spectral interference and critical spectrum effects. Combined with thermal expansion feedback and improved experimental signal processing, these enhancements will establish a comprehensive numerical framework for advanced LWR core design and safety analysis.

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