Computing Benchmark of Gadolinium-bearing Fuel Pins’ Depletion Skin Effect based on Deterministic and Monte Carlo Methods

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Abstract: Nuclear reactor core depletion and thermal-hydraulics coupling have long been calculation-intensive tasks challenging both nuclear industry development and academic research projects regarding computing budgets of memory and time. Albeit future evolution in smart computation hardware with artificial intelligence and quantum computing facilities embedded could continuously push the predictive modelling limit, the fundamental reactor physics model will still tip the balance in underpinning the prediction accuracy, as evidenced by a benchmark of two computational models in this work for characterising the depletion of highly self-shielded Gadolinium burnable poison-bearing fuel pins in assessing the British first European Pressurised Reactor’s start-up core performance. Specifically, a subgroup multi-annular-ring method is verified to efficiently represent the self-shielded skin effect, which addresses the deficiencies of classic equivalence models. The subgroup method is subsequently applied into a deterministic neutron transport code and a Monte Carlo stochastic code, respectively, for another benchmark. Resulting discrepancies in power peaking factors for the same assembly are less than 2% for the first fuel cycle, the agreement of which well demonstrates the validity of the proposed subgroup model. At the forefront of efforts to quantitatively understand the burnable poisons’ behaviour precisely for fuel optimisation (e.g., mitigating power peaking), this work could also be advantageously used for training purposes in boosting safety philosophy and public engagement in the roadmap for decarbonisation.

Keywords: Burnable poison depletion modelling; Computational reactor physics; Energy self-shielding; Gadolinium; Neutronics benchmark; Spatial self-shielding

1. Introduction

Continuously stable energy output capacity, zero-carbon emission, high energy density, and cost competitive advantages are strong incentives to support nuclear energy development as one of the main carbon-neutral solutions towards the British net-zero ambition [1]. Leveraging the economies of scale [2] in reducing the energy production costs, the philosophy of “a larger sized core is better” as agreed with the UK government’s vision has been implemented by two European Pressurised Reactors (EPR) [3] with gigantically volumetric cores being built up at the Hinkley Point C (HPC) nuclear power plant (NPP). Despite the costly delay [4] effects due to Brexit [5] and the COVID-19 pandemic [6, 7], the two units of reactors are projected to start commissioning...
(generating electricity) from around 2026 [8], supplying 2×1650 MWe for six million homes across the UK up to 2061 (commissioning limit). More importantly, the technology is capable of reducing carbon emissions drastically by 9 million tonnes per annum, not to mention the improved waste management claim [9] in terms of filtering gaseous radioactive waste and minimising the volume of liquid radioactive waste.

Benchmarks for neutronic analysis of the big nuclear reactor core is of practical importance, albeit the core design has previously been certified by the Office for Nuclear Regulation (ONR) [10] regarding safety, security, and environmental impact. There remain tremendous optimisation scopes on the initial fuel loading pattern, including Gadolinium (Gd) burnable poison pins arrangement in designated fresh assemblies to reduce power peaking [11, 12] for avoiding premature fuel failures at high burnup. Mocking up a realistic reference computation model for ongoing innovation has numerous impacts, e.g., facilitating intelligent decision making for regulatory authorities [13], boosting fuel economy [14] whilst reducing costs due to maintenance downtime [15].

Computing thermal flux, fission reaction rates, and hence predicting power distributions accurately are one of the foremost objectives of modelling a nuclear reactor core. Modern neutronics consist of two typical calculation steps, beginning from two-dimensional (2D) lattice-transport calculation [16, 17] to three-dimensional (3D) diffusion core computation [18]. Key procedures encompass homogenisation with preserved reaction rates, isotopic changes tracking with burnup (depletion), operation conditions parameterisation in branches, and multi-dimensional table interpolations [19], in which spatial homogenisation and group collapsing significantly mitigate the computational burden of heterogeneous components [20]. Relying on the preservation of reaction rates and eigenvalues in heterogeneous problems, homogenisation represents the realistic heterogeneity as averaged cross sections equivalent to the actual heterogeneous reactor with satisfactory accuracy. An intuitive treatment is adopting flux-volume weighting of cross sections, as detailed in [16, 20] in assembly homogenisation techniques, notably the classic equivalence theory [21, 22] as well as the subsequent introduction of discontinuity factors in forming a more generalised equivalence theory [23].

As an extension of the equivalence model, subgroup annular-ring treatment allows cross sections’ geometric variation in different radial rings to be explicitly tracked with sufficiently high resolution for representing the reactor physics precisely. Based on this philosophy, state-of-the-art computational codes (both off-the-shelf packages and application-specific custom code sequences) have advanced continuously with improved predicting accuracy, increased functionality, reduced computational burden and cost. Among such coupled calculation suites, this work employs two types of 2D lattice codes, i.e., WIMS (Winfrith Improved Multigroup Scheme [24], deterministic in nature), and Serpent (developed by VTT Technical Research Centre of Finland [25], stochastic in nature) for modelling the Gadolinium-bearing fuel pins of the British EPR startup core (initial fuel loading cycle). These versatile codes packages both feature general-purpose open structures and interfaces with other reactor physics or thermal-hydraulics software, hence highly suitable for benchmark study.

The present work is an extended version of the “Best Paper Award” winning paper [26] disseminated at the Third IEEE International Conference on Computing, Electronics and Communications Engineering (IEEE ICCECE 2020), entitled “Multi-ring Subgroup Method in Characterising Highly Self-shielded Gadolinium Burnable Poison Pins for the UK EPR Nuclear Fuel Assembly”. In addition to conducting a more critical survey of literature, two particular benchmarking problems of fuel assembly calculations are investigated in more depth as outlined in the flowchart at Figure 1 below. Firstly, the traditional equivalence theory-based one-zone approach is compared with the proposed sub-group multi-annular-zone method based on the same deterministic code (i.e., WIMS). Secondly, the sub-group method is further benchmarked based on two codes of diverse computing mechanism (i.e., deterministic versus stochastic) for the EPR full assembly verification.

The structure of the paper is divided into five sections. Following a brief introduction of the research scope in the current Section 1, the EPR first-core assembly geometry is specified in Section
2. The comparative study into Gadolinium pin models based on proposed subgroup method versus the classic equivalence approach is presented in Section 3. Based on the optimal predictive modelling method, the assembly power distribution results are obtained in Section 4 based on both deterministic and probabilistic calculations for statistic benchmarking. Section 5 concludes the research with an outlook of potential impact for nuclear industry and public engagement.

1. methodology benchmarking for Gadolinium-bearing fuel pins

![Diagram: Classic equivalence theory vs. subgroup multi-annular-ring method]

2. codes benchmarking to verify the methodology

Deterministic based vs. Monte Carlo based

Agreement?

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2. Computational Description of EPR Initial-loading Assemblies

Table 1 summarises the fuel assembly information of the gigantic EPR fresh core, including 241 fuel assemblies in 5 enrichment zones with different numbers of Gadolinium burnable poison pins (8wt%) positioning adhering to the design specification [27]. Detailed fuel zoning geometry of the whole core can be referred to the core design document [28] as well as the radial core layout shown in our recently published work in [29]. Each 17x17 square lattice consists of 264 fuel rods with M5 advanced cladding, and 25 guide thimbles for in-core instrumentation. With a 0.8 millimeter water gap separating adjacent assemblies, Figure 2 presents an octant radial description of an EPR assembly to be modelled based on the aforementioned two methods (classic equivalence theory versus proposed subgroup approach). Note that the advanced M5 cladding density is smeared over the gas that accommodates the fuel expansion and cladding creep with burnup, and spacer grids are not modelled (outside the scope). Normal operating conditions of the reactor (e.g., cold zero power, hot zero power, hot full power) are modelled, while transient behaviours under various accident conditions are not considered in the current benchmark.

![Diagram: Benchmark problems specification in this research.]

**Figure 1.** Benchmark problems specification in this research.

**Table 1.** Zone-wise initial fuel loading scheme of the UK EPR first core.

| Zone | Region-wise Enrichment | Number of Assembly | Gadolinium rods per Assembly | Uranium-235 in Gadolinium Rods |
|------|------------------------|--------------------|-----------------------------|-------------------------------|
| 1    | 4.2 wt%                | 72                 | 16                          | 2.2 wt%                       |
| 2    | 3.2 wt%                | 48                 | 20                          | 1.9 wt%                       |
| 3    | 3.2 wt%                | 24                 | 16                          | 1.9 wt%                       |
| 4    | 2.1 wt%                | 80                 | 8                           | 1.2 wt%                       |
| 5    | 2.1 wt%                | 17                 | 0                           | -                             |

As a 2D lattice code tailored for light-water reactor (LWR) geometries on various meshes, WIMS (Winfrith Improved Multi-group Scheme) produces burnup dependent fuel assembly homogenised cross sections and pin power peaking factors with reaction rates conservation. A fine 172 energy groups library based on JEF-2.2 tabulation of nuclear data [30] is collapsed into 6 groups...
to speed up computations. WIMS solves the transport equations in multiple stages, as illustrated in Figure 3.

![Gadolinium-bearing pins](image1)

**Figure 2.** Octant symmetry radial description of an EPR 4.2wt% fuel assembly with 16 Gadolinium pins (two depletion models benchmark based on diverse computation methods).

![Flowchart](image2)

**Figure 3.** Flowchart of computation modules developed in WIMS deterministic lattice transport code.

The default treatment for resonance capture is following the classic equivalence model procedure, which provides pin-averaged cross sections for energy groups in the resonance region ranging from 4 eV to 183 keV. While this method is applicable for simple geometries, it fails to reliably predict the spatial distribution of cross sections for more complex geometries such as burning a poison pin with strongly self-shielding skin effects. This motivates the development of a spatial discretisation-based subgroup code model in this work, in which the resonance treatment is extended to a wider range of geometries such as the multiple radial zones for Gadolinium-bearing pins. The group boundaries are specified in Table 2. Note that an 11-group energy condensation is employed in place of the traditional 6-group structure for the sake of an enhanced precision.

Regarding burnup analysis, cross sections parameterisation as a function of burnup is conducted for 18 months cycle in this work. Each assembly is irradiated up to 80 GWd/t to account
for localised axial peaking and correspondingly higher burnup nodes in subsequent whole core computation (using PANTHER or Serpent). Since the Xenon transient happens relatively fast, a small burnup step at the beginning is selected, i.e., 0.1 GWd/tU to settle Xenon to equilibrium as depicted in Figure 4 below, followed by slightly longer steps to enable other fission products to reach equilibrium.

### Table 2. Energy discretisation/condensation (11 groups) in WIMS deterministic code.

| Group Number | Upper Energy (MeV) | Group Number | Upper Energy (MeV) |
|--------------|-------------------|--------------|-------------------|
| 1            | 19.6403 E+00      | 7            | 1.1500 E-06       |
| 2            | 1.3534 E+00       | 8            | 972.0000 E-09     |
| 3            | 183.1564 E-03     | 9            | 400.0000 E-09     |
| 4            | 9.1188 E-03       | 10           | 220.0000 E-09     |
| 5            | 571.7032 E-06     | 11           | 80.0000 E-09      |
| 6            | 4.0000 E-06       | -            | -                 |

![Figure 4](image-url)  
**Figure 4.** Initial Xenon transient simulated at beginning of cycle 1 (4.2wt% assembly with 16 Gadolinium pins).

### 3. Skin Effect Benchmark of Self-shielding Gadolinium-bearing Fuel Pins

Two kinds of self-shielding effects are of particular research interest. On one hand, energy self-shielding mitigates the neutron capture in the resonance of fertile material. On the other hand, some of the thermal neutrons entering the fuel from the moderator are absorbed near the surface of the fuel (spatial self-shielding skin effect), i.e., not surviving to affect the interior thermal flux. From isotopic analysis, Gadolinium-157 and Gadolinium-155 are dominating the thermal neutron absorptions, with absorption cross sections equalling 254,000 barns and 61,000 barns [31], respectively. Serpent Monte Carlo code is employed to model the isotopic depletion, with results plotted in Figure 5 below.

![Figure 5](image-url)  
**Figure 5.** Atomic density of Gadolinium versus burnup for 2.1wt% assembly with 8 Gadolinium pins.

As illustrated above for the simulated atomic densities of Gadolinium with burnup, Gadolinium-155 and 157 both burn out from 10 GWd/tU. It is worth noting that Gadolinium-155
transmutes to Gadolinium-156 by capturing a neutron. Although exhibiting small capture cross sections, Gadolinium-156 can constantly feed Gadolinium-157 (extremely large absorption cross sections), indicating a residual poison penalty as Gadolinium cannot completely burns down. The outer portion of the fuel thus shields the interior. To characterise both self-shielding effects in Gadolinium-admixed fuel pins, the pin is sub-divided into annular segments of an equal area as already shown in Figures 1 and 2. The density change of Gadolinium-157 and Gadolinium-155 versus the assembly burnup for each radial ring is quantified. Note that 10 rings are selected as a preliminary proof-of-concept. Accordingly, characterising the Gadolinium burning in 10 radial zones within a pin is investigated using the aforementioned deterministic lattice code WIMS. By comparison, the modelling results in Figure 6 below illustrate the inaccuracy of classic equivalence model by default in WIMS. It is unrealistic to have such a nearly flat distribution of the Plutonium 239 density in different radial zones with burnup for our self-shielding fuel pins. The problem of the conventional equivalence theory-based approach is the pin-averaged cross sections being tracked (each radial zone treated with identical cross sections in 172 energy groups). Such a single-zone treatment arguably collapses all the radial zones down, cancelling out the desirable multi-ring computational effort for characterising the skin effect.

Figure 6. Computing results of Plutonium 239 density distribution based on classic equivalence-based method.

To address the problems, the proposed subgroup approach is developed in WIMS code for studying into the EPR fuel assembly. Simulated atomic density results of Gadolinium-157 versus the pin radial distance at different burnup levels are shown in Figure 7. Neutron absorption at the beginning of life (BOL) occurs largely at the fuel outermost surface. Gadolinium admixed in a pin depletes from the outside inwards, exhibiting a strong spatial self-shielding. Accordingly, the inner zones exhibit a slower burning down of Gadolinium. More pronounced flux depression occurs in the Gadolinium-bearing pin at BOL (by comparing the two curves in Figure 8). The characteristics of reaction rates in multiple radial zones are quantified in Figure 9 for BOC.

Figure 7. Proposed subgroup method based computing results of Gadolinium-157 atomic density variation in different annular zones of an EPR 3.2wt% fuel pin at different burnup stages.
Figure 8. Proposed subgroup method based BOL computing results for an EPR 3.2 wt% fuel pin with 8wt% Gadolinium (flux dip) vs. pin with no Gadolinium.

Figure 9. Proposed subgroup method based computing results of reaction rates distributions in EPR 3.2wt% fuel pins with and without Gadolinium. In particular, we demonstrate that the capture reaction rate distribution in the Gadolinium-admixed fuel pin exhibit the strong effect of spatial self-shielding, with the absorption rate at BOC picking up near the pin surface. We also observe that self-shielding is much less noticeable in pins without admixing Gadolinium, as evidenced by a less dramatic peaking of the capture rates towards the surface. Instead, the non-Gadolinium pins report much higher fission rates, giving rise to higher burnup in these pins. The importance of developing multi-radial-rings for burning Gadolinium pins is further quantified in Figure 10 with a comparative investigation.

Figure 10. Multiplication factor benchmark results for an EPR 3.2% assembly with 20 Gadolinium pins based on 1-zone treatment (classic equivalence method) vs. 10-zone treatment (proposed subgroup method).
Burning the Gadolinium-bearing fuel pin in one zone (equivalence theory) assumes a uniformly distributed Gadolinium, which overestimates the initial poisoning effect, as illustrated in the incorrect faster rate of Gadolinium burning out with a higher reactivity peak. In reality, at the beginning only the outermost Gadolinium acts as a black absorber for the incoming thermal neutrons. The incoming neutrons can only see the poison near the surface, irrespective of the Gadolinium density inside the pin. The depletion of Gadolinium-157 and Gadolinium-155 gradually reduces the spatial self-shielding, as shown in Figure 12 with a flattened flux distribution with burnup from beginning of cycle (BOC), to middle of cycle (MOC), and towards end of cycle (EOC). With the subgroup approach, the Plutonium-239 density in different radial zones with burnup is accurately demonstrated in Figure 12. As distinct from the problematic equivalence-based results in Figure 6, the proposed subgroup-based results in Fig. 11 report reasonable results for Plutonium and higher isotopes building up in the outermost zone where most of the resonance absorption in Uranium-238 happens. The increase in burdensome computation due to sub-dividing zones for ring-based depletion analysis is worth investigating in future optimisation research.

![WIMS Calculation Result of Pu-239 Density Distribution with Time](image)

**Figure 11.** Computing results of Plutonium 239 density distribution based on proposed subgroup method.

4. Benchmarking Assembly Calculations using Two Codes

Fuel assembly calculation results of the pin-wise radial power distribution are reported based on the precise subgroup computation of the Gadolinium-bearing pins. Here we illustrate the results for a 4.2wt% assembly with 16 Gadolinium pins in Figure 12 for both BOC and EOC, both under hot full power (HFP) and equilibrium Xenon conditions. Out of the concern for the reactor core’s thermal limit, the peak-to-average power density of the “hot” channel is calculated in WIMS (located in red circles). Poison pins (located in grey circles) exhibit low power at BOC, with the lattice power peaking factor decreasing with burnup as Gadolinium starts burning out from MOC. The blue and green circles represent locations for fuel rods without Gadolinium, and control rod guide thimbles, respectively. As reported in Figure 12, The resulting drop in thermal neutron absorption gives rise to higher power in these Gadolinium pins at EOC. For the second-round benchmark, the relative differences between WIMS and Serpent codes in power peaking factors are quantified in Figure 13 for BOC and EOC, respectively.

As compared with WIMS, the Serpent Monte Carlo code is free of discretisation in energy, free from numerical approximations, and with variance reduction techniques [29] applied. Examining the root mean square (RMS) and maximum (max.) discrepancies, WIMS and Serpent agree reasonably well, in particular for the purpose of predicting the “hot” rod location. The relative differences in power peaking factors are below 2% (based on RMS values) for both BOC and EOC, though the discrepancy increases slightly in the vicinity of Gadolinium-admixed rods and guide tubes. To improve the prediction accuracy further, the number of annular rings subdivision (currently 10 zones) merits justification by a sensitivity analysis supported by numerical simulations. Finite difference and source iteration [17] could be attempted. Interestingly, methodological implications from the skin effect study [32–35] in microwave [36, 37] and
millimetre-wave [38–43] electronics are arguably transferrable to the absorption skin effect here for Gadolinium-bearing rods. For instance, particular attention can be put on the meshing size optimisations in search for the minimum errors in neutron flux distributions with the minimum convergence time.

**Figure 12.** Computing results of a quarter assembly pin-wise radial power distribution using WIMS (for EPR 4.2wt% assembly with 16 Gadolinium pins).

**Figure 13.** Computing results benchmark (relative difference) for Serpent vs. WIMS in predicting pin-wise assembly power distributions (same quarter of assembly as Figure 12).

### 5. Conclusion

As a computational optimisation effort for light water reactor physics methods development, this work extends beyond the conference paper disseminated in IEEE iCCECE 2020 [26] by dual benchmarks to validate the proposed subgroup multi-radial-zone method in reliably predicting the fuel-assembly level reactor physics of the British first EPR reactor core at the first fuel cycle. For the first benchmark, deterministic lattice transport code WIMS is used for pin-cell level comparison research against the conventional equivalence theory based one-zone approach that is found to fail in characterising the realistic self-shielding behavior of Gadolinium poison pins. In response to the computational hurdle, the proposed subgroup multi-annular-ring approach well addresses this based on the layer-by-layer burning logic for the skin effect of interest. Based upon this, assembly-
level pin-wise power distributions are computed with burnup, then benchmarked statistically with Serpent, a state-of-the-art Monte Carlo code. The second benchmark results exhibit statistically good agreement, which verifies the subgroup model for the targeted fuel assembly calculations. Potentially, the demonstrated subgroup multi-region burning strategy could benefit the predictive modelling of other existing Generation III+ and future Generation IV reactor cores particularly embedded with self-shielded burnable poison rods or control rods. The precise model would advantageously inform the core performance optimisation targeting the balance between nuclear fuel economy and power peaking management, as well as guide the experimental integration of thermal-hydraulic facilities [44, 45] and sensor instrumentations [46–48] targeting the Defence in Depth [49] in nuclear energy safety.

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