*energies*

MDPI

*Article*

# Developing a Reactivity-Equivalent Physical Transformation to Simulate an Axially Heterogeneous Boiling Water Reactor

**Robert Mossop [1,*], Bruno Merk [1], Maulik Patel [1], Tetsushi Hino [2] and Aiden Peakman [1,3]**

[1] School of Engineering, University of Liverpool, Liverpool L69 3BX, UK
[2] Hitachi, Ltd., 7-1-1, Omika-cho, Hitachi-shi 319-1292, Ibaraki-ken, Japan
[3] National Nuclear Laboratory, Chadwick House, Warrington WA3 6AE, UK
* Correspondence: r.mossop@liverpool.ac.uk

**Abstract:** Hitachi is advancing their designs for a conceptual reactor called the resource-renewable boiling water reactor (RBWR), a concept reactor similar to the advanced boiling water reactor with a harder neutron spectrum. This design aims to minimise construction costs and waste production as well as to utilise separated plutonium and minor actinide fuel. However, the axial heterogeneity of the design poses calculation difficulties. The aim of this work is to use a known method, reactivity-equivalent physical transformation (RPT), for calculating fuel with double heterogeneity and apply it to a BWR-type fuel pin. This could reduce the calculation time needed for optimisation of the design of the RBWR. The objective of the study is to use SCALE 6.2 to produce an equivalent axial pin model by comparison with the burnup and neutron spectra of a radial model of the fuel. This model can then be used for 2D burnup calculations, and in future work will be used for the generation of two-group and multigroup cross-sections for further deterministic calculations as part of a two-step approach for analysis of the RBWR. The RPT method has been extensively tested on spherical fuel, and SCALE is a standard industry code. The initial radial model is a hexagonal assembly with 20% enriched $UO_2$ fuel in a zircaloy cladding, surrounded by light water moderator. The derived axial model has a water density distribution taken from Hitachi's RBWR designs. Criticality over 70 GWd/tU burnup is estimated using the model. The application of the RPT to the BWR pin was shown to be possible, but to have limitations with the introduction of additional radial complexity. For a single pin, excellent agreement between the radial and axial models could be found across a range of water densities, but in the case of an assembly level calculation distinct equivalence models were required for each water density. In addition, the produced RPT model is validated using SCALE's 3D Monte Carlo module, KENO.

**Keywords:** waste burner; axial heterogeneity; deterministic; RBWR



**Citation:** Mossop, R.; Merk, B.; Patel, M.; Hino, T.; Peakman, A. Developing a Reactivity-Equivalent Physical Transformation to Simulate an Axially Heterogeneous Boiling Water Reactor. *Energies* **2023**, *16*, 3359. https://doi.org/10.3390/en16083359

Academic Editor: Roman Vadimovich Davydov

Received: 23 February 2023
Revised: 1 April 2023
Accepted: 4 April 2023
Published: 11 April 2023



## 1. Introduction

The Generation IV reactor program seeks to improve several aspects of nuclear reactors, including safety, cost, and efficiency [1]. Improving sustainability also stands as one of the key goals for the successful large-scale deployment of future reactors. Generating energy sustainably and promoting long-term availability of nuclear fuel are extremely important in any scenario where the coverage of nuclear power is significantly expanded, and in response to questions about geological disposal and the cost of permanent storage of spent fuel, minimising long-term nuclear waste and reducing the stewardship burden are at the forefront of the conversation around civil nuclear power [2].

Hitachi's resource-renewable boiling water reactor (RBWR) is 'designed to improve the use of resources and reduce the load imposed on the environment by spent fuel' [3], while the concept is still based on a classical BWR plant design, which should reduce challenges with the implementation of a new technology by relying on several mature technologies from existing commercial BWR systems. By hardening the neutron spectrum

compared to a conventional BWR, the RBWR can reuse transuranic elements as fuel [4,5]. A report by Hitachi to the ICAPP 2019 [6] suggests that due to a discrepancy in results of both Monte Carlo and deterministic calculations performed on the RBWR core by the JAEA, several US universities, and Hitachi, a 'more sophisticated' understanding and an improved level of modelling of the heterogeneity in the axial direction of the fuel pin are required [7].

In a 2012 report by the University of Michigan, the following is noted: 'An inherent deficiency of the neutronics modelling described above is that it does not take accurate account of the axial variation of the neutron spectrum that is very significant in the RBWR cores and their interface with the reflectors. This is because the generation of the group cross-sections was performed using 2-D lattice calculations. The computational method used by Hitachi for the RBWR core designs has a similar deficiency' [8].

Thus, there is a strong demand to develop a new approach for a more robust cross-section preparation procedure that is able to handle the axial heterogeneity. One approach could be to move to a full 3D cross-section preparation using Monte Carlo methods, which would lead to significantly increased computational demand. While this approach provides the most accurate cross-sections, it is not practical or necessary for design activities requiring parametric studies. Based on this request, the approach should be applicable in a standard lattice calculation as is typical for the first step of the two-step procedure of light water reactor analysis.

The problem in the RBWR seems, therefore, comparable to the double heterogeneity problem of high temperature reactor (HTR) fuel based on tristructural isotropic (TRISO) fuel particles. This problem was discussed in a paper by Kim et al. (2004) as part of a preliminary assessment of lattice physics for HTR analysis by Argonne National Lab [9]. Kim and Baek (2005) of KAIST proposed a novel method called the reactivity-equivalent physical transformation for solving the double heterogeneity problem [10]. A general conceptual diagram of the method can be seen in Figure 1. For an HTR, the first step is achieved by smearing TRISO particle materials (which contain graphite and fuel) in a compact graphite region at the centre of the model to eliminate the complex single structures. This region is surrounded by pure graphite moderator (such as a pebble or block in a real case). This step will lead to an incorrect criticality result due to loss of the self-shielding effect caused by homogenization. In a second step, the radius of the smeared fuel region is adjusted to account for this and to match the criticality of the now-homogenized and densified fuel region and the surrounding graphite to the criticality of the heterogeneous composition. Key to the process is the fact that the material configuration is not changed—the number of particles in the region stays constant and only the geometric dimensions are adopted in the new reactivity-equivalent physical transformation (RPT) model to mimic the self-shielding. KAERI (Korean Atomic Energy Research Institute) developed a computer code for analysis of the HTR for treatment of the 'unique' HTR double heterogeneity problem, based on HELIOS/MASTER in 2008 [11]. Rohde et al. (2012) expanded the RPT method by modifying the way in which the TRISO particles were smeared in the transformed model, completely separating the different material regions in the particle [12]. This allowed for separate temperature assignment to different materials in the model, further improving the usefulness of the transformation for the cross-section preparation in reactor lattice codes. As of 2022, progress on the RPT method continues for TRISO spherical fuel. In their proposed Ring RPT method, Lou et al. (2020) correct the method for inclusion of burnable poisons [13]. Handling the problem of the fuel's double heterogeneity through the RPT and solving it in a lattice code provides significant benefit in terms of computational time, due to the nature of the difference between the deterministic method used in this study and a Monte Carlo (MC) route, noting that MC calculation routes are inherently computationally intensive [12,14,15]. The RPT has not yet been applied to fuel types outside of the area of TRISO based HTR fuel.

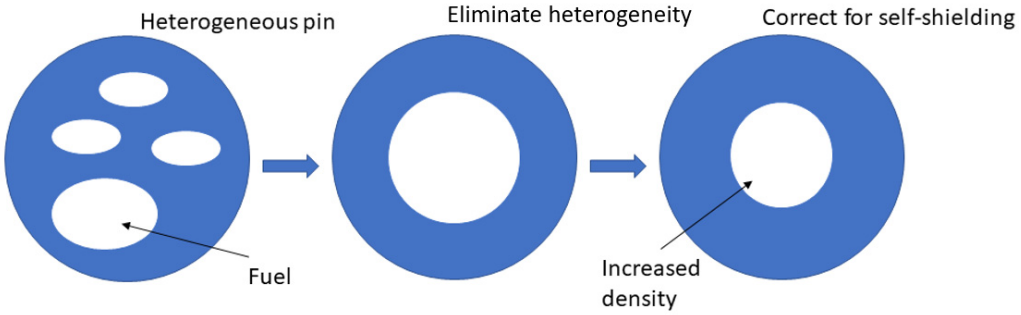


**Figure 1.** A diagrammatic representation of the core principle of previous uses for the RPT. A highly heterogeneous pin/fuel pellet is simplified to allow lattice calculations in 2D, and then the self-shielding differences which result from the geometric manipulation are corrected for by a manipulation of the density and radius of the fuel.

The current study investigates the applicability of the RPT method to the RBWR fuel pin, specifically focusing on the level of discrepancy between models of the pin produced for the axial and radial direction in a 2D calculation. An axial model of both a single pin and assembly, based on the RBWR design, are produced. The density and size of the fuel and moderator regions are changed, keeping the pitch and total mass of fuel and moderator constant. By using this adapted method of correction for self-shielding, heterogeneity in the axial direction, which is characteristic for RBWR fuel assemblies, could be calculated deterministically in a classical lattice code. As in the case of TRISO, the RPT method has the potential to reduce computation time for the design phase of the RBWR (or other axially heterogeneous reactor types) by expanding the applicability of deterministic codes through easing the production of homogenised and condensed cross-section libraries, an essential step for coupled neutronic/thermal hydraulic design and transient studies. The well-known lattice and burnup code system SCALE 6.2 is used for both models (classical radial as well as RPT corrected axial) to evaluate the question, 'Can the RPT be applied to an axially heterogeneous pin model of a BWR?'

## 2. Code Descriptions

Steady-state transport calculations and burnup calculations were performed using SCALE 6.2. SCALE 6.2 is a comprehensive modelling and simulation code package for criticality safety, reactor physics, radiation shielding, radioactive source term characterisation, and sensitivity and uncertainty analysis developed by the Oak Ridge Nuclear Laboratory (ORNL, Oak Ridge, TN, USA). Multigroup neutron energy libraries based on ENDF/B-VII.0 and ENDF/B-VII.1 data were used throughout this work. The specific structure used for these calculations is the 238-energy group structure. All calculations were performed with the TRITON module of SCALE 6.2. TRITON draws from several modules to perform calculations. T-XSEC is called to prepare multigroup cross-section libraries accounting for spatial and energy-dependent self-shielding. Libraries for each problem consist of microscopic cross-sections for each nuclide defined in the TRITON script. To build on the cross-section data, TRITON calls NEWT (New ESC-based Weighting Transport code), for the determination of the 2D neutron flux distribution. NEWT is 'a two-dimensional discrete ordinates transport code developed based on the Extended Step Characteristic (ESC) approach' [16].

Depletion calculations are performed using the ORIGEN depletion module, which is called by TRITON for time-dependent transmutation of each material. ORIGEN requires the neutron flux distribution and cross-sections as well as the user-defined material specifications. It provides new isotopic concentrations by performing depletion operations, cross-section collapsing, and flux normalisation.

Validation calculations were performed using the SCALE module KENO, specifically KENO-VI, which is a multi-group, flexible geometry 3D Monte Carlo transport calculator. In each validation case the energy groups used are kept the same between TRITON and KENO.

## 3. Model Descriptions for BWR Burnup Calculations

Unit or pin cell studies based on SCALE are performed for several scenarios relating to the production and implementation of a 2D 'RPT' transformed model. In all cases an RBWR-analogous uranium breeder reactor is used, consisting of a hexagonal fuel assembly with 20% enriched $UO_2$ fuel (see Figure 2). For burnup calculations applying the transformed model, effective multiplication factors were compared for different seed/blanket geometries to a burnup of 70 GWd/tU. Isotopic and spectral analyses were also carried out using the developed RPT model. For the RPT development, two models were created. The first is a hexagonal pin cell model of a uranium-breeder based on the geometry of the RBWR-TB2. The second is an axial model of a pin, made up of 40 sections of 10 cm height (see Figure 3). In the case of the calculations used to produce the RPT model, the fuel pin consists of 20% enriched $UO_2$ similar to the radial model, but for later calculations applying the equivalent model these sections can be filled either with the 20% enriched 'seed' or natural uranium 'blanket' as foreseen in the RBWR design, to test for the efficiency of different breeder reactor geometries.

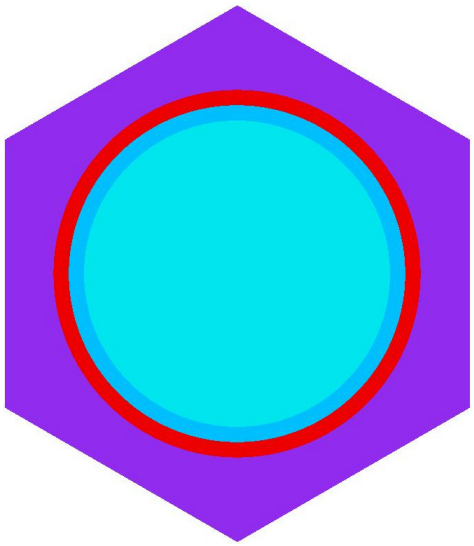

**Figure 2.** SCALE 6.2 model of radial RBWR-analogue pin-cell.

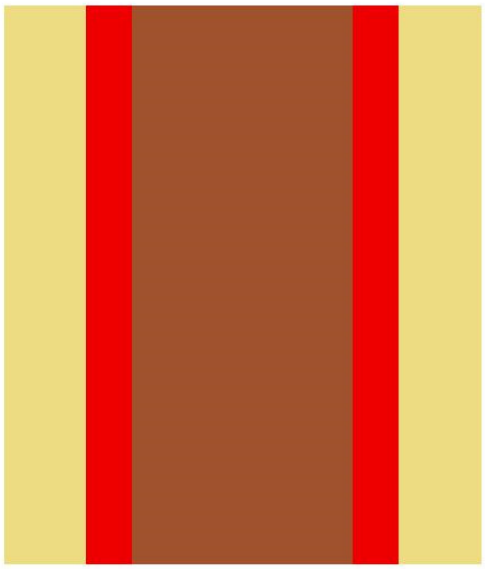

**Figure 3.** SCALE 6.2 model of a section of the axial pin model used for applying the RPT to an RBWR-analogue reactor.

### *3.1. RBWR-Analogue Radial Pin-Cell Model*

The radial pin-cell of a uranium-breeder based on the geometry of the RBWR-TB2 was produced to calculate reference values of neutron multiplication and energy distribution of the neutron flux, to which RPT-transformed models will be compared. Table 1 shows the main geometrical and operational parameters used in the simulations. Figure 2 displays the SCALE 6.2 model of the RBWR-analogue hexagonal pin cell which consists of fuel and cladding, surrounded by moderator. Reflective boundary conditions were applied to the system.

**Table 1.** RBWR-analogue pin-cell parameters.

| Parameter | Data |
|---|---|
| Fuel radius, mm | 3.00 |
| Zircaloy clad radius, mm | 3.60 |
| Pitch, mm | 9.10 |
| Fuel temperature, K | 850 |
| Natural Zr clad and moderator temperature, K | 620 |
| Fuel enrichment, wt% | 20 |
| Fuel density, g/cm$^3$ | 10.2540 |
| Moderator densities, g/cm$^3$ | 0.3–0.7 |

### *3.2. Axial Uranium Breeder Pin/Burnup*

Calculations on the axial direction were performed using a 400 cm long reactor pin discretized into sections of 10 cm height as a basis for later studies. In the first step, these sections consisted entirely of 20% enriched $UO_2$ fuel for the approach to produce the equivalent model, and thereafter consisted of either 20% enriched $UO_2$ or natural uranium in order to see the effect of different seed/blanket arrangements as proposed in the RBWR. For the later usage, the water density curve is important when investigating an axial cut of a boiling water reactor as it varies considerably along the height of the core. The opportunity to take this into account is foreseen through splitting the outer moderator region of the model into four 100 cm height sections, each with the opportunity to provide different water densities. The choice of four sections was determined, based on the current approaches for BWRs, to deliver a sufficient level of detail to gain useful insights into the behaviour of different sections of the pin without significantly increasing the computational time. Table 2 provides the data for the equivalent axial pin model, as a basis for the reactivity equivalent physical transformation to be applied.

**Table 2.** RBWR-analogue equivalence axial model parameters.

| Parameter | Data |
|---|---|
| Modified Fuel radius | To be determined |
| Modified Zircaloy clad radius | To be determined |
| Pitch, mm | 9.10 |
| Fuel temperature, K | 850 |
| Natural Zr clad and moderator temperature, K | 620 |
| Fuel enrichment, wt% | 20 |
| Axial region size for self-shielding calculation, cm | 10 |
| Calculated region sizes of seed/blanket structure, cm | 20/100 |
| Region sizes for water density distribution, cm | 100 |

### *3.3. Spatial Self-Shielding Effect*

Spatial self-shielding occurs when the fuel geometrically shields itself from neutron penetration due to the heterogeneous nature of the pin cell, resulting in a lower neutron flux inside the fuel rod compared to near the surface. As this effect is dependent on geometry, the process required by this paper's application of the RPT must account for a change in the self-shielding due to a change in the geometry.

Figure 4 shows that by reducing the radius and increasing the density of the fuel in the axial pin RPT model, there is an increase in the criticality. This is due, in part, to the reduction in self-shielded neutrons, but there may also be a spectral effect due to the respective increase in moderator region volume, as shown in Equations (1)–(5). The contribution of these two effects could be worthy of additional analysis, by separating the pin into several smaller regions to compare fluxes. However, this analysis was deemed unnecessary for an exploration of the applicability of the RPT in this case.

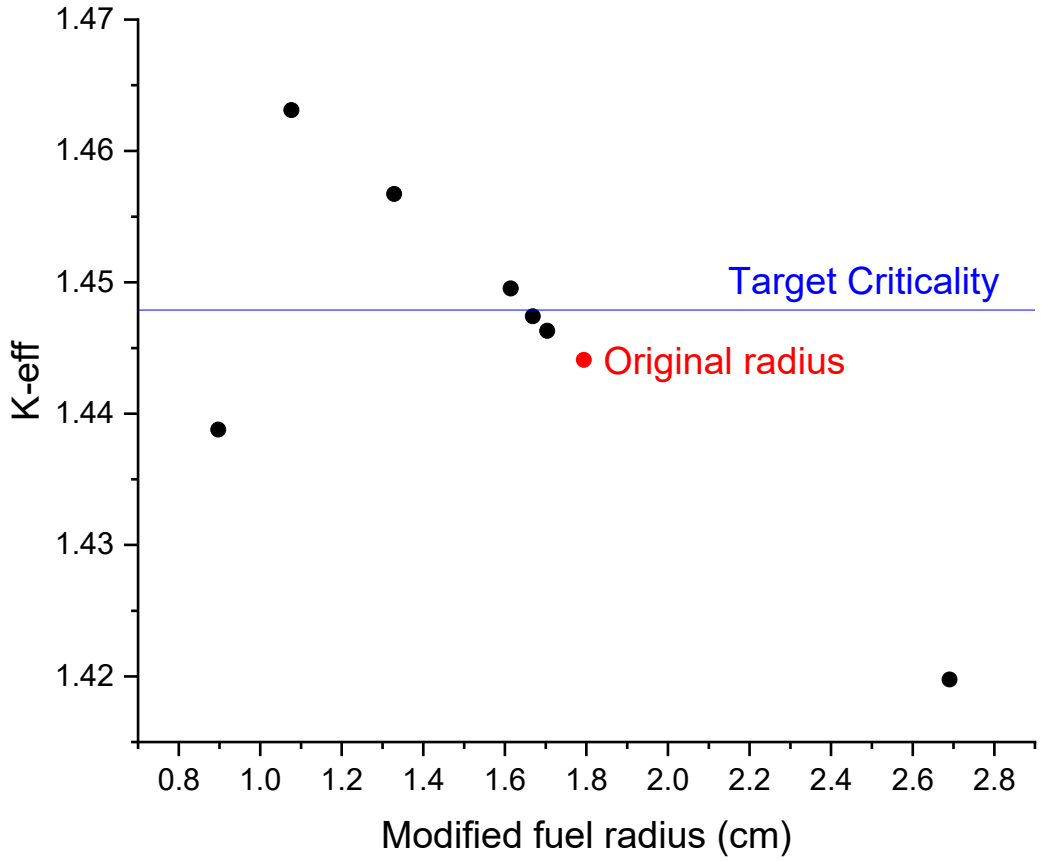


**Figure 4.** Effect of modification of the fuel radius with compensating density modification across several different modified fuel radii. It can be seen that the behaviour is predictable for most degrees of modification with higher criticality being calculated for denser fuel, due to the reduction in the effect of self-shielding.

### *3.4. Monte Carlo Validation*

Using the same unit cell model as was created for TRITON calculations (shown in Figure 2), multiple validation calculations were run using SCALE KENO-VI. The first point of validation was a direct comparison of the radial unit cell model to a 3D Monte Carlo extrapolation of the same unit cell. The Monte Carlo model was created with a single fuel material for this comparison, in order to evaluate the size of the difference between the two calculation methods before introducing axial heterogeneity through a seed and blanket structure.

When axial heterogeneity is added it is pivotal that the RPT-produced axial model is validated against a 3D calculation, as without this the only equivalence that is proven is for two one-dimensional models. Therefore, 3D Monte Carlo calculations for several seed/blanket axial geometries and varying void fractions were completed and compared against RPT-axial models, for various configurations relevant to future calculations for cross section production.

## 4. Results and Discussion

### *4.1. Producing the Equivalence Model*

#### 4.1.1. Effective Multiplication Factor

The first point of evaluation to determine the RPT radius is matching of the reference and the RPT model regarding the effective multiplication factor at a fresh steady-state, without burnup. This factor, $k_{eff}$, is the key value for the comparison between the two models to be matched in the RPT process. $\Delta pcm$ is the measure of the difference between the $k_{eff}$ of the pin model (RPT model) and of the radial unit cell model (reference), given by the equation:

$$\Delta\rho[pcm] = \frac{k_{eff}(axial) - k_{eff}(radial)}{k_{eff}(radial) * k_{eff}(axial)} * 10^5 \quad (1)$$

In order to keep both the mass of the fuel and moderator constant, as well as the pitch, a fuel diameter/width modification factor $(\alpha)$ is defined from which the density and width of each of the moderator, clad, and fuel can be defined. Therefore, trivially from $\alpha$ the following can be defined:

$$x_f = \alpha x_{f0} \quad (2)$$

$$x_m = P - x_{clad} - \alpha x_{f0} \quad (3)$$

$$\rho_f = \frac{\rho_{f0}}{\alpha} \quad (4)$$

$$\rho_m = \frac{x_{m0}\rho_{m0}}{P - x_{clad} - \alpha x_{f0}} \quad (5)$$

where $x_{f0}$, $\rho_{f0}$, $x_{m0}$, $\rho_{m0}$ are the initial widths and densities of the fuel and moderator, respectively, and $x_f$, $\rho_f$, $x_m$, $\rho_{m0}$ are the modified values [17–19]. These values are defined only by geometrically transforming the radial unit cell model to an axial pin model conserving the mass and number of particles of the fuel and moderator and conserving the pitch of the radial model. This is a straightforward geometric transformation, shown in the first step of Figure 5, using the ratios of the areas of the material regions in the hexagonal model and converting them directly into widths in the pin model. $P$ is the pitch, and the size, $x_{clad}$, and density of the cladding region of the model were kept constant, as varying it was found to have a negligible effect on results.

Figure 6 shows the discrepancy in $k_{eff}$ between the axial and radial models for four different water density calculations, each at steady state at zero burnup. The water density values were chosen to maximise similarity in the two models over a range which is relevant to RBWR/ABWR water density curves. The results obtained at a value of $\alpha$ between 0.9 and 0.95 are within a pcm difference of −200 to +100 for all water densities. For the value of $\alpha$ = 0.93, all pcm differences are <±50 pcm, showing a very good standard of agreement between the two models, at least for steady state criticality. However, it is necessary to expand on the investigation for this value to further implement the new equivalent model.

The next step of the analysis required to calibrate the RPT is to compare values of $k_{eff}$ over a burnup cycle. This is performed for a burnup up to 70 GWd/tU. As can be seen from Figure 7 in the case of 50% void, and as was seen for comparisons performed over the same burnup for 60% and 70% void, the pcm difference between the models remains consistent with what is found in the steady state analysis until a burnup of 20 GWd/tU or higher. At this point the discrepancy between the two models begins to increase, which is a consequence of the change in the fissile material due to the breeding of plutonium and the related change in the neutron spectrum. This effect produces a discrepancy of more than 100 pcm at very high burnup. In the 60% void case there was a maximum difference of 77 pcm, and for 70% void this was 62 pcm across the same burnup length.

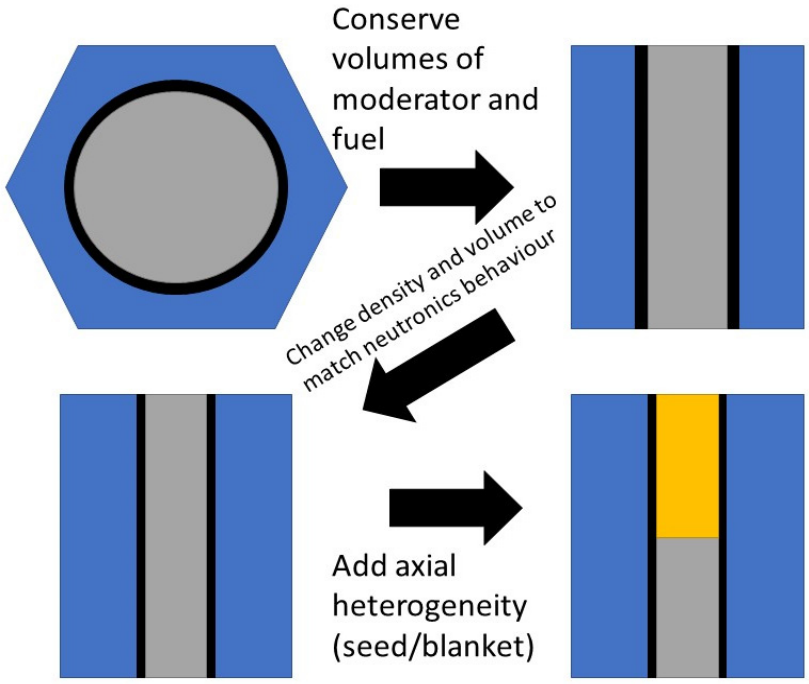


**Figure 5.** Simple diagrammatic representation of the processes undertaken as part of this work.

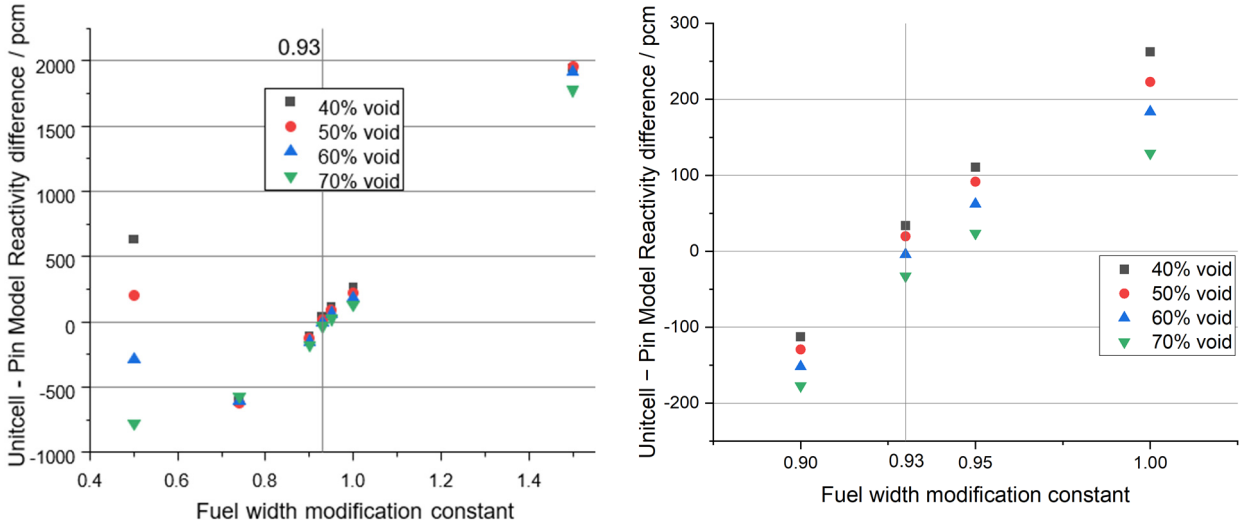


**Figure 6.** Reactivity difference between the axial and radial models of the pin in pcm units. When $\alpha$ is significantly below 1, with highly dense fuel represented in the model, the behavior of the pin model is inconsistent across different void fractions. The best agreement is found at a width reduction of 0.93, where the difference between the transformed pin model and the unit cell radial model is below 30 pcm across all void fractions calculated. Figures (**left**) and (**right**) are the same set of data, with different axis scaling.

#### 4.1.2. Spectral Comparison

Following the investigation of the $k_{eff}$ development over burnup, the next, more detailed step will be the comparison of the neutron spectra. The neutron spectra of the two models were investigated as a follow-up metric by which to evaluate the RPT. Due to the high enrichment of the fuel and relatively small pitch in the fuel assembly of the RBWR, the model produces a much harder neutron spectrum than a classical LWR, as shown in Figure 8. Figure 9 shows that for the fast spectrum, there is a strong correlation between the two models, as there are no energy brackets of the SCALE-defined 238-group structure within this range where the number of interactions in either model varies from

the other by more than 1%. At lower, thermal energies within the two models there are larger differences, even up to around 3% at ~1 eV. The normalisation of lower absolute numbers of interactions leads to these comparably large values.

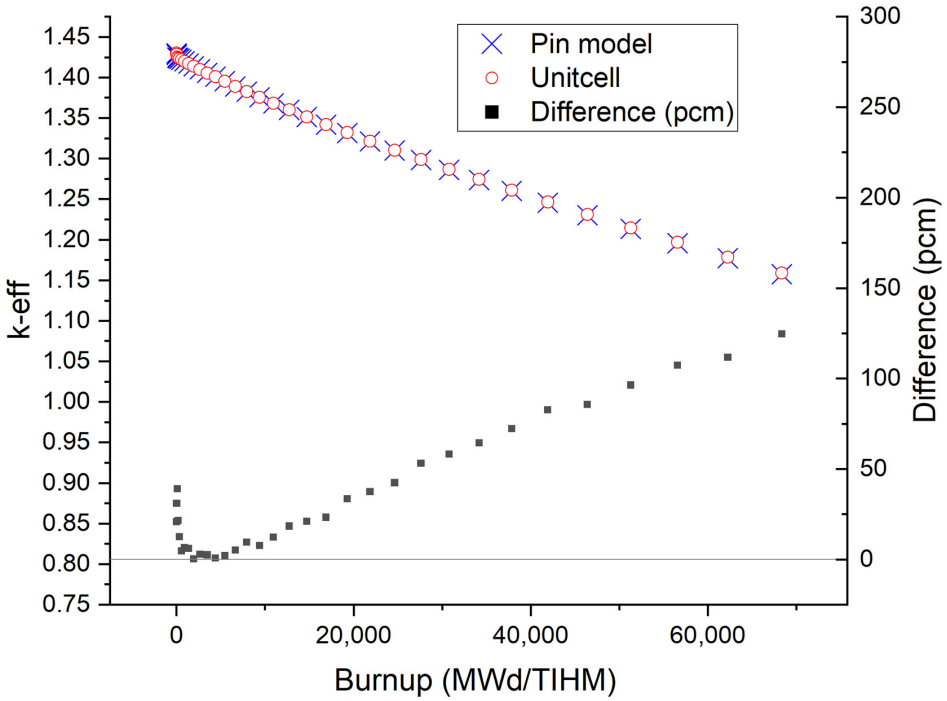


**Figure 7.** Difference in k-eff, the effective neutron multiplication in the model, between the axial RPT model of the pin and the radial unit cell model across a standard burnup cycle. As the pin reached high burnup (>50 GWd/tU), the difference in criticality between the two models increased to >100 pcm. This calculation was performed with a void fraction of 50%. In the cases of 60% and 70% void, the axial model showed more similar behaviour at high burnup.

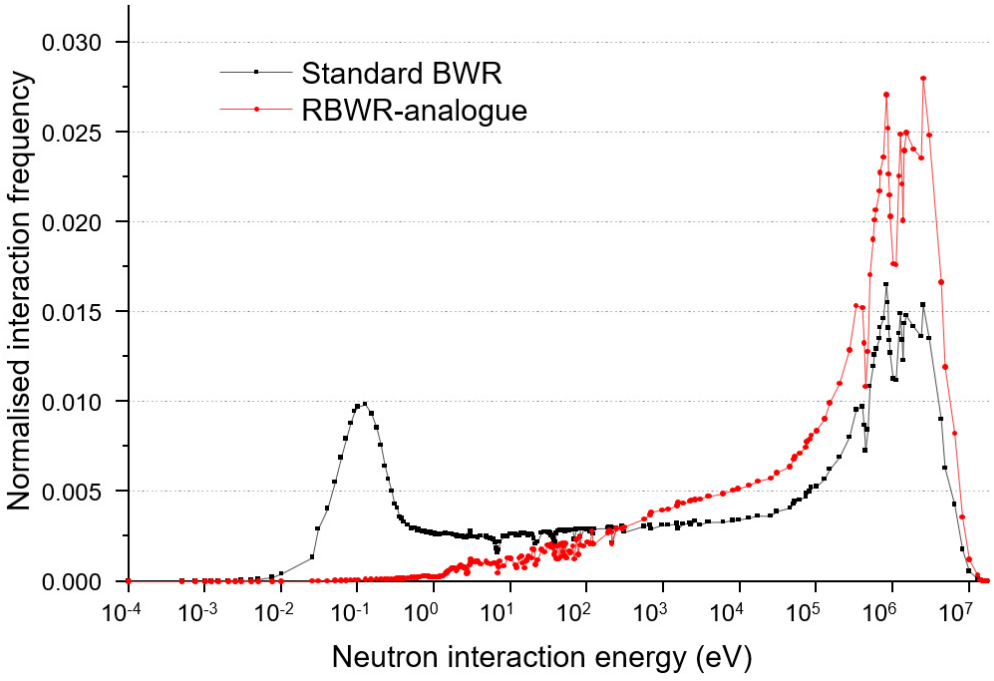


**Figure 8.** Comparison of neutron energy distribution between the RBWR-analogue calculated reactor used in this work and a standard BWR as calculated from a simple example case from the SCALE user guide. Both calculations were run at steady state before any depletion.

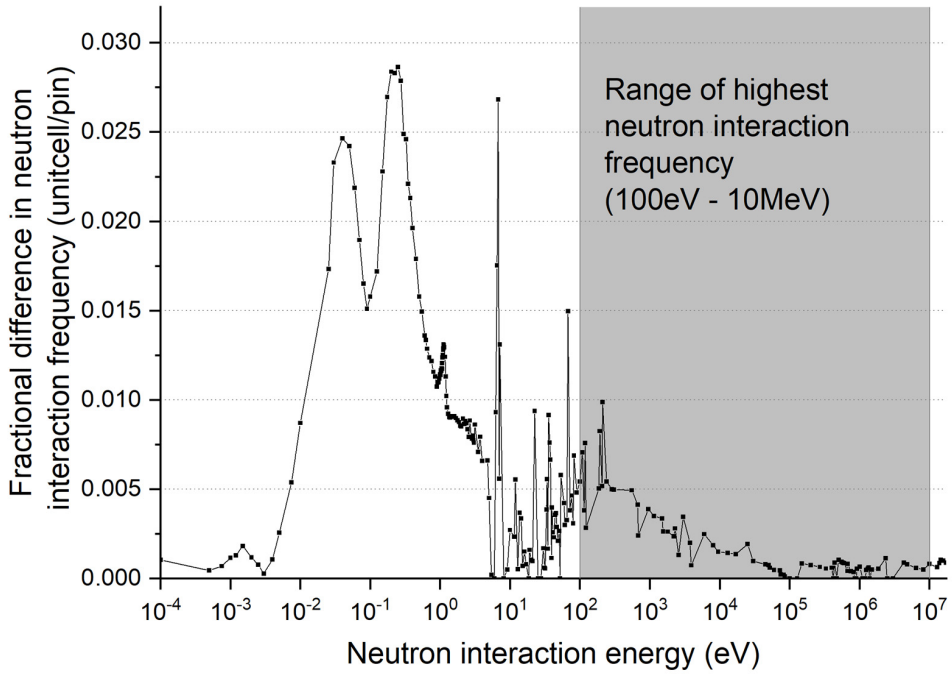


**Figure 9.** Fractional difference in neutron interaction frequency between the unit cell and RPT pin models calculated across a 238-energy group spectrum. In the energy range of highest interaction frequency for this pin, agreement of within 1% is seen between the axial and transformed radial models. Outside of this most-frequent range, higher discrepancies between the models can be found but very few interactions between neutrons of energies lower than 100 eV take place in the breeder reactor, as can be seen in Figure 8. Fractional difference is calculated using $\frac{2(unitcell-pin)}{unitcell+pin}$ to normalise values for energy groups of lower interaction frequency.

### *4.2. Applying the Equivalence Model*

The RPT model was used to investigate the effect of different levels of heterogeneity on the breeding capabilities of the RBWR-analogue reactor with varying seed and blanket arrangements along the length of the pin. This was achieved by changing the placement of some parts of the fuel within the pin and running a burnup calculation as before. In each case, the amount of highly enriched uranium fuel was kept constant, but the geometry of seed and blanket regions across the height of the pin were changed. Calculations were run for repeated regions of seed and blanket of 100 cm, 40 cm, 20 cm, and 10 cm height. For the evaluation TRITON is used for observing the number densities of several main actinides, particularly fissile plutonium isotopes which were tracked at the same set of burnup points.

At a first glance of Figure 10 it is clear that by the end of the burnup cycle the smaller seed and blanket regions lead to a pin which can produce more fissile plutonium. This is also seen in the comparison between Figures 11 and 12, where the same comparison of 100 cm/20 cm seed and blanket regions is seen, but with the data split into different regions of the reactor. There are different observations to make. First the increase in the plutonium amount in the seed is slightly higher in the 100 cm case than in the 20 cm case. Second, in the case of the 100 cm height blanket regions, the natural uranium at the centre of the region, 50 cm from its closest highly enriched uranium region, produces a negligible amount of fissile plutonium. Thus, the observation in the blanket is clear—there are simply not enough neutrons reaching all areas of the breeding blanket to create a significant amount of neutron capture in U-238 to breed Pu-239 when the blanket area is 100 cm long. The other observation needs a bit more of an explanation but thinking about the different structure of power production in the seed and in the blanket gives an answer. In the 20 cm case, the power production in the blanket region will already be significant due to the strong breeding of Pu which typically dominates fissile content after a burnup of 30 GWd/tU and higher in an LWR. Thus, in the 20 cm case, the local burnup in the seed will be lower since

some burnup is already created in the blanket. In contrast, in the 100 cm case, due to the weak breeding, almost all burnup is accumulated in the seed and there is a clear correlation between the neutron flux, or the power produced in a fuel, and the plutonium bred due to the exposure to the neutron flux. It can be observed in all calculations of the seed that the Pu production increases almost linearly with the burnup. Based on this observation, the slightly increased Pu content in the seed of the 100 cm case can be explained with the higher local burnup there, while the global value is still lower, as in Figure 10.

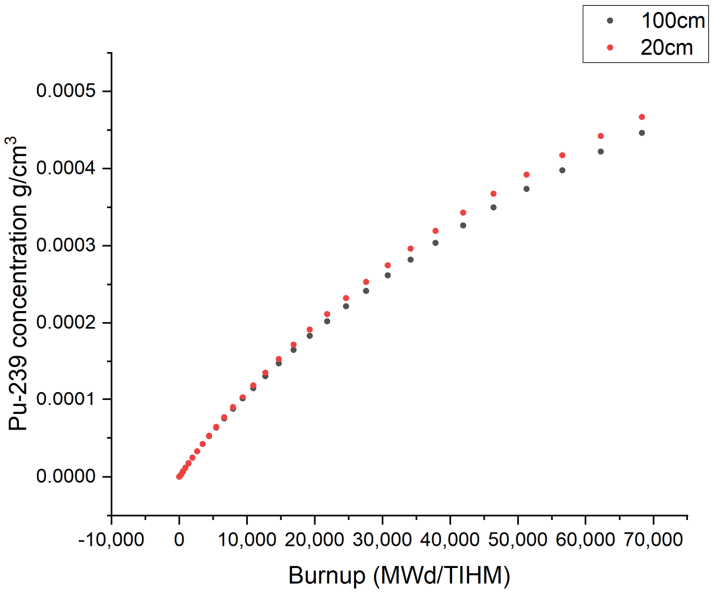


**Figure 10.** Pu-239 concentration across a burnup cycle ending at 70 GWd/tU, averaged across the whole pin. The two different models are referred to by their seed and blanket region sizes of 20 cm and 100 cm. The difference in plutonium production is similar at low burnup, but at higher burnup the 20 cm seed/blanket model produces more Pu-239.

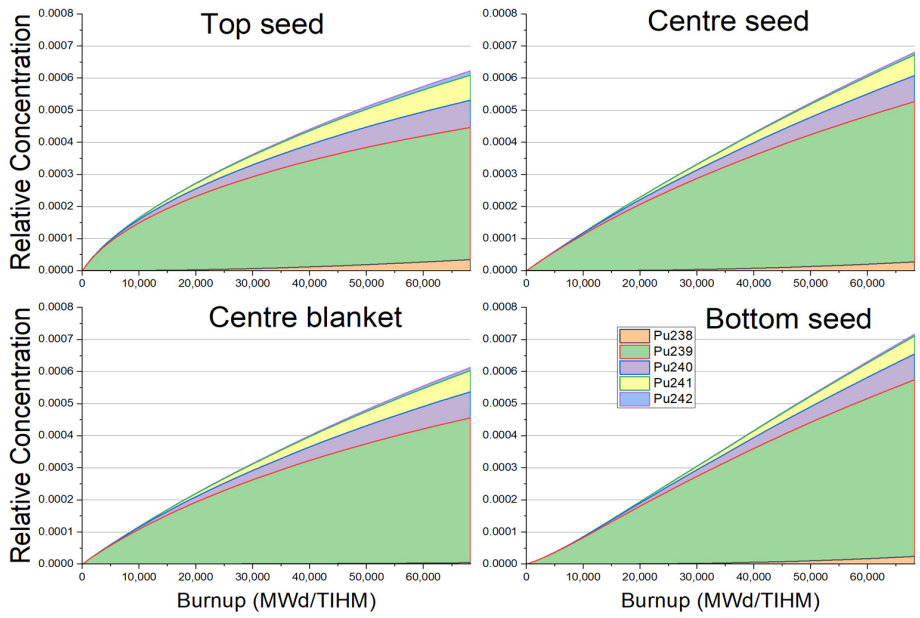


**Figure 11.** Concentrations of different plutonium isotopes throughout a burnup cycle, for a seed and blanket structured pin with regions of 20 cm size. The production of fissile plutonium (Pu-239 and Pu-241) in the top seed is faster at the start of the burnup cycle, in the region where the water density is lowest. The opposite is true for the bottom of the reactor pin. The central blanket region produces less plutonium than any seed region, but still yields over 70% of the plutonium of the central seed region.

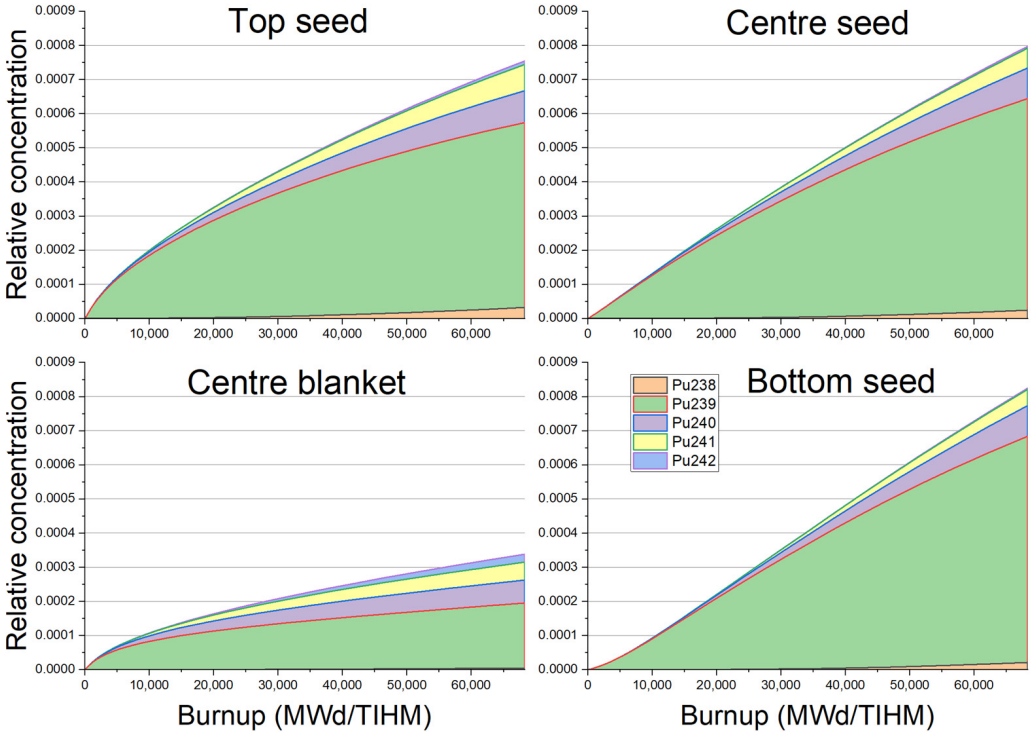


**Figure 12.** Concentrations of different plutonium isotopes throughout a burnup cycle, for a seed and blanket structured pin with regions of 100 cm size. The production of fissile plutonium (Pu-239 and Pu-241) in the top seed is faster at the start of the burnup cycle, in the region where the water density is lowest. The opposite is true for the bottom of the reactor pin. The central blanket region produces less plutonium than any seed region.

In addition, Figures 10 and 11 show that the different water densities across the height of the reactor have a noticeable effect on the plutonium production, and particularly by looking at the differences between the top and bottom seed regions for the 100 cm seed/blanket model, it can be observed that the effect is for both the quantity and quality of the plutonium produced. In the case of the top seed region, very high-quality plutonium is produced quickly at low burnup, but this is not extended to high burnup points.

### *4.3. Reapplying the Results to a Full Assembly Model*

After using the radial unit-cell model as a proof of concept for the equivalence procedure as a first step, it is possible to apply the process to a more realistic full assembly model. The new model includes areas of improved moderation (see Figure 13) which change the fuel width modification needed to produce an axial model with similar behaviour, but this time for the full fuel assembly. The effect on criticality is given in Figure 14 for different water densities. In order to produce cross-sections for the equivalent full assembly models, different width modifications in the RPT model are required for each water density due to the larger effect of the radial heterogeneity, paired with the effect of different spatial self-shielding. The results of the procedure are shown in Figure 15. $\alpha$ values for water densities of 0.3, 0.4, 0.5, and 0.6 were found to be 0.90, 0.74, 0.74, and 0.60, respectively.

### *4.4. Validation Results*

Figure 16 shows the pcm difference over the same burnup cycle as used elsewhere in this work, in this case between a 3D Monte Carlo calculation (as described briefly in Section 3.4) and a single material axially homogeneous RPT-transformed pin model. The maximum pcm difference is around 100, showing a very strong level of agreement between the two models, as would be expected.

Figures 17 and 18 show the results of the validation of the 2D RPT axial model with a seed and blanket structure. In all of these cases, the RPT model was 'calibrated' using a case with 50% void fraction and 50 cm repeating seed and blanket axial regions. The results clearly show that for the calibration case there is very good agreement between 3D Monte Carlo and RPT. The results also include comparisons for void fractions and seed and blanket geometries which are not the calibration case, to show the robustness of the RPT method. It is shown that the RPT calibration is relatively robust to changes to void fraction in the model, but responds far less well to changes in the axial heterogeneous geometry.

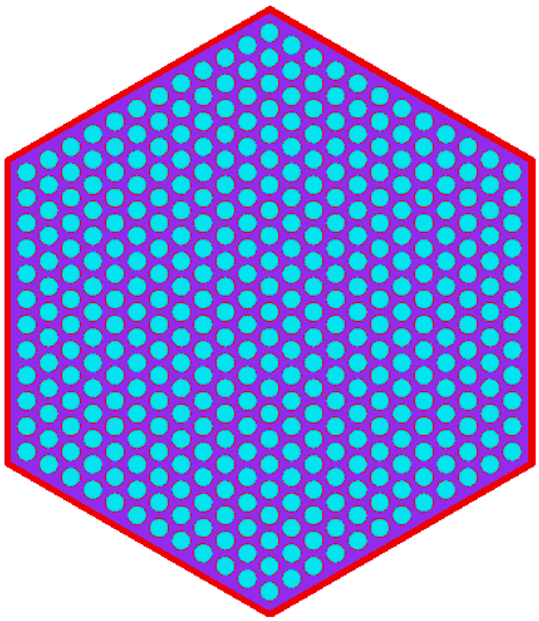

**Figure 13.** SCALE 6.2 model of radial RBWR-analogue assembly.

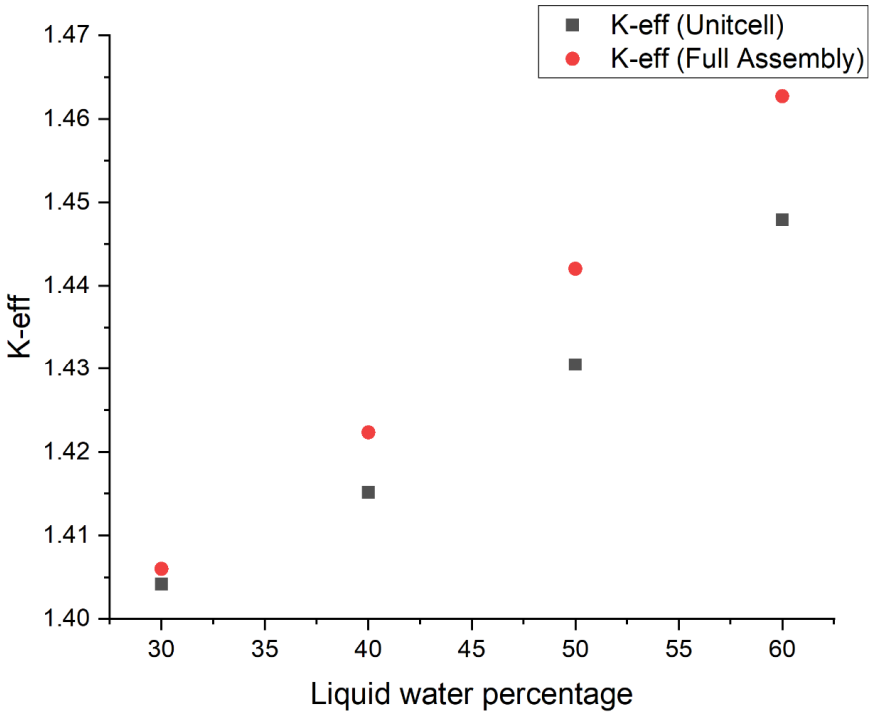


**Figure 14.** Effect of areas of increased moderation on the criticality of the radial model. At lower void fractions the effect is shown to be greater, up to a difference around 1000 pcm at the lowest void fraction of 60% water density.

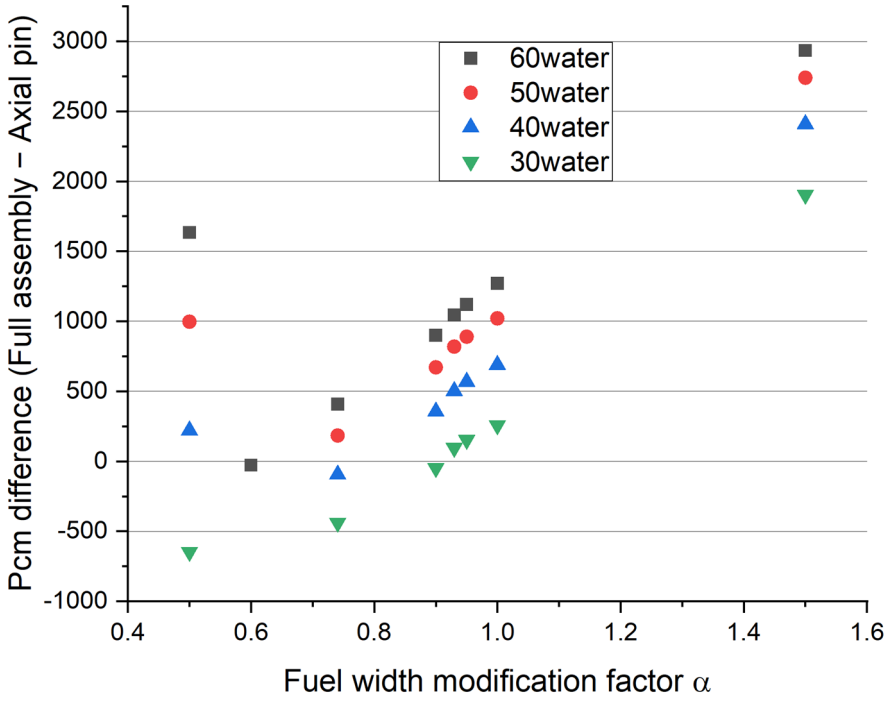


**Figure 15.** Difference in pcm units between the k-eff values of the full assembly radial model and an equivalent axial pin model modified by the given fuel width modification factor. Different factors for modification are required to minimise the difference in behaviour between the two models, with the largest modification required for the lowest void fraction, as expected.

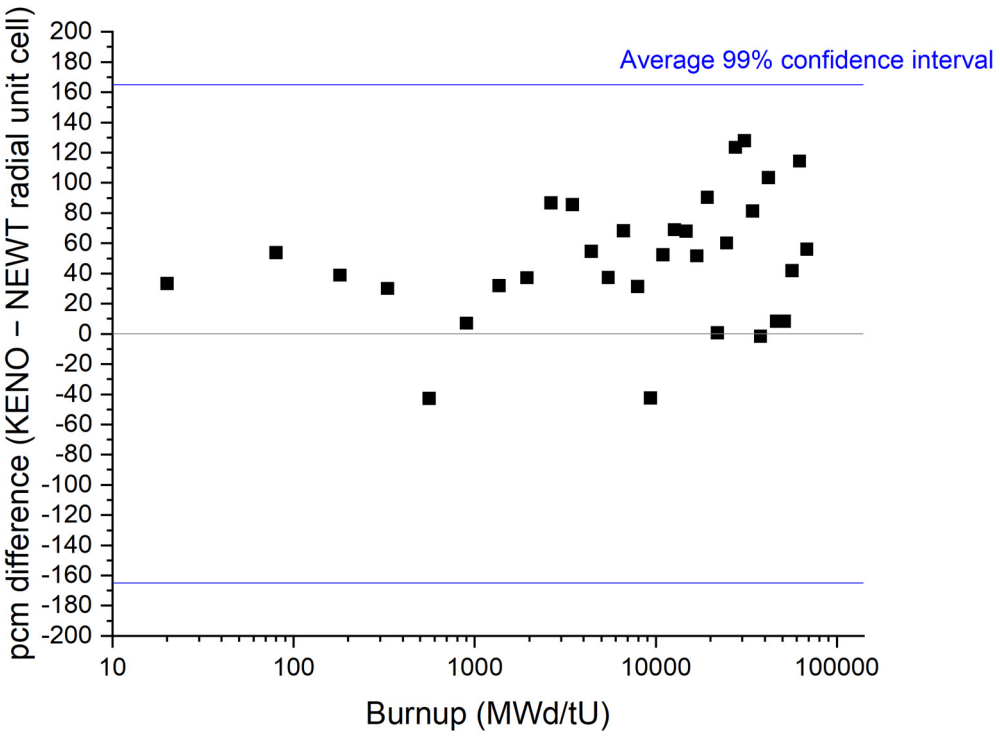


**Figure 16.** Difference in pcm units between the k-eff values over ~75 GWd/tU burnup between the radial unit cell model from which the RPT is calibrated, and a 3D SCALE KENO model of the same geometry and material composition. In both cases there is only a single fuel material in the pin. For the entirety of the burnup cycle the difference remains within the 165 pcm 99% confidence interval determined by the Monte Carlo statistics used in the KENO 3D model.

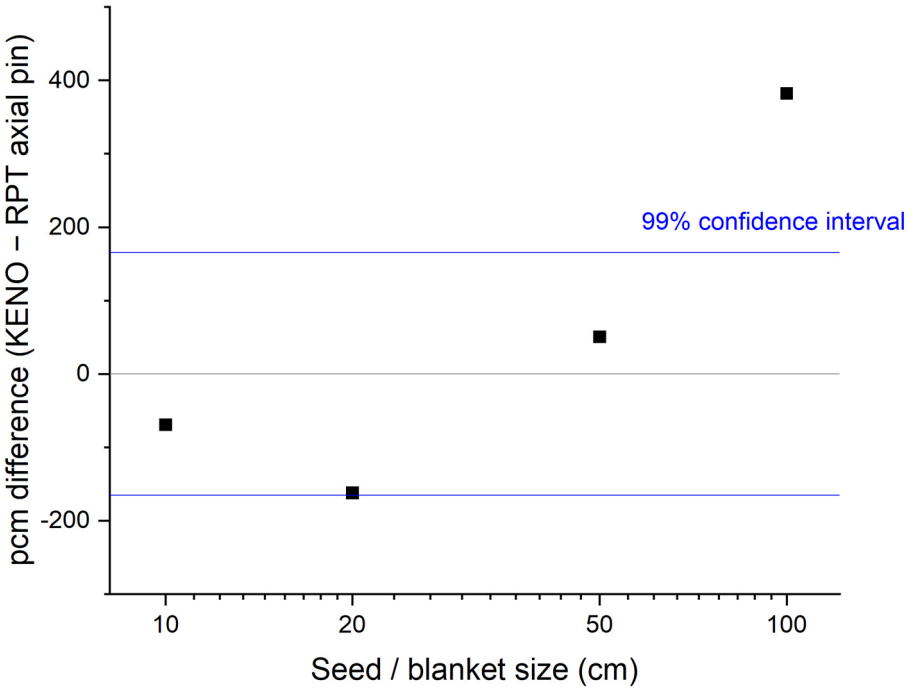


**Figure 17.** Difference in pcm units between the k-eff values of the 3D SCALE KENO and an equivalent axial pin model modified by the given fuel width modification factor. In this case, a seed and blanket geometry of 50 cm regions and a void fraction of 50% is used to calibrate the RPT. The results show that, firstly and most importantly, axial heterogeneity can be successfully modelled by the RPT method in 2D, and that the method requires recalibration for different axial geometries to be well-validated.

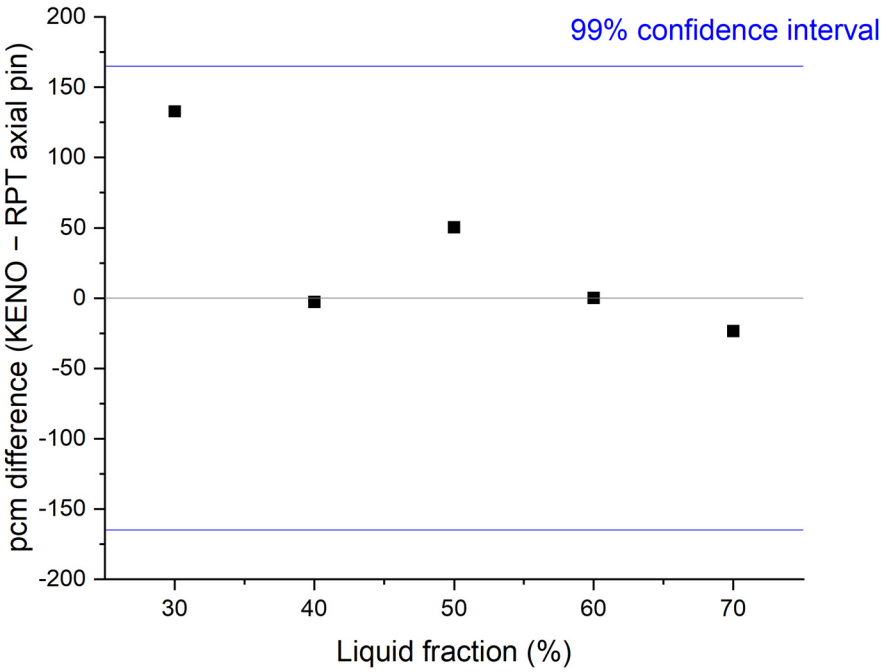


**Figure 18.** Difference in pcm units between the k-eff values of the 3D SCALE KENO and an equivalent axial pin model modified by the given fuel width modification factor. In this case, a seed and blanket geometry of 50 cm regions and a void fraction of 50% is used to calibrate the RPT. The results show that, firstly and most importantly, axial heterogeneity can be successfully modelled by the RPT method in 2D, and that the method is relatively robust against requiring recalibration for changes in water density.

## 5. Discussion and Conclusions

Development of reactor designs such as the RBWR is important for progression of the nuclear industry towards providing solutions to one of its most difficult problems—the demand of improving the fuel usage—as well as to develop promising solutions for the waste management. Both are required to improve the already good sustainability of nuclear energy to a new level that will allow widespread use of nuclear energy as a core contributor to a future net zero society [20]. Lattice physics computation is a computationally less-intensive tool when compared to Monte Carlo simulations, which for a reactor design early in the iteration stages can be extremely useful. In addition, lattice calculations build the backbone of all later core simulations and transient studies since the lattice simulations are the key step for the cross-section preparation for the widely used nodal core simulators, which are used for neutronic/thermal hydraulic coupled analysis. To support the later application of these coupled core simulators, the application of the reactivity-equivalent physical transformation process to an axially heterogeneous boiling water reactor pin was adapted from another application and investigated. Two models, one a radial representation of an RBWR-analogue pin and the other an axial representation, were produced. Through several stages of analysis and comparison using the code system SCALE 6.2, it was possible to apply the transformation process to these models and produce an equivalence model which could then be used to examine some properties of axially heterogeneous pins without the need for 3D Monte Carlo simulations.

The equivalence model was produced by varying the density and size of the moderator and fuel regions of the axial model and then comparing with the radial model, using several different properties as comparators [21]. The first comparison was the steady-state criticality. In this case, it was found that for void fractions of 30–70%, a fuel width reduction constant of 0.93 provided an equivalence model with <50 pcm difference to the radial model. The models were then compared across burnup, which provided further evidence of the efficacy of the reactivity equivalent physical transformation, with a maximum of ~100 pcm difference between the models even at very high burnup points. A spectral analysis was then performed, showing that the models were very consistent across all energy groups for neutron interaction frequency, and particularly consistent in the energy region of most interest between 1 keV and 100 MeV.

There were limitations to the model in both the burnup and spectral comparisons. At very high burnup an increasing level of disparity between the models was observed. This may have been caused by the Pu production and the appearance of fission products in the fuel, which would have had an amplified impact on the criticality and the evolution of the self-shielding of the modified model which would require further adjustment or an optimization not singularly based on fresh fuel. In the case of the spectral analysis, normalisation accounts for some of the larger discrepancies at low energy, wherein there are far fewer interactions, and the effect of small discrete differences between the models' interaction frequency appears as large fractional differences.

The model was then used to investigate the effect of heterogeneity, and more specifically the seed/blanket breeder structure of concept reactors such as the RBWR, on plutonium production. Applying the equivalence model, it was found that for larger areas of seed/blanket, blanket regions would not produce as much fissile plutonium as for smaller seed/blanket geometries. This is due to the lack of neutron penetration into large blanket regions past a few mean free paths.

Based on all of the above, it is clear that the application of the reactivity-equivalent physical transformation to fuel geometries, outside of its current use cases, has the potential to be a very powerful tool. However, the RBWR-analogue reactor which is used for all of the calculations in this work is not a realistic reactor. In the case of more complex and continuous water density distributions, the model may require such a level of detail that the computational advantage is lessened [22], but there is still a great opportunity to use this approach for the essential cross-section preparation required for coupled 3D core analysis and transient studies [23].

**Author Contributions:** Conceptualization, R.M. and B.M.; methodology, R.M.; validation, R.M.; investigation, R.M.; resources, B.M. and T.H.; data curation, R.M.; writing—original draft preparation, R.M.; writing—review and editing, M.P., A.P. and B.M.; supervision, M.P., A.P. and B.M.; funding acquisition, A.P. and T.H. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by Hitachi Ltd., specifically through a funded studentship from the Centre for Technology Innovation—Energy, Research and Development group.

**Data Availability Statement:** The data presented in this study are available on request from the corresponding author. The data are not publicly available due to some data sets being proprietary.

**Conflicts of Interest:** The authors declare no conflict of interest.

## References

1. Merk, B.; Litskevich, D.; Bankhead, M. iMAGINE-A disruptive change to nuclear or how can we make more out of the existing spent nuclear fuel and what has to be done to make it possible in the UK? *ATW Int. J. Nucl. Power* **2019**, *64*, 353–359.
2. Merk, B.; Litskevich, D.; Whittle, K.; Bankhead, M.; Taylor, R.; Mathers, D. On a Long Term Strategy for the Success of Nuclear Power. *Energies* **2017**, *10*, 867. [CrossRef]
3. Kito, K.; Hino, T.; Matsumura, K.; Matsuura, M. Hitachi's Vision for Nuclear Power and Development of New Reactors. *Hitachi's Nucl. Power Bus.* **2020**, *69*, 156–162.
4. Hino, T.; Nagayoshi, T.; Mitsuyasu, T.; Ohtsuka, M.; Moriya, K. Development of RBWR (Resource-renewable BWR) for Recycling and Transmutation of Transuranium Elements (1)—Overview and core concept. In Proceedings of the ICAPP2015, Nice, France, 3–6 May 2015.
5. Hino, T.; Miwa, J.; Mitsuyasu, T.; Ishii, Y.; Ohtsuka, M.; Moriya, K.; Shirvan, K.; Seker, V.; Hall, A.; Downar, T.; et al. Core Design and Analysis of Axially Heterogeneous Boiling Water Reactor for burning Transuranium Elements. *Nucl. Sci. Eng.* **2017**, *187*, 213–239. [CrossRef]
6. Hino, T.; Miwa, J.; Murakami, Y.; Mitsuyasu, T.; Soneda, H.; Lindley, B.; Tollit, B.; Smith, P.; Shirvan, K.; Downar, T.; et al. Core Design of RBWR (Resource-renewable Boiling Water Reactor) and Benchmark Calculation of Core Analysis Tools. In Proceedings of the ICAPP2019, Juan-les-Pins, France, 12–15 May 2019.
7. Hino, T. Research needs for BWR core and core analysis. In Proceedings of the Conference and Workshop on the Research Needs of Boiling Water Reactors, Bangor, UK, 25–27 October 2016.
8. Lui, Y. A Full Core Resonance Self-Shielding Method Accounting for Temperature-Independent Fuel Subregions and Resonance Interference. Ph.D. Thesis, University of Michigan, Ann Arbor, MI, USA, 2015.
9. Kim, T.; Yang, W.; Taiwo, T.; Smith, M. Preliminary assessment of lattice physics capabilities for VHTR analysis. In Proceedings of the ANS Winter Meeting, Washington, DC, USA, 14–18 November 2004.
10. Kim, Y.; Baek, M. Elimination of double-heterogeneity through a reactivity-equivalent physical transformation. In Proceedings of the International Conference on Nuclear Energy Systems for Future Generation and Global Sustainability, Tsukuba, Japan, 9–13 October 2005.
11. Noh, J.; Kim, K.; Kim, Y.; Lee, H. Development of a computer code system for the analysis of prism and pebble type VHTR cores. *Ann. Nucl. Energy* **2008**, *35*, 1919–1928. [CrossRef]
12. Rohde, U.; Merk, B.; Baier, S.; Fridman, E.; Dürigen, S.; Kliem, S.; Weiss, F. Development of a reactor dynamics code for block-type HTR at Forschungszentrum Dresden-Rossendorf. In Proceedings of the Fachtag der KTG: "Aktuelle Themen der Reaktorsicherheitsforschung in Deutschland", Dresden, Germany, 7–8 October 2010.
13. Kim, Y.; Kim, K.; Noh, J. Preservation of Fuel Characteristics in the RPT Method. In Proceedings of the Spring Meeting of the Korean Nuclear Society, Gapyoung, Republic of Korea, 22 December 2006.
14. Miwa, J.; Hino, T.; Mitsuyasu, T.; Nagaya, Y. Whole-core Monte Carlo burnup calculation for RBWR by parallel computing. In Proceedings of the Joint International Conference on Supercomputing in Nuclear Applications + Monte Carlo 2020, Chiba, Japan, 18–22 May 2020.
15. Fridman, E.; Merk, B. Modification of the Reactivity Equivalent Physical Transformation Method for HTGR Fuel Element Analysis. In Proceedings of the 5th International Topical Meeting on High Temperature Reactor Technology, Prague, Czech Republic, 18–20 October 2010.
16. Rearden, B.; Jessee, M. *SCALE Code System, Manual*; Oak Ridge National Laboratory: Oak Ridge, TN, USA, 2017.
17. Lynch, S. Reactivity-Equivalent Physical Transformation Model or Pin Cell Arrays. Bachelor's Thesis, Massachusetts Institute of Technology, Cambridge, MA, USA, 2010.
18. Goluoglu, S.; Williams, M.L. Modeling Doubly Heterogeneous Systems in SCALE. *Trans. Am. Nucl. Soc.* **2005**, *93*, 963–965.
19. Rohde, U.; Baier, S.; Duerigan, S.; Fridman, E.; Kliem, S.; Merk, B. Development and verification of the coupled 3D neutron kinetics/thermal-hydraulics code DYN3D-HTR for the simulation of transients in block-type HTGR. *Nucl. Eng. Des.* **2012**, *251*, 412–422. [CrossRef]
20. Baldova, D. Feasibility Study on High-Conversion Th-U233 Fuel Cycle for Current Generation of PWRs. Ph.D. Thesis, Czech Technical University in Prague, Prague, Czech Republic, 2014.

21. Lou, L.; Chai, X.; Yao, D.; Peng, X.; Chen, L.; Li, M.; Yu, Y.; Wang, L. Research of ring RPT method on spherical and cylindrical Double-Heterogeneous systems. *Ann. Nucl. Energy* **2020**, *147*, 107741. [CrossRef]
22. Kulikowska, T. *Reactor Lattice Codes*; Lecture; Institute of Atomic Energy: Otwock, Poland, 2000.
23. Downar, T.; Hall, A.; Jabaay, D.; Ward, A.; Greenspan, E.; Ganda, F.; Bartoloni, F.; Bergmann, R.; Varela, C.; DiSanzo, C. *Technical Evaluation of the HITACHI Resource—Renewable BWR (RBWR) Design Concept*; Technical Report; Electric Power Research Institute: Palo Alto, CA, USA, 2012.