

Characterisation and Transport Modelling of Spent Nuclear Fuel from LWR SMRs

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ABSTRACT

It is commonly assumed that light water reactor (LWR) small modular reactor (SMR) spent nuclear fuel (SNF) can be disposed of in a similar manner as conventional LWR SNF [1][2]. However, some differences resulting from smaller core sizes have been reported [3]. Furthermore, fuel burnup in some LWR SMRs designs can be higher, up to 65 MWd/kgU [1], or significantly lower, below 20 MWd/kgU, than in current nuclear power plants (NPPs). In comparison, the burnups in current NPPs are typically up to 55 MWd/kgU [4]. This paper aims to compare LWR SMRs with different design burnups, and to some extent enrichments, and the resulting radionuclide release rates from a KBS-3 type repository. LDR-50 and the Rolls-Royce SMR have been selected for the assessment due to the large difference in their fuels design burnups, up to 18MWd/kgU and 65 MWd/kgU respectively, and the publicly available LDR lite benchmark model specifications for the LDR-50 [5]. The assessment will provide better understanding on how much the burnup affects disposability of LWR SMR SNF.

Characterisation of SNF for the two selected LWR SMR designs, LDR lite and the Rolls-Royce SMR, was performed using the continuous-energy Monte Carlo code Serpent version 2.2.2 [6]. The computational model was defined as a 2D infinite lattice geometry with reflective boundary conditions, representing typical 17x17 square lattice LWR fuel assemblies. Burnup simulations utilize Serpent's internal depletion solver [6] and repeated transport calculations to predict the isotopic inventory of a single fuel assembly at a time. Three different fuel assembly types were evaluated for the LDR lite, whereas only a single generic assembly was modelled for the Rolls-Royce SMR to provide a conservative estimate despite limited availability of design-specific information.

The radionuclide transport near-field model, used in this study, was based on earlier models for KBS-3 type repository [7]. The model consisted of a leaking copper canister, a bentonite buffer surrounding it in a deposition hole, and a backfilled disposal tunnel section. Diffusion was the main mode of radionuclide transport in the near-field model.

The SNF characterisation showed that the Rolls-Royce reactor had a larger inventory of fission products and a smaller inventory of fissile materials. The activity of the inventory was thus higher, leading into larger release rates from the repository. However, it needs to be determined to what extent this effect is due to the larger amount of SNF deposited in a single canister when using the Rolls-Royce assemblies and to what extent due to the discharge burnup. Both SMRs also had significantly lower peak annual release rates than the reference fuel, likely due to the omitting of activated impurities in the SMRs.

It also needs to be emphasised that the characterisation work had a lot other of assumptions as well. Thus, the results of this paper are indicative and can mainly be used as a first step in understanding how burnups affect the disposability of LWR SMR SNF. More thorough assessment needs to be carried out for the reactors that are designed to operate on either such high or low discharge burnups.

1 INTRODUCTION

Small modular LWRs differ from conventional LWRs on multiple aspects such as their power density, output power and reliance on passive safety systems. Their output power ranges from 10 MW_e in micro reactors up to 300 MW_e in larger models [8]. Their design is often simpler than in conventional NPPs and, due to the lower power density [8], they

can use passive cooling systems such as gravity or natural circulation of coolant.

Despite the differences, the reactors rely on conventional UO₂ fuel and light water coolant and thus it has been assumed that their SNF and low- and intermediate level waste (LILW) can be disposed in similar ways as ones produced by conventional NPPs [1][2]. Some differences in reactor core material activation [9][10] have been estimated with the main impact on volume of material to be disposed. The fuel enrichment and burnup however have a larger impact

on the properties of the spent nuclear fuel, with lower burnups leading to lower radioactivity and decay heating power, but higher post-irradiation reactivity [3] and vice versa on higher burnups.

The burnups and enrichments reported for LWR SMRs range from low values such as 20–25 MWd/kgU and 2–3% ^{235}U for the Finnish district heating reactor LDR-50 [11] up to high burnups such as 65 MWd/kgU for the Rolls-Royce SMR and high enrichment such as 19% ^{235}U for the STAR ENERGY SA SMR [1]. The differences raise the research question of this study: *How does SNF from LWRs using different burnups and to some extent enrichments differ.*

To answer this question, this paper compares and characterises the SNF of two LWR SMRs with different design burnups, enrichments and dimensions to determine how the radionuclide content of their respective SNFs differ. This is followed by comparing the resulting radionuclide near-field release rates from a KBS-3 type deep geological repository (DGR).

The Rolls-Royce SMR and LDR lite have been selected for the comparison. The former was selected as it had one of the highest discharge burnups of the current LWR-SMR designs, while the latter due to its low burnup and enrichment, and the availability of public model specifications [5] LDR lite is the publicly available benchmark specification for the Finnish LDR-50 SMR currently developed by Steady Energy.

The characterisation of the SNFs was performed using the continuous-energy Monte Carlo code Serpent version 2.2.2 [6] and is discussed further in Section 2. Assessing the radionuclide release rates from the DGR near-field was carried out by simulating the repository radionuclide transport in the vicinity of a leaking disposal canister, through the bentonite buffer and a section of the backfilled tunnel. The radionuclide transport is further discussed in Section 3.

2 SNF CHARACTERISATION

2.1 SNF Characterisation

The characterisation of SNF for the selected LWR SMRs is performed using the continuous-energy Monte Carlo neutron transport code Serpent version 2.2.2 [6]. The modelling approach chosen describes a typical 17x17 square LWR fuel assembly in an axially infinite 2D lattice geometry with reflective boundary conditions to effectively neglect axial leakage effects. Results are normalized to a

power density corresponding to full power operation. Burnup calculations utilize Serpent's integrated depletion solver, which iteratively couples neutron transport with isotopic depletion across discrete fuel burnup intervals. This methodology enables precise estimation of the nuclide inventory throughout the fuel lifecycle. The activation of cladding and steel components are included in the simulations and all assemblies are subject to an additional 30-year decay period following the removal from the core to more accurately represent the final disposal conditions. To mitigate inaccuracies resulting from isotopic results being averaged across the geometry, burnable materials are divided into burnup regions. All fuel rods, cladding tubes, and guide tubes are treated as separate depletion regions, and the rods doped with burnable absorbers are further subdivided radially into 10 equal-volume rings. The model geometry and depletion divisions are visualised in Figure 1.

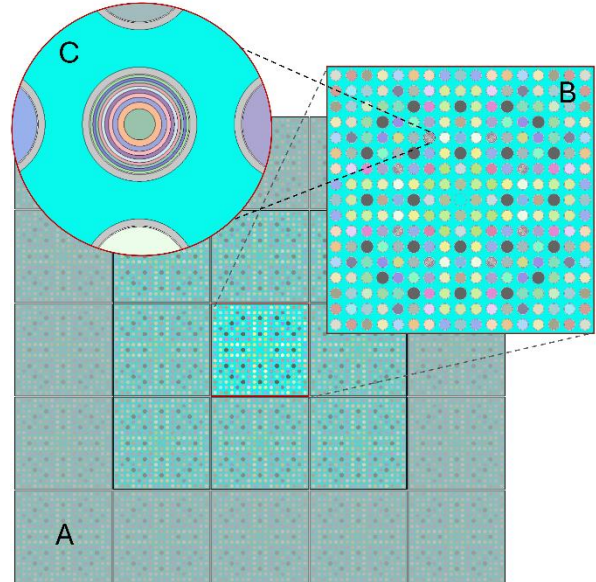


Figure 1: A) The modelled single assembly forms an effectively infinite lattice geometry that continues in both coordinate directions using reflective boundary conditions. B) The assembly geometry, the different colours represent depletion zones. C) The gadolinium doped fuel rods are further divided into 10 radial depletion zone rings.

The model specifics of the LDR lite are well documented in [5]. The 50 MW_{th} district heating reactor core is small, consisting of 37 PWR low enriched uranium (LEU) fuel assemblies with an active height of 100 cm and a total initial heavy metal mass of 5300 kg. The calculation model of the LDR described in this paper is based the published specifications of the LDR lite. For the LDR fuel case three distinct fuel assembly configurations are modelled. Assembly types B and C consist of fuel

enriched to 2.4% ^{235}U , whereas assembly type A is enriched only to 1.5% ^{235}U . Each assembly incorporates burnable Gd_2O_3 absorber intermixed into the fuel across eight rods with absorber concentrations of 9.0%, 5.0%, and 6.0% for assembly types B, C, and A respectively. Fuel assembly types B and C are depleted for approximately three full power operational cycles, achieving a cumulative discharge burnup of 18 MWd/kgU. In contrast, assembly type A represents a centrally positioned assembly depleted over a single operational cycle reaching a lower discharge burnup of only 6 MWd/kgU.

The Rolls-Royce SMR is considerably larger than the LDR lite with an operational power of 1358 MW_{th}. Detailed design specifications for the reactor are not readily available. Therefore, the information available in the NEA SMR handbook [1] is utilized along with conservative assumptions to achieve results fit for a preliminary analysis. The core of the Rolls-Royce SMR contains 121 PWR fuel assemblies at enrichments up to 4.95% ^{235}U . Active height of the core is specified at 280 cm, resulting in an initial heavy metal mass of approximately 48 500 kg. The use of gadolinium based burnable absorbers is mentioned in the specification sheet. Therefore, for this paper it is assumed that the absorber placement and concentration is equal to that of the LDR assembly type B with eight rods at 9.0% of Gd_2O_3 . Due to the preliminary nature of the study, only a single fuel assembly type is modelled, with fuel rods enriched to reported maximum of 4.95% ^{235}U and depleted to a discharge burnup of 65 MWd/kgU. By modelling the highest enrichment assembly type, conservative estimates for disposal of all possible assembly types are obtained. Specifications for both SMRs assemblies are summarised in Table 1.

Table 1: Assembly specifications for the two SMRs

Assembly type	Initial ^{235}U enrichment	Initial Gd concentration
LDR lite - A	1.50%	6.00%
LDR lite - B	2.40%	9.00%
LDR lite - C	2.40%	5.00%
Rolls-Royce SMR	4.95%	9.00%

2.2 Canister loading

Criticality safety assessments for the different SNFs were outside the scope of this study. For the conventional SNF, a reference inventory and canister loading by [12] used also in [7] were used in this paper. For the LDR and Rolls-Royce SMR, it was

assumed that an EPR-style disposal canister fitting four 17x17 assemblies [12] would be used.

Earlier preliminary criticality safety calculations for the LDR lite fuel have been carried out in [13] which showed that 2.4% ^{235}U SNF could be disposed in such a canister with a fresh-fuel assumption, meaning that no burnup would need to be accounted for (burnup-credit). For this paper, the burnup of the LDR lite fuel is 18 MWd/kgU. Thus, an assumption of loading a canister, with the SNF mass of four 100 cm assemblies was made. For the assemblies, the ones enriched to 2.4% U-235 with 5% Gd were selected for a conservative assumption regarding radionuclide transport modelling.

For the Rolls-Royce SMR, unfortunately no criticality safety assessments for the EPR-style disposal canister have been published. As it has the same enrichment as the EPR fuel, but a higher burnup, a rough preliminary assumption was made that four Rolls-Royce SMR assemblies could be disposed in the canister. This assumption should however be investigated further. As the Rolls-Royce SMR assemblies are larger than the LDR lite ones, also the canister considered in this study has 2.8 times the SNF mass respectively.

3 RADIONUCLIDE TRANSPORT MODELLING

The radionuclide transport modelling in this paper adopts the approach described in [7] for the Posiva repository in the reference case (BS-RC). The approach was selected as it has been used for the KBS-3 type of repository and thus uses realistic input parameters and boundary conditions suitable for the SMR SNF comparison.

According to the approach, the radionuclide transport model is split into near-field and geosphere models. However, for this paper, only a near-field model is considered. The near-field model consists of a disposal canister filled with SNF, bentonite filled deposition hole, a section of the backfilled disposal tunnel and interfaces to the surrounding bedrock. A pinhole is assumed to appear in the canister 1000 years after disposal as in the BS-RC scenario [7]. The modelling was carried out using GoldSim software. The inventory of the SNF is split into the fuel pellets, the cladding, other metal parts and the instant release fraction (IRF). However, as the inventory in the IRF was not determined (Section 2), it is also omitted here.

In the approach, the main release processes of the near-field model include the degradation of the SNF inventory, diffusion through the small defect in

the canister, diffusion through the bentonite and backfill, and finally advective transport from the near-field model to the geosphere. In total, there are three release points to the geosphere-model; one from the disposal hole, the second from the tunnel excavation damage zone and the third from the deposition tunnel [7]. The main retention mechanisms are linear sorption on the solid materials and the solubility of the elements including radionuclides and stable isotopes.

In this paper, same input parameters and model geometries are used as in [7] but the radionuclide inventory inside the copper canister is changed to the inventories of LDR lite and Rolls-Royce SMR from Section 2. For the SMR inventories, no non-radioactive isotopes of the inventory species were added. For this study, the length of the disposal canister is not varied, despite the different lengths for the LDR lite and Rolls-Royce assemblies compared to the reference fuel. Instead, the mass and resulting inventory is based on the characterisation work but inserted into a canister used for the reference fuel [7]. The relevant radionuclide transport occurs from the top of the canister, and thus the effect of the length of the canister below the pinhole in the canister is small.

The near-field model results were verified against the results of [7] for generic Finnish conventional SNF, and those results are also used to compare the two SMRs here (without IRF) as seen in Section 4.2.

4 RESULTS

4.1 SNF Characterisation

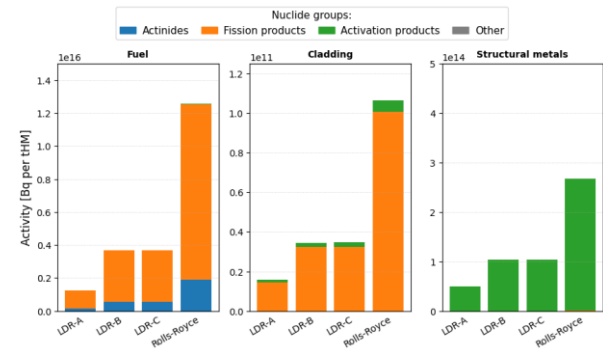
The simulations produced time-dependent isotopic compositions for each modelled assembly type. For the LDR, assemblies reached the specified discharge burnup of 6 MWd/kgU or 18 MWd/kgU over one or three full-power operational cycles, respectively, while the Rolls-Royce SMR assembly attained a discharge burnup of 65 MWd/kgU over a slightly longer, but comparable operational period. The substantially higher power density of the Rolls-Royce SMR core compared to the LDR core accounts for the significantly greater achieved fuel burnup. Assembly specific burnup parameters are summarised in Table 2.

Table 2: Assembly burnup periods

Assembly type	Burnup MWd/kgU	Total depletion time days
LDR lite - A	6.0	560
LDR lite - B	18.0	1682
LDR lite - C	18.0	1682
Rolls-Royce SMR	65.0	2041

The results follow the expected trend, higher burnup scenarios show greater depletion of fissile isotopes and production of fission products, accompanied by increased build-up of higher actinides such as americium and curium. The high burnup Rolls-Royce scenario resulted in significantly larger inventories of fission and activation products both in fuel and structural components, attributable to its longer irradiation time and higher cumulative neutron fluence. These are visualized in Figure 2 across material wise categories for all assembly types.

A)



B)

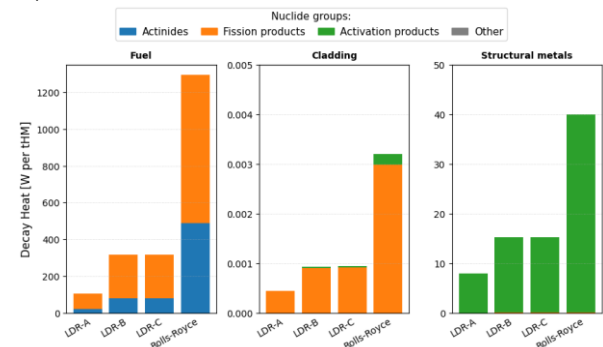


Figure 2: Material-wise burnup inventories at EOL after a 30-year decay period. Nuclide tallies are grouped into actinides, fission products, and activation products to illustrate the composition of the materials in further detail. A) Activity in becquerels normalised to tons of initial heavy metal. B) Decay heat in watts normalised to tons of initial heavy metal.

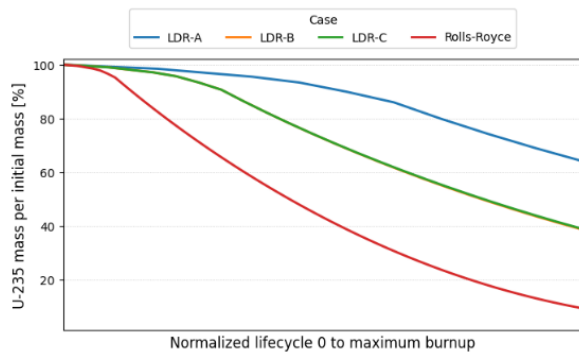


Figure 3: Relative evolution of initial fissile mass across the full operation periods as defined in Table 1 for each assembly type. X-axis is normalized for equality and is not to scale between the cases.

Interestingly, even the higher burnup LDR assemblies B and C retain substantial residual fissile inventories at end-of-life (EOL). This is visualised in Figure 3 by plotting relative initial fissile inventory across the operation period. The relative residual ^{235}U inventory of the LDR high-burnup assemblies at EOL is nearly four times that of the Rolls-Royce SMR, indicating that fuel utilisation efficiency is greatly limited by core design and operational constraints. The high residual ^{235}U inventory may, for example, influence repository criticality assessments.

The isotopic burnup inventories at EOL and after the 30-year post removal decay period include actinides, fission products, and activation products, present in fuel, cladding, and guide tubes. The selection of nuclides chosen for further safety analyses follows the set of 41 key nuclides identified in [14] as most relevant to repository safety, based on long-term radiotoxicity, heat generation potential, and mobility under disposal conditions. The results presented here provide the basis for the subsequent analysis of radionuclide release and transport behaviour in the KBS-3 disposal concept.

4.2 Radionuclide release rate

To compare the SNFs with each other, the release of the key mobile radionuclides for the KBS-3 specified in [7] from the near-field into fracture intersecting a deposition hole were analysed. The results are presented in Figure 4, Figure 5 and Figure 6. The total release, peak release rate and the time of the peak, over the 1 000 000 years of simulation for the fracture intersecting the bentonite buffer, are presented in Table 3.

Table 3: Total release, peak release rate and time of the peak in the fracture intersecting the bentonite buffer, during the 1 000 000 simulated years.

	Reference fuel	LDR lite	Rolls-Royce SMR
Total release [GBq]	6.8	2.9	8.9
Peak release rate [Bq/yr]	50200	8670	9880
Time of peak release rate [a]	3300	140000	350000

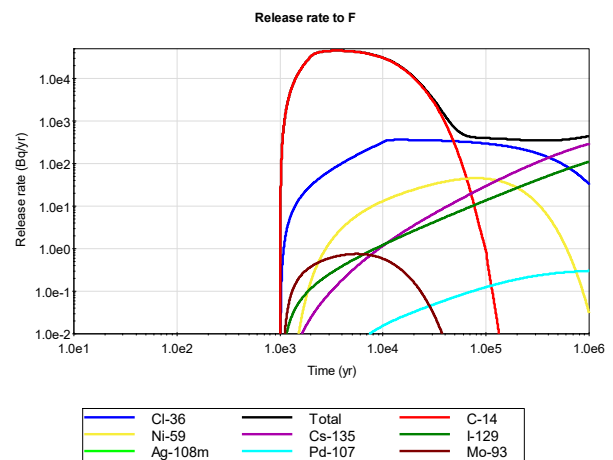


Figure 4: Release rates of the key mobile radionuclides into a fracture intersecting the deposition hole, for the reference fuel excluding IRF.

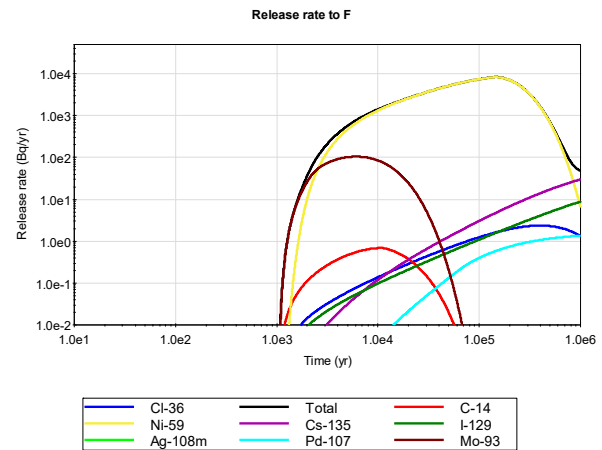


Figure 5: Release rates of the key mobile radionuclides into a fracture intersecting the deposition hole, for the LDR lite spent fuel.

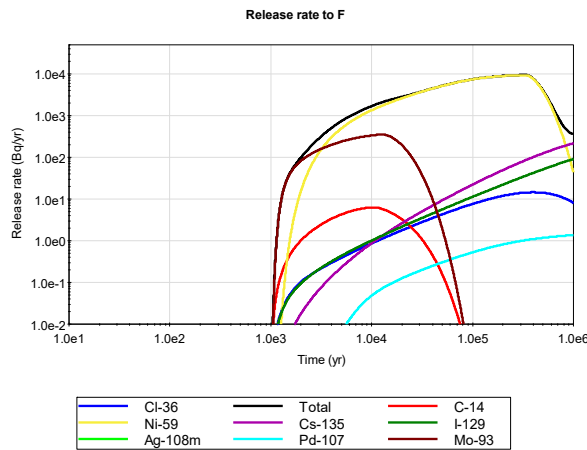


Figure 6: Release rates of the key mobile radionuclides into a fracture intersecting the deposition hole, for the Rolls-Royce SMR spent fuel.

5 DISCUSSION

5.1 SNF Characterisation

In the LDR lite assemblies, the usage of the initial fissile inventory is low due to the lower burnup. This means that a low amount of the fissile material is depleted into fission products. This could lead to higher risk of post-irradiation criticality incidents, but due to the low initial enrichment, the post-irradiation multiplication factor is likely low and a fresh fuel assumption for a disposal canister could possibly be made [13].

It should also be noted, that for the LDR reactor, the LDR lite benchmark parameters are preliminary, and later actual operation would show what burnups are achievable. The LDR reactor does not inherently mean low burnup operation, but low power density. This could in theory lead into longer operation periods without refuelling.

The Rolls-Royce reactor on the other hand depleted a larger fraction of the initial fissile material due to its higher burnup. This led into a larger inventory of fission products. However, it should be considered that only one assembly type was modelled here, and it most likely represents the hottest assembly using the assumed operating parameters of this paper. Further investigation using more realistic operating parameters should be carried out if such become available for the Rolls-Royce SMR.

For both reactors a cooling time of 30 years was used. Realistically this would be adjusted to fit the realistic decay heat and radioactivity of the SNF, so it could be shorter for a low-burnup SNF or longer for a higher burnup one.

5.2 Radionuclide transport modelling

When comparing both SMR SNF release rates to the reference fuel, it can be seen that the relationships between some of the radionuclides greatly differ. In the reference fuel, ^{14}C is the main contributor to the dose, while in the SMRs they are ^{59}Ni and ^{93}Mo . All three radionuclides are mostly present in the other metal parts. Nitrogen impurities are one of the main contributors to ^{14}C production in the metallic parts of the assemblies [15]. Impurities were excluded from the calculations of Section 2.1, which could explain the drastic decrease of ^{14}C in the SMR SNF. ^{36}Cl release is also significantly lower in the SMR-SNF. It is also mainly present in the zircaloy and other metallic parts and is an activation product of chlorine impurities. For a more thorough analysis of the differences between the conventional SNF and the SMR SNF, characterisation including impurities should be carried out.

The higher release of nickel and molybdenum observed in the SMR SNF likely stems from usage of steel with a higher Ni and Mo contents [5], resulting in the high amount of activated ^{59}Ni and ^{93}Mo .

Other radionuclides, present mainly in the SNF such as ^{135}Cs and ^{129}I have fewer relative differences between the reactors, especially when comparing the reference fuel and the higher burnup Rolls-Royce SMR fuel.

When comparing the two SMRs, the effects of the different enrichment and burnup can be observed. The total release from the near-field is three times larger in the Rolls-Royce reactor when compared to the LDR lite. However, it should be noted that the mass of Rolls-Royce reactor SNF in the canisters for the is 2.8 times the mass of LDR lite fuel. One option for the disposal of the small LDR lite assemblies or canisters could be stacking two of them on top of each other if both mechanical strength of the canister and the bedrock as well as criticality safety would allow to do so [13].

Another aspect to investigate further is the effect of the higher burnup on the degradation rates of the different SNFs. In this study the degradation rates of the fuel pellets, the cladding and other metal parts were assumed constant and same for all the reactor types, but higher burnups lead into a more degraded fuel and vice versa with low burnups. If this effect would be considered in the degradation rates of the model, the release rates of the high-burnup SMR would likely be higher than with the current assumption, while the values for lower burnup respectively lower.

Interestingly, despite the large difference in the total release rate, the peak release rate between the

SMRs is rather small (14%). This could be explained by the solubility limit of nickel ($8.30\text{E-}4$ mol/l [7]), but nickel did not precipitate in the model. Further investigation to understand the difference between the rates should be carried out.

When comparing the peak annual release rate to the reference fuel, the values for both SMRs are significantly lower. However, this is most likely explained by the lack of impurities leading to ^{14}C activation in the SMRs.

To better understand how large effect the burnup has on the increased release rate, it would be useful to compare canisters with a normalised SNF loading. While this would not depict a realistic disposal scenario, it would isolate the changes in radionuclide release solely to the burnup. Another option when comparing SMRs would be to compare disposed SNF per unit of energy produced. The comparison would then better answer the question on whether SMRs produce more SNF in comparison to conventional NPPs, discussed for example by [17], and if so, under what operating conditions. However, even with such comparison it should be noted, that a reactor solely producing district heat would probably be very different from a reactor producing electricity.

The comparison of the LDR lite and Rolls-Royce SMR release rates (Figure 3 and Figure 4) shows that the shape of some radionuclide graphs are tilted towards later time for Rolls-Royce SMR. This is explained by the different locations of these radionuclides in the inventory. For example, there is relatively more ^{59}Ni and ^{93}Mo in the fuel and the cladding in comparison to the other metal parts in the Rolls-Royce SMR than in LDR lite (

Table 4). As both the fuel and the cladding have slower degradation rates than the other metal parts, the radionuclides in Rolls-Royce SMR case are released slower than in the LDR lite case. The differences in the inventories result from the different activation of the fuel parts in the Rolls-Royce SMR and LDR lite.

Table 4: ^{59}Ni and ^{93}Mo inventories in LDR lite and Rolls-Royce SMR spent fuels.

	Inventory	Fuel	Cladding [%]	Other metal parts [%]
LDR lite				
^{59}Ni	360 GBq	$1.4\text{E-}11$	$5.7\text{E-}13$	~ 100
^{93}Mo	4.6 GBq	$2.2\text{E-}5$	$3.8\text{E-}7$	~ 100
RR-SMR				

^{59}Ni	2.3 TBq	$2.3\text{E-}11$	$7.8\text{E-}12$	~ 100
^{93}Mo	47 GBq	$1.1\text{E-}4$	$1.7\text{E-}6$	~ 100

6 CONCLUSIONS

In this study, characterisation of two LWR-SMRs, the LDR lite and the Rolls-Royce SMR were carried out using Serpent. The former reactor had a lower fuel enrichment and discharge burnup than the latter. The post-irradiation activity, decay heat and radionuclide inventories were determined. The characterisation showed that with the lower burnup of the LDR lite, less fissile material was converted into fission products during reactor operation when comparing to the original ^{235}U mass, than with the Rolls-Royce reactor. The radionuclide inventory of the high-burnup reactor was actinide rich and full of fission products. Thus, both the activity and decay heat of the Rolls-Royce SMR were significantly higher than with the LDR lite.

For the radionuclide transport modelling, a simple near-field transport model consisting of a SNF filled copper canister with a small pinhole appearing at 1000 years, a bentonite filled deposition hole and a backfilled section of the disposal tunnel was created in GoldSim software. Radionuclide release rates to an advective fracture intersecting the deposition hole were determined.

The results showed that the radionuclide releases differed significantly between the reference fuel of conventional LWR power plants and with the two LWR SMRs. The total release was the highest for the high-burnup Rolls-Royce SMR and the lowest for the low-burnup LDR lite. However, the characterisation work excluded contaminants in the SMR fuel and thus releases of radionuclides such as ^{14}C and ^{36}Cl , typically associated with activation of contaminants, were significantly lower for the SMR SNFs than the conventional LWR SNF. Therefore, including contaminants in SNF comparisons is important in future studies on the topic.

It could however be noted that the share of ^{59}Ni and ^{93}Mo , both nuclides activated in the steel parts of the fuel assemblies, were higher in both SMRs than in the reference fuel. This is likely due to different steel composition in comparison to the reference fuel.

When comparing the two SMRs, expectedly the Rolls-Royce assemblies lead to higher release rates than the LDR lite. This is both due to the higher discharge burnup and longer assembly size of the former. For a more thorough assessment of the discharge burnups effect only, a comparison with canisters loaded with equal SNF masses should be performed. However, even without the inclusion of contaminants and their activation products, and the

difference in canister loading, the high-burnup Rolls-Royce SNF had the highest total release from the near field. Thus, further studies to understand the disposability of high-burnup fuel in a KBS-3 repository are highly recommended. Such studies should include comparison of longer cooling times and more realistic canister loading. In addition, the effect of the geosphere on the transport modelling should be included.

Further, in assessing the long-term safety of repository for spent SMR fuel, topics like the SNF's potential for criticality, fuel dissolution rate at relevant chemical conditions, radiation effects on the canister performance, effect of heat generation on the near-field evolution and gas generation from the SNF need to be addressed.

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