

Criticality Sensitivity Analysis of a Generic Spent Nuclear Fuel Disposal Cask

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ABSTRACT

Criticality safety is one of the key challenges in the design of disposal concepts for spent nuclear fuel. This work presents a criticality sensitivity analysis of a generic spent nuclear fuel disposal cask concept proposed within the EURAD-2 WP17 project (CSFD – Criticality Safety for Final Disposal). The study aims to quantify the impact of relevant design and degradation parameters on the effective neutron multiplication factor and to provide input for the derivation of spent fuel loading curves.

Fresh fuel configurations are considered as a reference, including uranium enrichments of 2 %, 3 %, 4 %, and 5 % and two common fuel assembly types (16×16 and 17×17). Several criticality-relevant cases are investigated, focusing on the positioning of fuel assemblies within the cask boxes, variations in water density, variations in the pin-by-pin lattice pitch, and changes in the thickness of structural material between assembly compartments. In addition, long-term degradation effects are addressed by analysing stainless steel insert corrosion and the formation of a magnetite layer, which may influence neutron moderation and reflection behaviour over disposal timescales.

All calculations are performed using the Serpent2 Monte Carlo code with nuclear data libraries ENDF/B-VII.1 and ENDF/B-VIII.1, allowing for comparison of cross-section impacts on sensitivity results. The outcomes of this work contribute to a better understanding of parameter-driven uncertainties in disposal cask criticality assessments and support the development of robust safety margins for final repository concepts.

Keywords: *spent nuclear fuel disposal, criticality safety, sensitivity study*

1 INTRODUCTION

The disposal of spent nuclear fuel is one of the major challenges in modern nuclear energy, as it requires ensuring safety over timescales of thousands to hundreds of thousands of years. Spent fuel contains highly radioactive and long-lived radionuclides, which necessitates the development of reliable disposal solutions. Deep geological repositories are widely considered the most viable option, combining engineered and natural barriers to isolate the waste from the biosphere [1].

A key aspect of repository safety is criticality safety, which ensures that no uncontrolled nuclear chain reaction can occur under any conditions, including potential material degradation or changes in environmental parameters over time. Maintaining the effective neutron multiplication

factor (k_{eff}) well below unity is therefore essential for the design and safety assessment of disposal systems. Within this context, the EURAD-2 programme, and in particular the Criticality Safety for Final Disposal (CSFD) - work package 17, addresses key methodological and technical challenges associated with demonstrating long-term subcriticality in geological disposal systems [2,3].

Disposal cask concepts typically involve multiple fuel assemblies arranged within structured compartments, using materials that provide mechanical stability and influence neutron moderation and reflection. Water, in particular, plays a significant role as a moderator, and its presence or variation in density can strongly affect system reactivity. These systems must remain subcritical throughout their entire lifetime, including during long-term degradation processes such as corrosion of structural materials or the formation of secondary compounds [4].

Given the complexity of these systems and the range of uncertainties involved, sensitivity analysis is a crucial tool for understanding how variations in design and environmental parameters impact criticality. It enables the identification of the most influential factors affecting k_{eff} and supports the development of conservative safety margins and optimized cask designs.

The objective of this study is to perform a criticality sensitivity analysis of a generic spent nuclear fuel disposal cask. The focus is on quantifying the impact of key design parameters, fuel configurations, and long-term degradation effects on neutron multiplication. In addition, the study aims to provide input for the derivation of spent fuel loading curves.

The remainder of this paper is organized as follows: first, the methodology and cask model are described, followed by a presentation of the analysed cases and input parameters. The results of the sensitivity analysis are then discussed, and finally, the main conclusions and implications for disposal system design are provided.

2 METHODOLOGY

2.1 Description of the Disposal Cask Model

The analysis is based on the EURAD-2 WP17 Task 5 reference model [5], version 6.2.1, which represents a simplified disposal canister for PWR fuel. The canister consists of a cylindrical copper shell (outer diameter 100 cm, inner diameter 90 cm, height 440 cm) with an internal stainless-steel insert. The insert contains four rectangular compartments (25×25×410 cm) arranged symmetrically with a spacing of 5 cm. Radial and axial cross-sections are presented in Figure 1.

Due to geometrical symmetry, only one quarter of the system is modelled, corresponding to a single fuel assembly, with reflective boundary conditions applied on the symmetry planes and black boundary condition at the outside surface of the copper shell.

Each compartment hosts a 17×17 or 16×16 PWR fuel assembly, modelled at the pin level with explicit representation of fuel, gap, and cladding. Simplifications include the omission of guide tubes, grid spacers, and end hardware. The active fuel region is centrally positioned, while non-active regions are replaced by water.

All void spaces within the compartment are assumed to be fully flooded with water, providing conservative moderation conditions. The main materials included in the model are UO₂ fuel, Zircaloy cladding, stainless steel, copper, and light water, all assumed homogeneous and at room temperature.

The reference configuration assumes intact geometry with nominal dimensions and material compositions, serving as a baseline for subsequent sensitivity analyses.

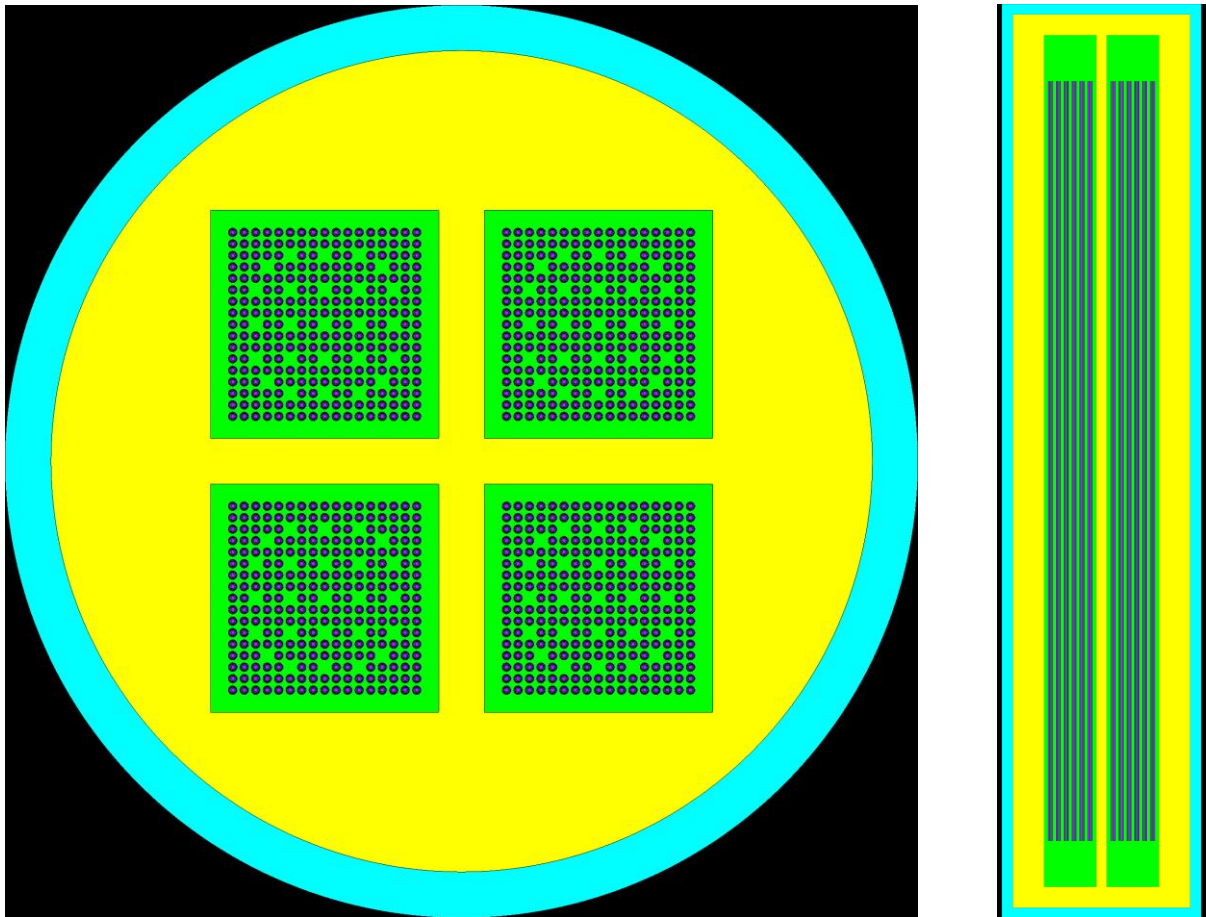


Figure 1: Horizontal and vertical cross-sections of the disposal cask model showing the copper overpack, stainless-steel insert, and fuel assembly compartment layout (17×17 configuration)

2.2 Fuel Characteristics

Four uranium enrichment levels are analysed: 2 wt.%, 3 wt.%, 4 wt.% (reference case), and 5 wt.% in ^{235}U .

The fuel assemblies are based on a typical 17×17 (pellet diameter of 0.8166 cm, cladding outer diameter of 0.955 cm and rod pitch of 1.26 cm) and 16×16 PWR lattice (pellet diameter of 0.8195 cm, cladding outer diameter of 0.95 cm and rod pitch of 1.2319 cm). The active fuel length in both cases is 365.76 cm and is centrally positioned within the rod and cask.

Fuel material is assumed to be uranium dioxide (UO_2), with isotopic compositions corresponding to the specified enrichment levels. The fuel is modelled as fresh, and thus no burnup credit is applied. This represents a conservative assumption, as the absence of neutron-absorbing fission products leads to higher reactivity.

2.3 Computational Approach

All criticality calculations are performed using the Serpent2 [6] Monte Carlo transport code. The Monte Carlo method enables high-fidelity simulation of neutron transport by tracking individual particle histories and probabilistically modelling interactions such as scattering, absorption, and fission. The Serpent2 (version 2.2.0 is used) is a Monte Carlo particle transport code widely used for academic studies, and is currently employed in over 150 universities and research institutions for a broad spectrum of reactor physics applications, from group constant generation and burnup calculations to research reactor modelling. Developed at the VTT Technical

Research Centre of Finland since 2004, Serpent is available for distribution through VTT and two data centres: the OECD/NEA Data Bank and the Radiation Safety Information Computational Centre (RSICC) in the United States, with various licensing options available for non-commercial research and education as well as commercial use.

The effective neutron multiplication factor (k_{eff}) is used as the primary metric for assessing criticality. For each configuration:

- A sufficient number of neutron histories (e.g., 30000) is simulated to ensure statistical convergence
- Multiple independent cycles are used to reduce bias (200 inactive plus 2000 active cycles)
- Convergence is verified through standard deviation and stability of k_{eff} values

The simulations assume:

- Steady-state conditions
- Isotropic neutron emission from fission sources
- Reflective and black boundary conditions

To assess the impact of nuclear data uncertainties, calculations are performed using two evaluated nuclear data libraries:

- ENDF/B-VII.1 [7]
- ENDF/B-VIII.1 [8]

These libraries provide cross-section data for neutron interactions across a wide energy range. They are used here to assess the sensitivity of the results to nuclear data selection. By comparing results obtained with both datasets, the sensitivity of calculated reactivity to nuclear data selection is evaluated.

3 RESULTS AND DISCUSSION

This section presents the results of the criticality calculations and their sensitivity to selected design and environmental parameters. The analysis is structured to first establish a reference case, followed by systematic variation of moderation conditions, geometrical parameters, and long-term degradation effects. The focus is placed on identifying dominant contributors to reactivity changes and assessing their relative importance for criticality safety.

3.1 Reference Case Results

The reference case provides a baseline for evaluating the impact of design and environmental variations on system reactivity. The calculated effective multiplication factors for both fuel assembly types and all enrichment levels are summarized in Table 1 and illustrated in Figure 2.

As expected, the effective multiplication factor increases monotonically with fuel enrichment for both 17×17 and 16×16 assembly types. For the 17×17 configuration, the system transitions from clearly subcritical at 2 wt.% enrichment ($k_{\text{eff}} \approx 0.885$) to supercritical already at 4 wt.% ($k_{\text{eff}} \approx 1.047$), with further increase at 5 wt.% ($k_{\text{eff}} \approx 1.089$). A similar trend is observed for the 16×16 lattice, although with consistently lower k_{eff} values due to its reduced moderation-to-fuel ratio and slightly tighter geometry. In this case, the system remains subcritical up to 4 wt.% ($k_{\text{eff}} \approx 0.980$) and becomes marginally supercritical at 5 wt.% ($k_{\text{eff}} \approx 1.018$).

The comparison between assembly types indicates that the 17×17 configuration is systematically more reactive by approximately 600–700 pcm across the analysed enrichment range.

This difference can be attributed to the larger moderator volume fraction in the 17×17 lattice, which enhances neutron thermalization and increases the probability of fission, while the slightly lower uranium inventory in the 16×16 lattice further contributes to this difference. While this behaviour is consistent with expectations, it highlights that lattice geometry remains a non-negligible design parameter even under otherwise identical conditions.

The comparison of nuclear data libraries reveals small but systematic differences. Calculations performed with ENDF/B-VII.1 consistently yield slightly higher k_{eff} values than those obtained with ENDF/B-VIII.1. The observed deviations range from approximately 20 pcm to 160 pcm, with larger differences appearing at higher enrichments. Although these discrepancies are relatively modest compared to typical safety margins, they are not negligible in the context of sensitivity analysis and may influence the ranking of dominant parameters. This suggests that nuclear data uncertainty should be considered as a relevant contributor to overall reactivity uncertainty.

It should be noted that all statistical uncertainties are low ($1\sigma \approx 10 - 13$ pcm), indicating good convergence of the Monte Carlo simulations. Therefore, the observed trends are dominated by physical effects rather than statistical fluctuations.

Due to space limitations, the remainder of the analysis is restricted to the 4 wt.% enrichment case, which is considered representative of typical PWR fuel.

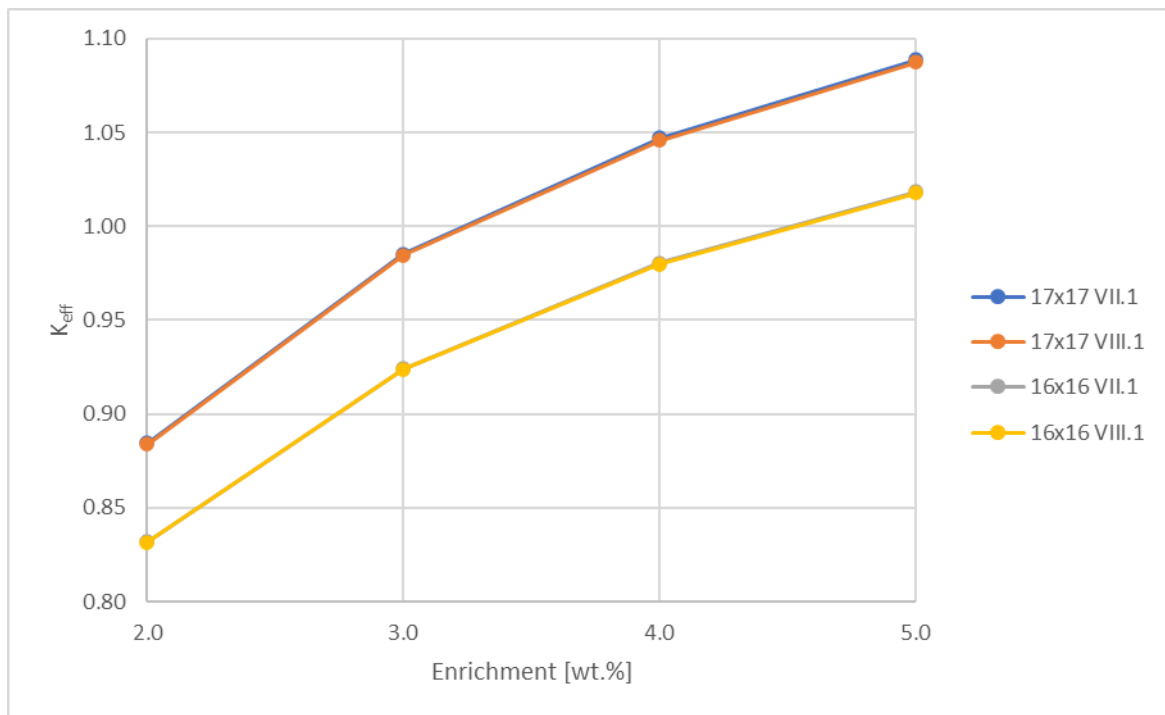


Figure 2: Effective multiplication factor (k_{eff}) as a function of fuel enrichment for 16×16 and 17×17 assemblies in the reference configuration

Table 1: Multiplication factors for the reference case

	ENDF/B-VII.1		ENDF/B-VIII.1		Diff. VII.1- VIII.1
17x17					
Enrichment	k_{eff}	1σ	k_{eff}	1σ	[pcm]
2.0	8.84650E-01	0.00012	8.83857E-01	0.00012	79.3
3.0	9.85514E-01	0.00012	9.84619E-01	0.00011	89.5
4.0	1.04720E+00	0.00011	1.04577E+00	0.00011	143.0
5.0	1.08897E+00	0.00011	1.08739E+00	0.00010	158.0
16x16					
2.0	8.31913E-01	0.00013	8.31564E-01	0.00013	34.9
3.0	9.24189E-01	0.00012	9.23982E-01	0.00012	20.7
4.0	9.80442E-01	0.00012	9.80007E-01	0.00012	43.5
5.0	1.01854E+00	0.00012	1.01785E+00	0.00012	69.0

An additional sensitivity test was performed to assess the impact of boundary conditions. By replacing the black boundary condition at the cask surface with a hypothetical periodic boundary condition in a compact hexagonal arrangement (Figure 3), the multiplication factor increased by approximately 538 pcm. This represents a significant reactivity increase and indicates that the assumed external boundary condition has a strong influence on neutron leakage. However, such configuration is not physically realistic for disposal conditions and overestimates the degree of neutron reflection.

This result nevertheless exposes a limitation of the current model: the absence of a realistic representation of surrounding materials (e.g., buffer, host rock) introduces uncertainty in the treatment of neutron leakage. As a consequence, the reference case may not fully capture realistic boundary effects that are expected in a repository environment. Further refinement of the external geometry is therefore recommended particularly for improved safety margin quantification.

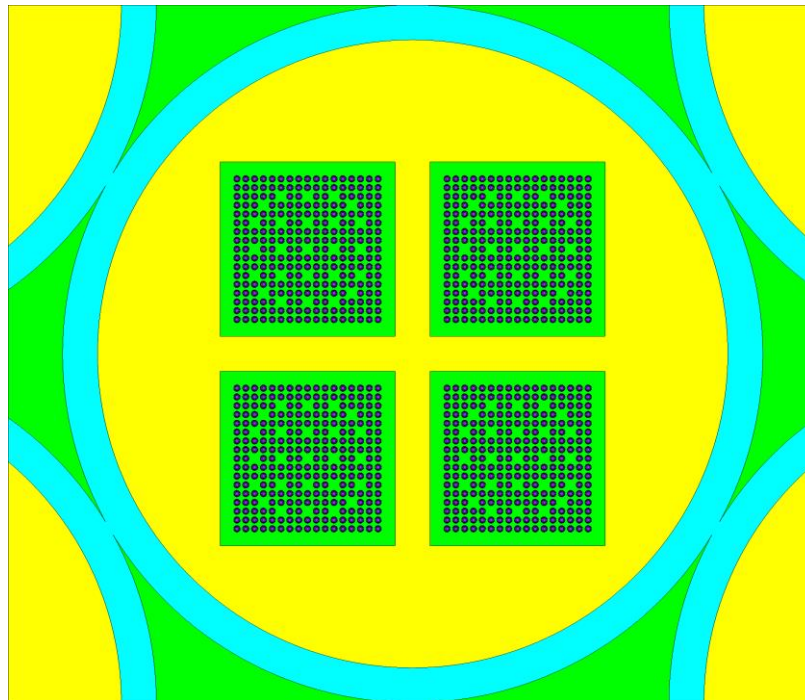


Figure 3: Representation of a hypothetical periodic boundary condition used to assess the impact of reduced neutron leakage compared to the reference black boundary condition

3.2 Sensitivity to Moderation Conditions

The impact of water density on the effective multiplication factor is presented in Figure 4. As expected, moderation conditions play a dominant role in determining system reactivity, given that all void spaces are assumed to be water-filled in the reference configuration.

The results indicate a monotonic decrease in k_{eff} with decreasing water density. No distinct maximum in reactivity is observed within the analysed range, which suggests that the system is under-moderated at nominal conditions. In other words, the reference configuration does not contain sufficient moderator to achieve optimal neutron thermalization, and any reduction in water density further degrades moderation efficiency, leading to a lower probability of thermal fission.

This behaviour is consistent with the relatively compact lattice geometry and the presence of structural materials (e.g., stainless steel insert), which reduce the moderator-to-fuel ratio compared to typical reactor conditions. As a result, neutron spectra remain relatively harder, and additional moderation would be required to reach peak reactivity.

From a safety perspective, this trend is relevant but should be interpreted with caution. While reduced water density (e.g., due to partial voiding or drying) leads to lower reactivity in this configuration, the opposite scenario - namely full saturation or potential ingress of additional moderating material - remains more limiting. The assumption of fully flooded conditions in the reference case is therefore conservative, but it may not fully envelope all possible long-term evolution scenarios, particularly if changes in geometry or material composition occur simultaneously.

It should also be noted that the absence of a clear moderation peak limits the identification of a “worst-case” density within the analysed range. This introduces some uncertainty in defining bounding conditions, especially if the system were to evolve towards configurations with increased moderation (e.g., due to degradation-induced porosity or redistribution of materials).

Overall, the sensitivity analysis confirms that moderation conditions are a key driver of reactivity, but their effect is strongly coupled with geometric and material parameters. Consequently, water density variations should not be evaluated in isolation, since their impact may be either amplified or mitigated by concurrent changes in system configuration.

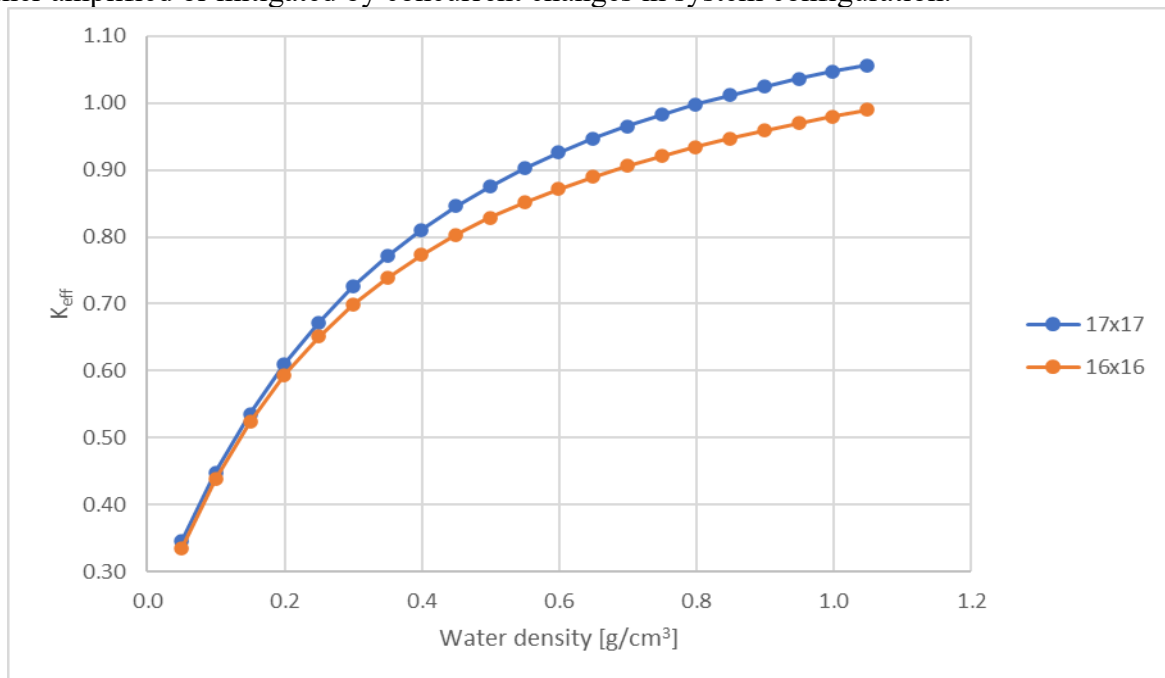


Figure 4: Dependence of k_{eff} on water density, illustrating the sensitivity of system reactivity to moderation conditions.

3.3 Sensitivity to Geometrical Parameters

The influence of geometrical variations on system reactivity was analysed through three main parameters: (i) fuel assembly positioning within the stainless-steel insert, (ii) thickness of the stainless-steel walls separating individual compartments, and (iii) pin-by-pin lattice pitch.

The effect of eccentric fuel positioning was evaluated by shifting the assembly along the diagonal of the compartment, both towards the centre of the cask and towards the outer wall (Figure 5). The results presented in Figure 6 indicate a relatively modest but systematic impact on k_{eff} . A shift towards the centre leads to a slight increase in reactivity, while displacement towards the outer boundary results in a decrease. This behaviour is primarily driven by changes in neutron leakage and coupling of the fuel assemblies between neighbouring compartments: configurations closer to the centre benefit from increased neutron reflection due to surrounding material and stronger neutron coupling of the fuel assemblies, whereas outward shifts enhance neutron escape and reduce fuel assembly coupling. Although the observed reactivity variation is limited, the trend is consistent and indicates that positioning tolerances may contribute to overall uncertainty, especially when combined with other effects.

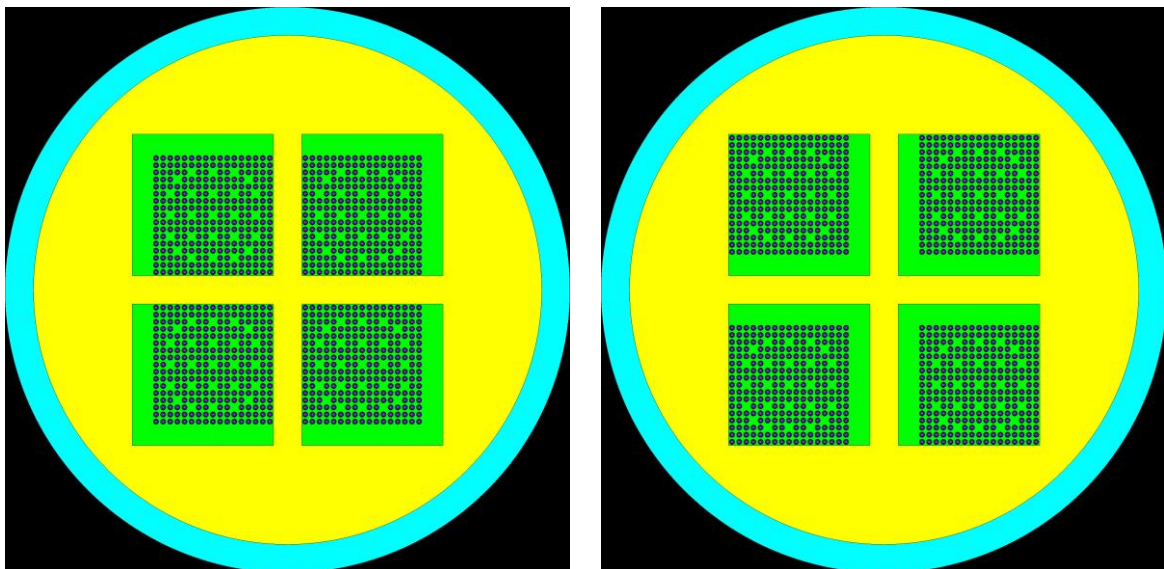


Figure 5: Schematic representation of diagonal fuel assembly repositioning within the compartment, illustrating inward and outward displacement relative to the cask centre

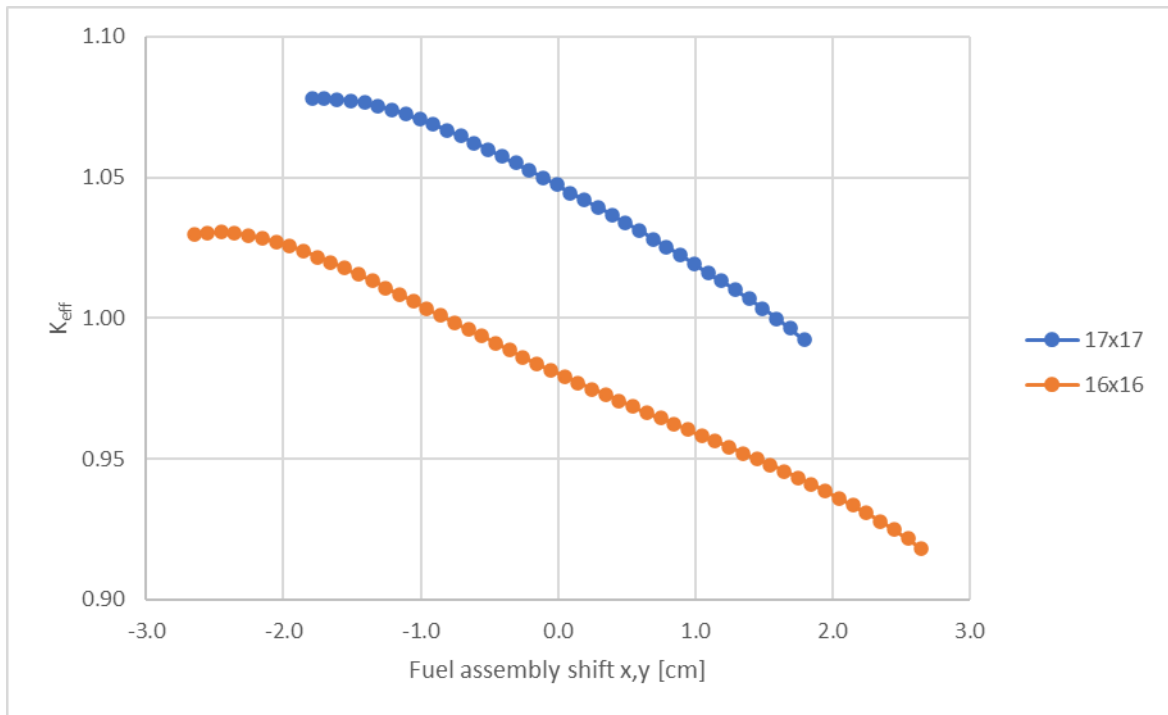


Figure 6: Variation of k_{eff} as a function of fuel assembly displacement from the compartment centre towards the outer boundary.

The thickness of the stainless-steel walls between adjacent compartments was varied to assess its role as a structural and neutronic barrier (Figure 7). As shown in Figure 8, increasing the wall thickness leads to a decrease in k_{eff} . This effect can be attributed to the reduced neutron coupling between neighbouring fuel assemblies, as thicker steel layers introduce additional absorption and scattering. Conversely, thinner walls allow for increased neutron interaction between compartments, effectively increasing system reactivity. Compared to fuel repositioning, this parameter exhibits a more pronounced impact, suggesting that structural design choices governing compartment separation are more influential from a criticality perspective.

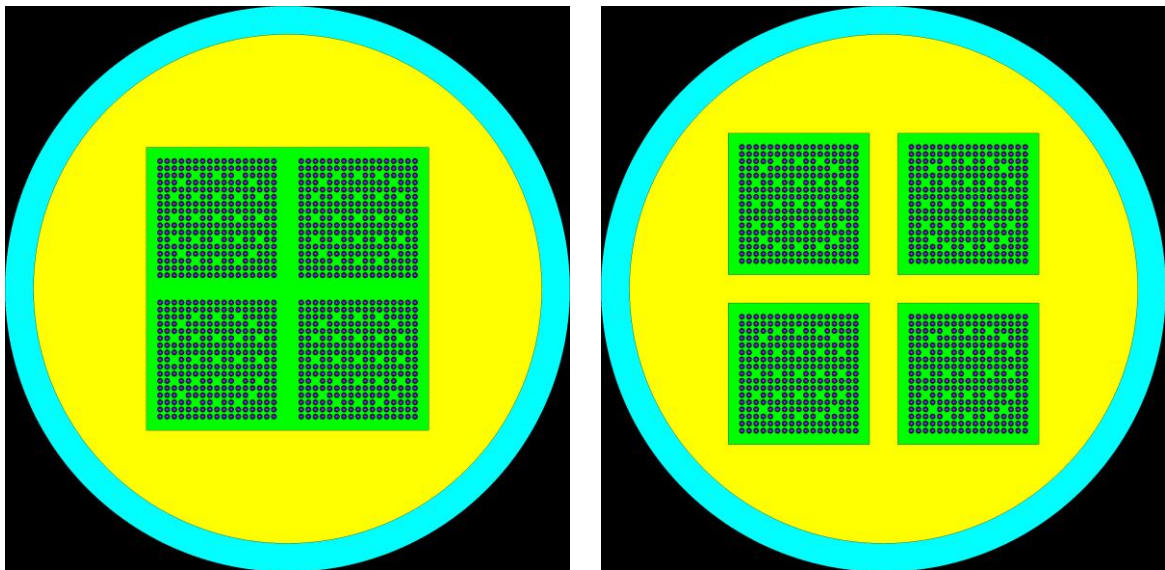


Figure 7: Schematic of the variation in stainless-steel wall thickness separating adjacent fuel assembly compartments

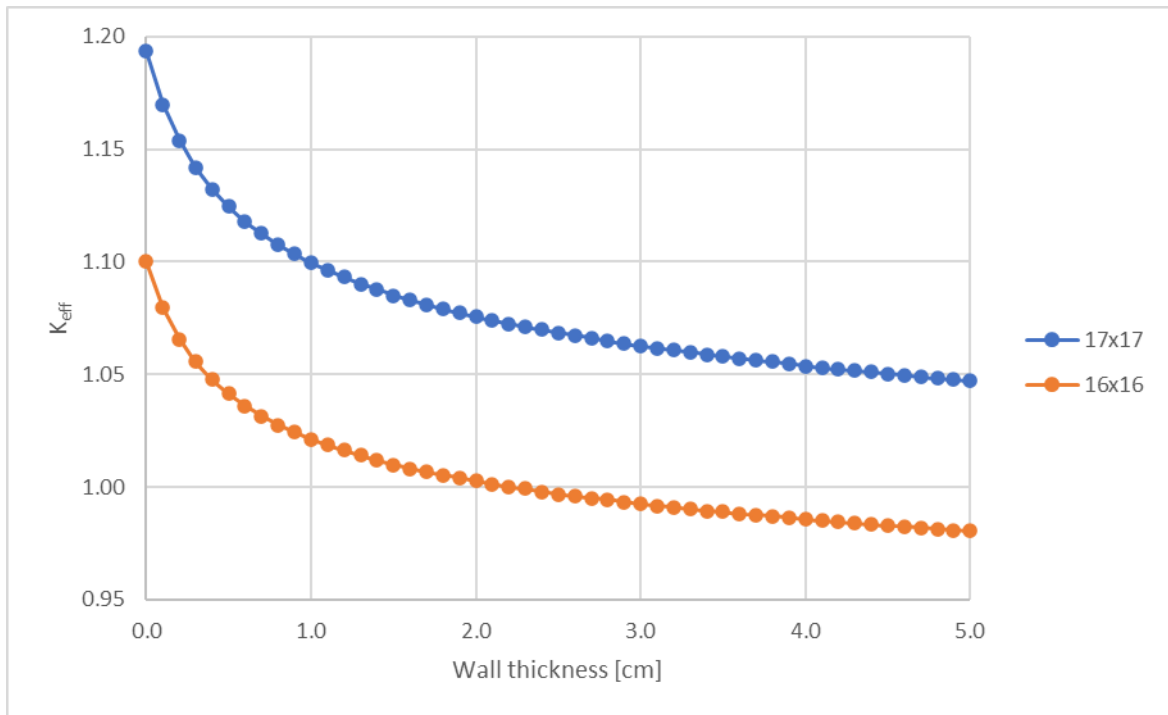


Figure 8: Effect of stainless-steel wall thickness on k_{eff} , showing reduced neutron coupling with increasing structural separation

The variation of pin-by-pin pitch within the fuel assembly (Figure 9) shows the strongest geometrical influence on reactivity (Figure 10). An increase in pitch results in higher k_{eff} , reflecting improved moderation conditions due to a larger moderator-to-fuel ratio. In contrast, a reduction in pitch leads to a more compact lattice with reduced moderation efficiency and consequently lower reactivity. This trend is consistent with classical lattice physics behaviour and confirms that even relatively small changes in lattice spacing can significantly affect neutron spectrum and neutron multiplication. The sensitivity to pitch is notably higher than for the other geometrical parameters considered, indicating that assumptions related to fuel geometry are critical for reliable reactivity predictions.

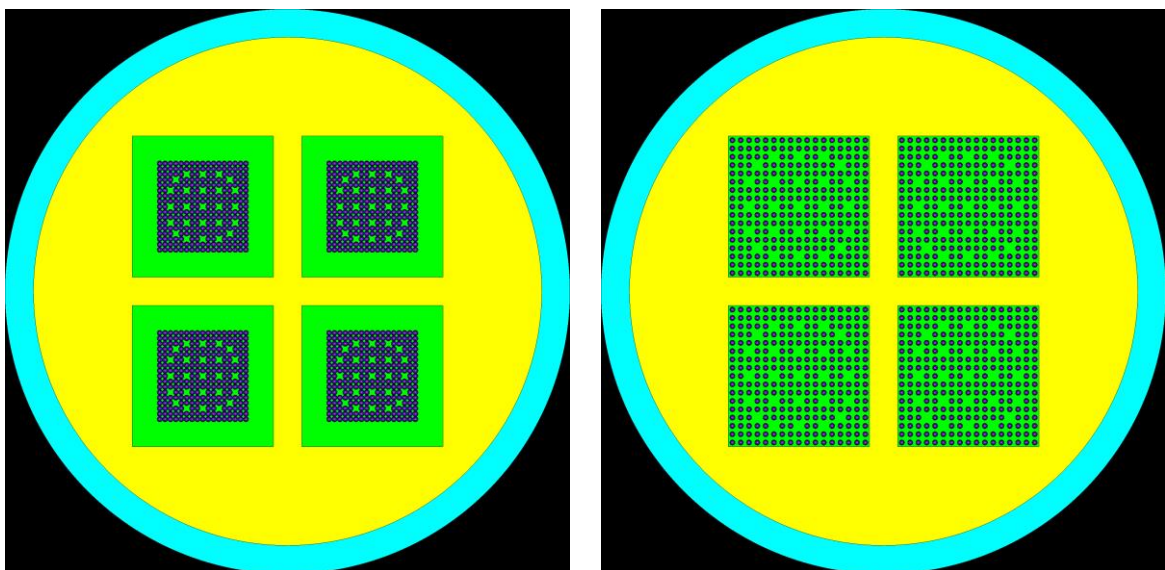


Figure 9: Illustration of pin-by-pin lattice pitch variation within the fuel assembly

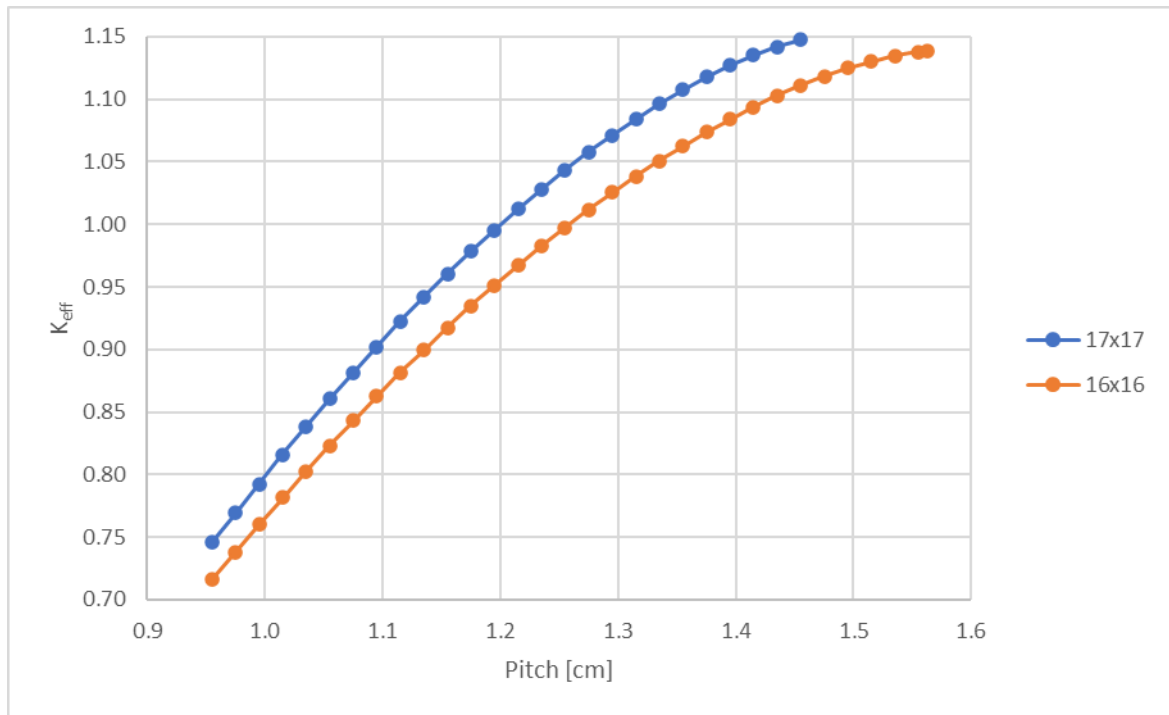


Figure 10: Dependence of k_{eff} on lattice pitch, highlighting the impact of moderator-to-fuel ratio on system reactivity.

3.4 Impact of Degradation Effects

Long-term degradation processes represent one of the main sources of uncertainty in disposal system criticality assessments, as they may significantly alter both material composition and geometry over repository timescales. In this study, degradation of the stainless-steel insert was modelled through progressive corrosion and the associated formation of magnetite (Fe_3O_4), which is expected under reducing repository conditions typical of deep geological environments.

The corrosion process was simplified by assuming a gradual conversion of stainless steel into magnetite, while conserving the original metallic constituents and introducing additional oxygen required for the formation of oxides. A Pilling–Bedworth ratio (PBR) of 2 was applied, meaning that the corrosion product occupies approximately twice the volume of the original steel. Consequently, the formation of magnetite leads not only to material substitution but also to significant volumetric expansion, which affects the spatial distribution of materials within the cask (Figures 11 and 12).

The impact on the effective multiplication factor is shown in Figure 13. The results indicate a non-linear response of k_{eff} to the progression of corrosion. In the initial stages, the replacement of stainless steel by magnetite generally leads to an increase in reactivity. This behaviour can be attributed to two combined effects: (i) magnetite has a lower density and lower neutron absorption capability compared to stainless steel, and (ii) volumetric expansion lower leakage from the fuel area, locally improving moderation conditions.

As corrosion progresses further, the spatial redistribution of materials becomes more dominant. In advanced stages, magnetite may approach or even come into contact with the fuel rods, effectively modifying the local moderation and reflection environment. In the 17×17 configuration, the most extreme case analysed corresponds to magnetite encompassing an entire row of fuel rods. This results in a noticeable decrease in k_{eff} , indicating that degradation-induced geometry changes can locally decrease neutron economy. However, such configurations are highly idealized and represent limiting scenarios rather than realistic outcomes.

The 16×16 configuration shows a similar trend. Due to the smaller amount of structural material available, the extent of magnetite formation is limited and does not reach configurations

where entire fuel rod rows are affected. As a result, the reactivity decrease in advanced stages remains moderate. This highlights the importance of initial design features, as the amount and distribution of structural material directly constrain the potential impact of degradation processes.

Despite the observed increase in reactivity, several limitations must be emphasized. First, the corrosion model assumes homogeneous and uniform transformation of stainless steel into magnetite, which is unlikely in realistic conditions where localized corrosion, cracking, or fragmentation are expected. Second, potential removal or redistribution of corrosion products (e.g., due to groundwater flow) is not considered. Third, the interaction between corrosion and other processes, such as changes in water chemistry, porosity development, or mechanical deformation, is neglected.

From a safety perspective, the results suggest that degradation effects can contribute to increased reactivity, particularly when they lead to improved moderation or reduced neutron absorption. However, the magnitude of this effect remains strongly dependent on the assumed evolution pathway. Given the large uncertainties associated with long-term material behaviour, these scenarios should be interpreted as sensitivity cases rather than predictive representations.

Overall, the analysis indicates that degradation-induced changes in material composition and geometry may represent a non-negligible contributor to reactivity uncertainty. Therefore, they should be considered in combination with other parameters, rather than analysed independently, when defining conservative safety margins for disposal system design.

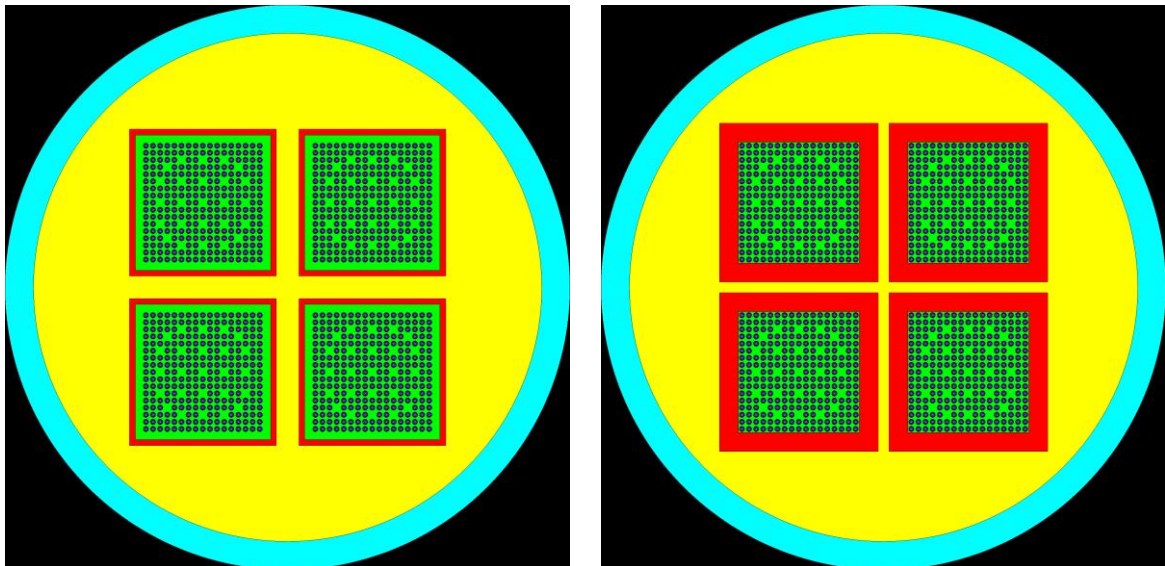


Figure 11: Initial stage of stainless-steel corrosion showing material recession and corresponding magnetite formation with volumetric expansion towards the fuel assembly boundary.

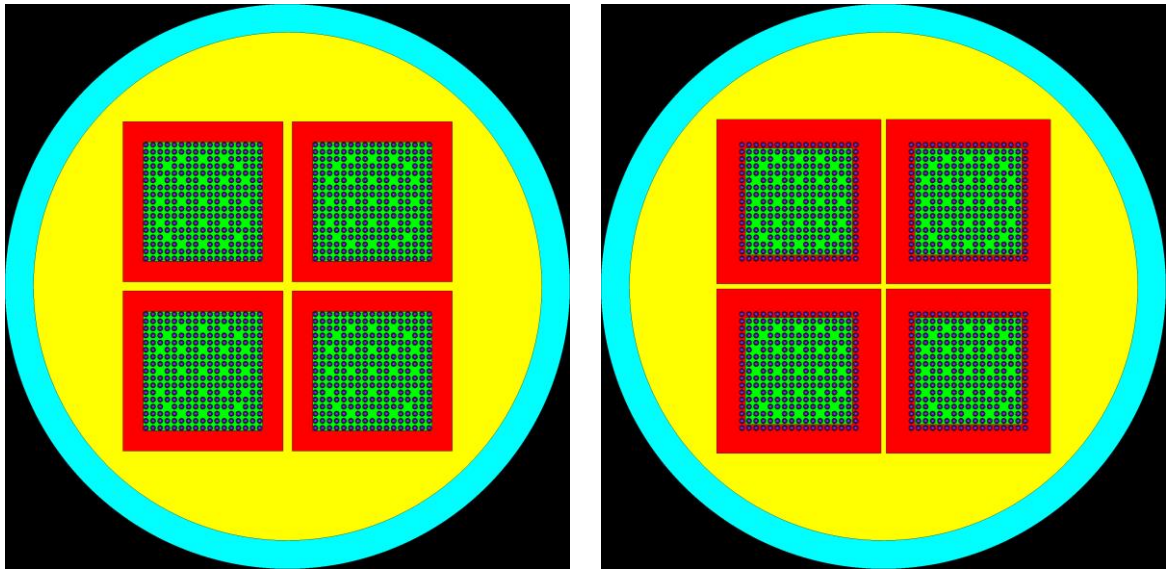


Figure 12: Advanced corrosion stages illustrating magnetite expansion into the fuel region, including contact with fuel rods and complete coverage of a fuel rod row.

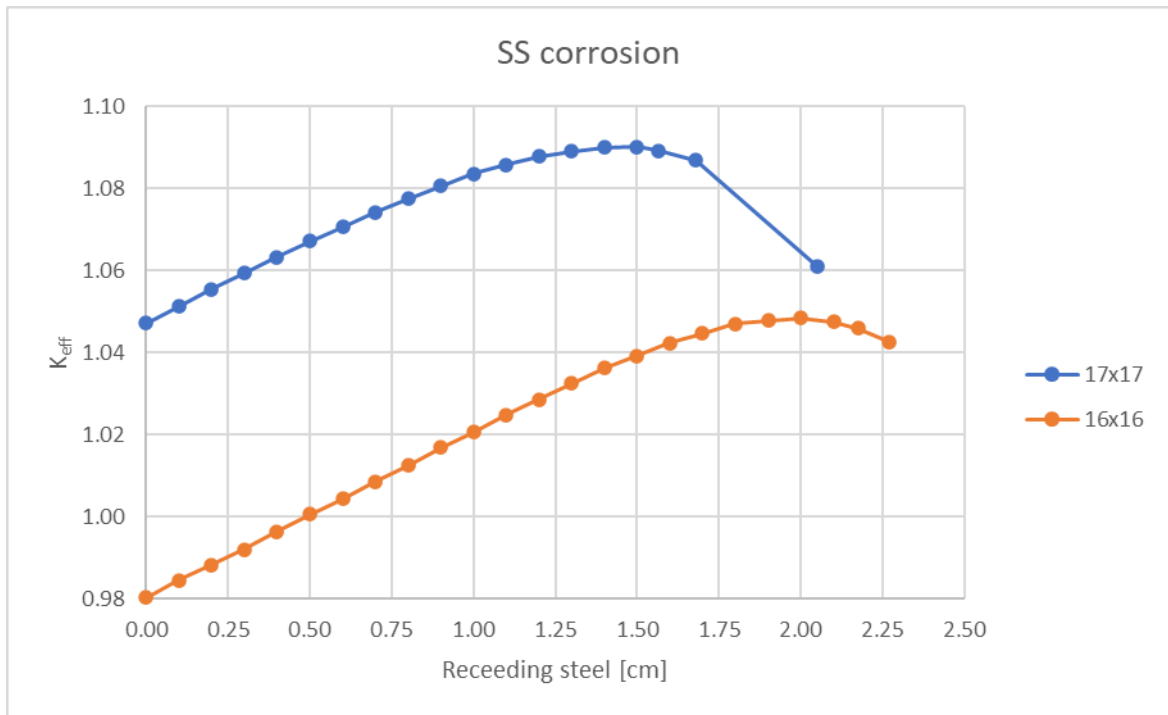


Figure 13: Variation of k_{eff} as a function of corrosion progression, showing the combined effects of stainless-steel replacement by magnetite and associated geometric changes.

4 CONCLUSIONS

This work presents a sensitivity analysis of a generic spent nuclear fuel disposal cask, with the objective of identifying the most influential parameters affecting the effective neutron multiplication factor and supporting the development of conservative safety margins.

The results confirm that fuel enrichment and lattice geometry are primary drivers of system reactivity. The reference case shows that the 17×17 configuration is consistently more reactive than the 16×16 lattice, mainly due to a higher moderator-to-fuel ratio and, to a lesser extent, a higher uranium content. In addition, the comparison of nuclear data libraries indicates systematic differences on the order of up to ~160 pcm, which, although relatively small, are not negligible for sensitivity ranking and should be considered as a contributor to overall uncertainty.

Among the analysed parameters, moderation conditions emerge as one of the dominant factors. The monotonic dependence of k_{eff} on water density suggests that the system remains under-moderated within the investigated range, with no clear reactivity maximum identified. This complicates the definition of bounding conditions, as potential changes in geometry or material distribution could shift the system towards more favourable moderation.

Geometrical parameters show a non-uniform influence on reactivity. Variations in pin-by-pin pitch have the strongest effect, directly impacting moderation efficiency and neutron spectrum. Changes in stainless-steel wall thickness between compartments also affect reactivity through neutron coupling, while fuel assembly positioning has a comparatively minor but systematic impact. These results indicate that assumptions related to fuel geometry and structural design can significantly influence the outcome of criticality assessments.

The analysis of degradation effects demonstrates that corrosion of the stainless-steel insert and formation of magnetite can lead to substantial changes in reactivity. In early stages, reactivity tends to increase due to reduced absorption and improved moderation, while advanced stages introduce complex geometric effects with less predictable behaviour. However, these results are strongly dependent on simplified assumptions regarding corrosion mechanisms and material redistribution processes.

Several limitations of the present study should be emphasized. The model assumes idealized geometry, homogeneous material transformations, and fully flooded conditions, without accounting for coupled processes such as mechanical deformation, localized corrosion, or changes in boundary conditions due to surrounding repository materials. In particular, the absence of a realistic external environment introduces uncertainty in neutron leakage and reflection effects. As a result, the presented sensitivities should be interpreted as indicative trends rather than strict bounding cases.

Overall, the study highlights that criticality behaviour in disposal systems is governed by a complex interplay of fuel characteristics, moderation conditions, geometry, and long-term degradation processes. No single parameter can be considered in isolation, and combined effects may lead to non-intuitive or non-linear outcomes. Therefore, future work should focus on coupled multi-parameter analyses, improved modelling of degradation pathways, and inclusion of realistic repository boundary conditions. Such developments are necessary to reduce uncertainties and to establish robust and defensible safety margins for spent nuclear fuel disposal systems.

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