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Innovative Investigation of Reflector Options for the Control of a Chloride-Based Molten Salt Zero-Power Reactor

Bruno Merk [1,*], Anna Detkina [1], Seddon Atkinson [1], Dzianis Litskevich [1] and Gregory Cartland-Glover [2]

[1] School of Engineering, University of Liverpool, Liverpool L69 3GH, UK; a.detkina@liverpool.ac.uk (A.D.); Seddon.Atkinson@liverpool.ac.uk (S.A.); d.litskevich@liverpool.ac.uk (D.L.)
[2] Daresbury Laboratory, Scientific Computing Department, Science and Technology Facilities Council, SciTech Daresbury, Cheshire WA4 4AD, UK; greg.glover@stfc.ac.uk
* Correspondence: b.merk@liverpool.ac.uk

Abstract: Molten salt reactors have gained substantial interest in the last years due to their flexibility and their potential for simplified closed fuel cycle operations for massive net-zero energy production. However, a zero-power reactor experiment will be an essential first step into the process delivering this technology. The choice of the optimal reflector material is one of the key issues for such experiments since, on the one hand, it offers huge cost savings potential due to reduced fuel demand; on the other hand, an improper choice of the reflector material can have negative effects on the quality of the experiments. The choice of the reflector material is, for the first time, introduced through a literature review and a discussion of potential roles of the reflector. The 2D study of different potential reflector materials has delivered a first down-selection with SS304 as the representative for stainless steel, lead, copper, graphite, and beryllium oxide. A deeper look identified, in addition, iron-based material with a high Si content. The following evaluation of the power distribution has shown the strong influence of the moderating reflectors, creating a massively disturbed power distribution with a peak at the core boundary. This effect has been confirmed through a deeper analysis of the 2D multi-group flux distribution, which led to the exclusion of the BeO and the graphite reflector. The most promising materials identified were SS304, lead, and copper. The final 3D Monte Carlo study demonstrated that all three materials have the potential to reduce the required amount of fuel by up to 60% compared with NaCl, which has been used in previous studies and is now taken as the reference. An initial cost analysis has identified the SS304 reflector as the most attractive solution. The results of the 2D multi-group deterministic study and the 3D multi-group Monte Carlo study have been confirmed through a continuous energy Monte Carlo reference calculation, showing only minor differences.

Keywords: nuclear; nuclear reactors; reactor physics; nuclear experiments; zero-power reactors; modelling and simulation; molten salt reactors

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1. Introduction

Zero or very low power experiments are recognized as the first step into a new reactor technology, historically [1] as well as in the recently published new development process [2] and in recently initiated programs [3]. The major point in the past has been to test new configurations in safe settings and to use the opportunity of these highly flexible experiments to create an accelerated learning curve at the beginning of a new technology. In new programs, there is the additional demand to provide safety demonstrations and to validate code systems to assure the quality of the predictions for the next step, while using this multi-fold opportunity for learning in manufacturing and educating future reactor physics experts [4].

The first part of this current series of publications on zero-power studies delivers on the importance of a zero-power reactor experiment for the process of developing a new, innovative reactor concept in the form of a molten salt fast reactor, and the challenges due to the homogeneous core composition (unity of coolant and fuel) are worked out [5]. The second part delivers on new approaches for the control and shutdown of a homogeneous core experiment [6]. This will be complemented by this study of the choice of the neutron reflector as an essential part of efficiently operating small reactor cores, especially in the case of the fast neutron spectrum.

The reflector is an essential part of all operating reactors, as well as for a wide variety of reactor experiments. However, the reflector sometimes fulfils completely different demands in different reactors (e.g., protecting essential components versus improving the neutron economy) and can be formed easily out of coolant, normal structural materials of the reactor, or from a special material.

In light water reactors, the reflector is just provided by the light water coolant and the core barrel; partly, the outer row of the low leakage loading could also be seen as a kind of reflector. The major function of the reflector materials in LWRs is to protect the pressure vessel from high-energy neutron flux to keep the fluence on the vessel within an acceptable limit over the lifetime [7]. In high-temperature reactors such as the AVR [8] and the THTR [9], the major aim of the reflector is to improve the neutron economy; thus, graphite is used as the reflector and it is also used as a structural material.

It is interesting to recognize that the relative size of the reflector significantly decreases with increasing core size. This demonstrates that the relevance of the reflector decreases with a decreasing surface to volume ratio. An interesting and relatively new approach is the proposed use of BeO reflectors. In the micro-reactor U-Battery concept, this approach has been proposed to reduce the core size. In comparison with the classical graphite reflector, a clear size reduction can be achieved; however, this size reduction comes with a significant cost due to the more exotic reflector material [10].

Sodium-cooled fast reactors are significantly different in the design of the reflector, due to the closed system and the high-energy fast neutron flux, resulting in different approaches. The reflector in a SFR such as the pool type PFBR [11] comprises several rings, starting with the breeding blanket to improve neutron economy while breeding fresh fissile material, followed by a steel reflector and a B_4C shield, which can be seen as the core. This area is followed by the internal vessel storage for the fuel, required due to the high decay power of the fuel assemblies when unloaded from the core. The internal storage is surrounded again by a stainless steel reflector and, finally, a large B_4C shielding to prevent the heat exchanger containing secondary sodium from the high energy neutron flux, which could otherwise lead to activation of this secondary coolant. It is impressive to see the dimensions: while the core consists of approximately nine inner rings, the outer structure consists of 14 rings leading to an increase in the size of the rings to ~200 core assemblies compared with ~1300 assemblies in the outer structure. New investigations have recently been delivered with the aim of replacing a part of the reflector with a more advanced material like ferroboron [12]. Other recent studies have assessed the impact of reflector material on the core design for SFR. Delivering a mixed spectrum core design [13] or a compact sodium-cooled breed-and-burn reactor design [14] would demonstrate the opportunities and the influence which can be created through innovative reflector applications.

The very significant role of the reflector in critical experiments is maybe best demonstrated by the last documented criticality accident at Sarov (Arzamas-16) on 17 June 1997 [15]. This accident was caused when reproducing an experimental setup which had been already used in the 1970s. "He [the experimenter] had taken the dimensions for all of the system components from the original 1972 logbook. However, when he copied down the inside and outside dimensions of the copper reflector (167 and 205 mm, respectively), he incorrectly recorded the outside dimension as 265 mm". When the experimental setup had been assembled, this change in the reflector led to a prompt critical spike and the ~6.5 day excursion. In general, in most nuclear experiments, the reflector is an essential piece for improving the neutron economy, leading to a reduced demand for fissile material and thus reducing the cost. However, the reflector has the potential not only to reduce costs but also to influence the results of future experiments, which can lead to significant problems; e.g., in YALINA experiments, the idea of supporting the fast reactor's configuration by a decoupled thermal system with the aim of boosting criticality has led to some really surprising and hard to explain results [16] caused by the penetration of thermal neutrons into the fast region [17]. Thus an improper decoupling of the fast system from the thermal system has finally taken place in a real experiment.

An additional challenge for future projects is the required and requested flexibility of a multi-purpose facility for reactor physics of advanced molten salt-based reactor systems which may need different reflectors for each technology considered, which, in turn, may have contrasting neutron spectra. The primary focus of this work is on a fast system, but with a clear outlook into flexible multi-purpose operations for the long term. This formed a secondary focus, keeping in mind the view and the requirements of the reflectors that are suitable for a potential future experimental investigation of a thermal core. The investigation started from a generic reflector which has been used in the previous studies [5,6] and proceeded into an investigation to support the right choice of the ideal reflector for a molten salt zero-power reactor answering the research question "Which reflector material will assure the best possible performance in a fast reactor experimental configuration?".

The investigation started with a discussion of the different roles of the reflector, followed by a broad investigation of different potential materials and a refined investigation of a down-selected number of attractive materials. It finished with a verification of the results with alternative calculation methods and a test of the stability of the chosen material for the control and shutdown proposals of [6].

2. The Role of the Reflector

Some of the different roles a reflector can play in a nuclear reactor and in nuclear experiments have already been discussed in the review of existing solutions in the introduction. However, it is important to collect all the functions of the reflector and all the requirements of the reflector in the case of a zero-power experiment; both points will be delivered in this section.

Theoretically, the main aims of a reflector that surrounds a nuclear reactor or experiment are:

- Saving neutrons by improving neutron economy,
- Protecting the environment from radiation,
- Protecting the experiments from the environmental influence,
- Potential control of the moving reflector, carrying the control system via rods or drums,
- Possibility for massive cost savings.

The potential savings of adding a reflector to a zero-power reactor core has been investigated based on SCALE/POLARIS calculations for different enrichments and the related critical radius. Both different systems use a NaCl reflector; while the salt system is slightly different, one system is based on a eutectic NaCl-UCl_X fuel, 42.5% NaCl-40.5 UCl_4-17% UCl_3 (denoted 42.5% NaCl), and a second heavy metal rich system on 20% NaCl-56.35% UCl_4-23.65% UCl_3 (denoted 20% NaCl) [5]. For both salt systems, the volume gain achieved through adding a 30 cm thick NaCl reflector has been determined and is given in Figure 1. There is a clear trend that the gain will increase with decreasing core size and increasing enrichment, which seems to be natural, while the gain for the heavy metal rich system is not very pronounced and may even be explained by the slightly reduced core size. However, it is clear from the figure that the volume of the fuel required for the experiment can be reduced by between 30 and 45% when a 30 cm thick NaCl reflector is applied.

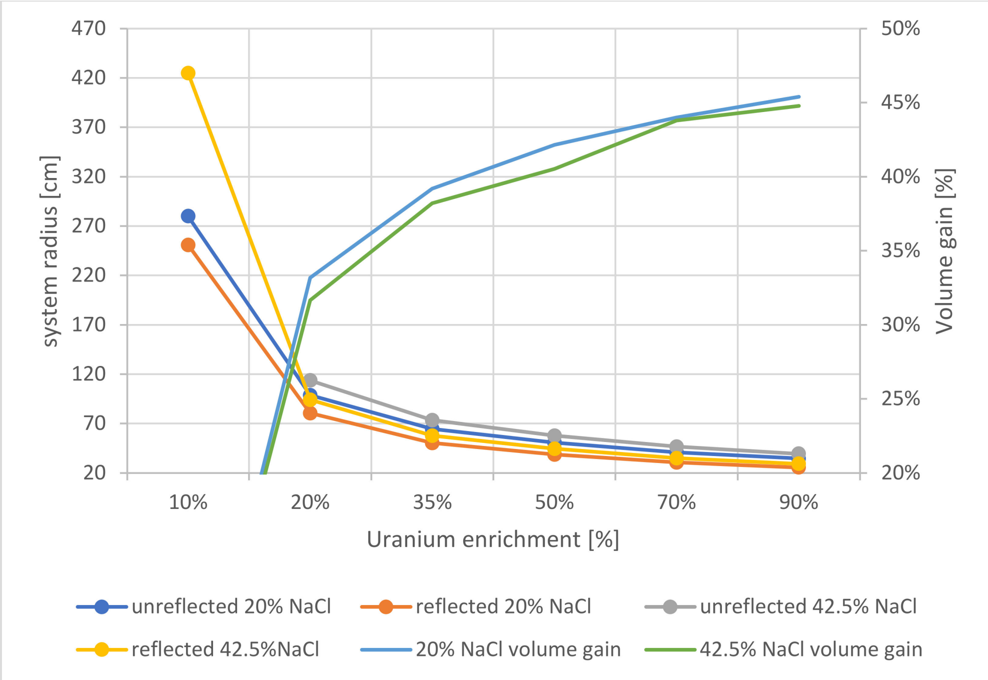

Figure 1. Generic 2D calculated system size depending on the fuel enrichment for the eutectic and the heavy-metal-rich system, and the fuel volume reduction achieved through a 30 cm thick NaCl reflector calculated with SCALE/POLARIS [5].

In addition to the potential gain and the protective effect of the reflector in nuclear reactors, some very specific demands on the reflector have to be kept in mind for a zero-power experiment, with some additional specifics for a molten salt reactor experiment:

- The reflector should save as many neutrons as possible—reducing costs and reducing the core size or enrichment.
- The reflector should only have a limited effect on the neutron core spectrum, which will have an influence on the power production/neutron flux at the core boundary in the spatial, as well as the energy distribution.
- The reflector should be usable for all temperature ranges of the experiment.
- The reflector should not disturb potential kinetic experiments—the long life-time of neutrons (e.g., in graphite or neutron production)—in the YALINA experiment.
- The reflector should cause only limited disturbance of the natural neutron flux distribution of a homogeneous fast system.
- Through the use of the reflector, the zero-power core will deviate from the future power-producing core. However, the issue of bias/reproducibility factors should be as limited as possible.
- The reflector could act as a moderator for the thermal system or could provide additional neutrons, e.g., a hybrid system as in the YALINA experiments.

The core study will focus on the experiments for the fast system as envisaged for iMAGINE [2], which ultimately will be a large-scale system operating on spent nuclear fuel without prior reprocessing [18]. Thus, the design of the zero-power reactor, as well as the experimental equipment and the experiment itself, will require some substantial innovation to allow as much reproducibility/transferability of the experiments through special approaches [19] to draw conclusions for the larger-scale systems foreseen in the process of developing an advanced reactor system as described in [2]. However, the zero-power system will provide a technological testing case for the new technology as well as a solid basis for the validation of modern modelling and simulation tools through experiments [4], which will help significantly in reducing the challenges of reproducibility.

In addition to the iMAGINE-related investigations, some outlook will be given on the multi-purpose use for future investigations of a thermal system in the study.

3. Codes and Data

Based on the given salt system investigation [20] for iMAGINE and the dimensions study [5], the applied standard salt composition for the study for the nominal case is the heavy-metal-rich composition 20%NaCl-56.35%UCl_4-23.65%UCl_3. This composition was originally studied for the required thermo-physical properties by [21]. In addition, some comparative studies have been based on the eutectic 42.5% NaCl-40.5 UCl_4-17% UCl_3. The salt system has been chosen to be similar to the salt system envisaged for the iMAGINE proposal. From reactor operation point of view, the key parameter to obtain for self-sustained operation on spent nuclear fuel is the high possible loading for heavy metal, which is decisive to achieve sufficient breeding. However, the salt system is currently to be seen as an initial primary candidate of choice based on the UK experience in working with chlorine salt melts, but for the final decision, the corrosion control opportunities have to be investigated.

The simulations for this step of the study of the zero-power reactor configurations were mainly performed using the TRITON/NEWT sequence of the SCALE code system [22], applying TRITON for the preparation of the shielded multi-group cross-section set and NEWT for the 2D transport solutions for the core part of the study. This was complemented with the use of Keno VI (multi-group as well as continuous energy) for creating 2D cross-checking solutions, as well as for the following 3D studies using the multi-group solver and the continuous energy solver for cross-testing. For TRITON, the v7-252 cross-section set of the SCALE package was used, which was based on ENDF/B 7.1. The sequence and the cross-section set was also the basis for the multi-group cross-section preparation for the multi-group (MG) Keno VI calculations, while the continuous energy version used the ce_v7.1_endf library of the SCALE package.

For the TRITON/NEWT study, two specific 2D models for a fast molten salt reactor was built for the simulation (Figure 2). Both NEWT models reflected a 2D quarter of the core with x-y discretization consisting of the ring core (with added ring-shaped discretization for the evaluation of the power distribution) and the steel vessel surrounded by reflector, while the rest of the cell was filled with vacuum using reflective boundaries at the bottom and the left side and vacuum boundaries at the other two sides. The 2D and 3D Keno VI models shown in Figure 3, reflecting a cylindrical core surrounded by a vessel and a reflector on all sides for the 3D model and reflective boundary conditions at the top and bottom for the 2D model, were used for cross testing with the NEWT results.

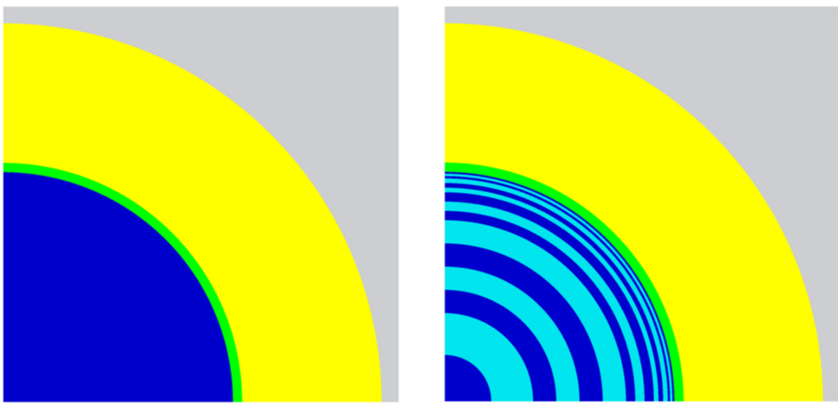

Figure 2. TRITON/NEWT model for the 2D study of reflector materials (**left**) and for the analysis of the variation of the effect of different reflector thicknesses (the thickness of the green reflector region is varied). The evaluation of the power distribution in the 2D system is based on a ring structure in the core (**right**). Molten salt core—blue; steel vessel—light green; reflector—yellow; surrounding vacuum—grey.

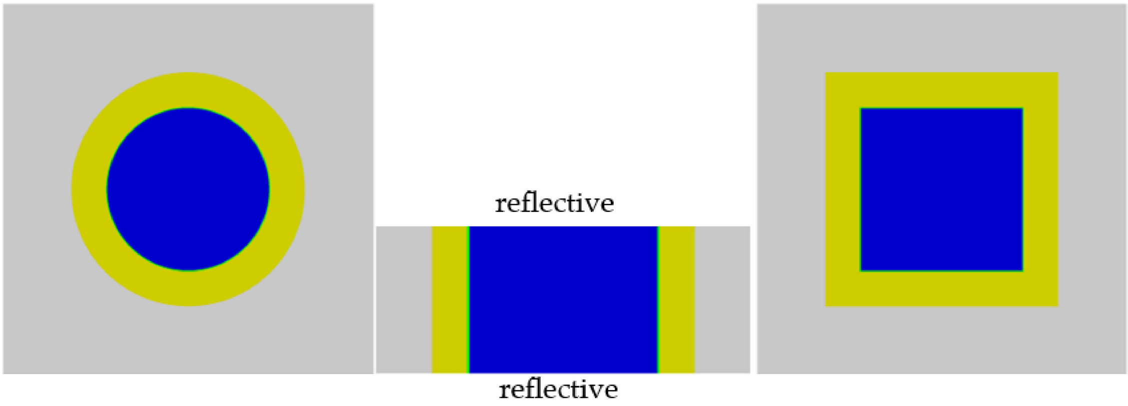

Figure 3. General 2D (**left** and **centre**) Monte Carlo model of the configuration (**left**, top view x-y; centre, front view x-z) and 3D (**left** and **right**) Monte Carlo model of the configuration (**left**, top view x-y; right, front view x-z) with a molten salt fuel core (blue), a stainless steel vessel (light green), the reflector (yellow), and a vacuum (grey) used for the validation of the results and the 3D studies.

4. Test of Different Materials

The study of the optimization of the reflector was, in the first step, based on the 2D critical reference system with the following dimensions: a core radius of 49.4 cm in a 2 cm thick SS304 vessel surrounded by a 30 cm thick NaCl reflector (see the arrangement given in Figure 2) and calculated using TRITON/NEWT. The reflector material choice for the investigation was driven, in a first step, by looking into traditional materials used in nuclear reactors and critical experiments; in the second in the second step, by looking into materials which came under discussion in the last years. Following this first insight, the driver was to create a deeper understanding of the effects of different alloying elements of stainless steel with the view of leveraging this knowledge for potential optimization. The results of all steps will be finally used for a down-selection for deeper studies.

In the first analysis, typical materials used in nuclear reactors and experiments were investigated, and the change in criticality is shown in Figure 4. The strong influence of the reflector on the system's criticality is visible between the helium case (the reference for a non-reflected system) with k_{eff} = 0.7434 and the graphite case with k_{eff} = 1.1903, which would, in the end, reflect a massive difference in the required amount of fissile material for the experiment, leading ultimately to massive cost savings. Beside graphite, the investigated high-density metals led to a clear increase in criticality, while the low-density light metal sodium, as well as water and the shielding material ferroboron [12], led to a reduction of criticality compared with the reference material, NaCl.

In the next step (Figure 5), the study was widened, on the one hand, to more exotic materials for reactor use, which are sometimes proposed for future reactor systems or for very specific issues in reactors. On the other hand, a more in-depth analysis was performed to understand the large difference between carbon steel containing 99% iron and 1% carbon (k_{eff} = 1.1271) and stainless steel SS304 (k_{eff} = 1.155). This was achieved by systematically studying the separate effects of the main alloying elements: chrome, nickel, manganese, and silicon, each singled out in a composition with 20% of the alloying element in 80% iron. The results of this single-effect study are shown in Figure 5. The study of the alloying elements indicated a strong influence appearing in the case of the addition of silicon. In addition, the study of alternative reflector materials indicated a very high k_{eff} for using BeO as the reflector material. Two other often-proposed hydrogen rich reflector materials, polyethylene and ZrH_2, do not deliver the expected improvement in criticality when used as reflector materials.

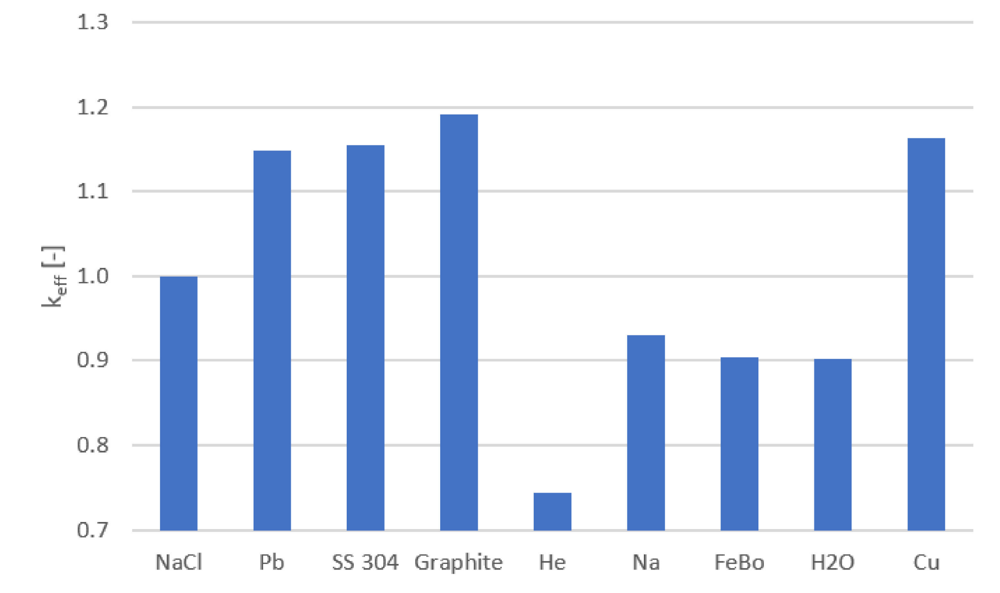

Figure 4. Analysis of the effect of a 30 cm thick reflector made from different materials used in nuclear reactors and experiments on the criticality of the studied 2D test core.

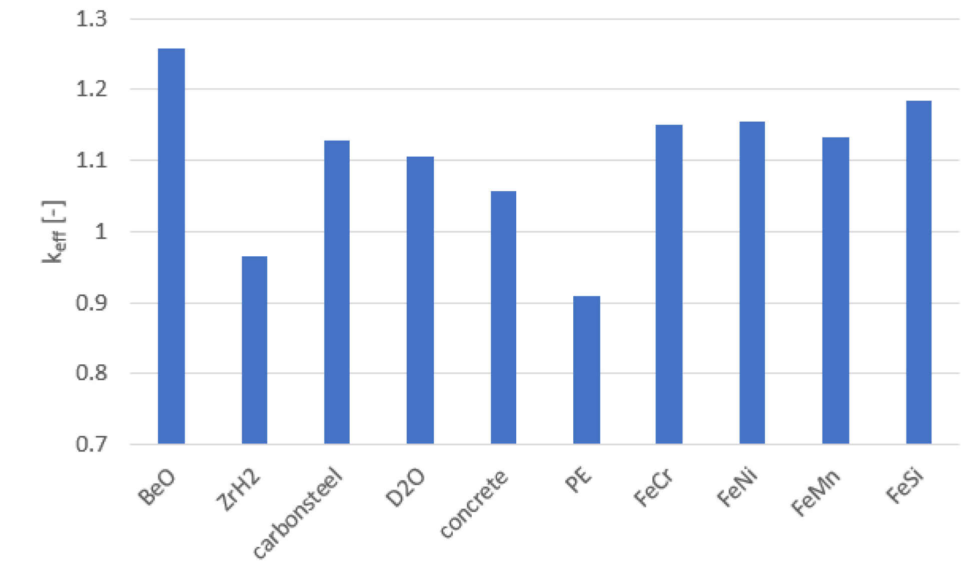

Figure 5. Analysis of the effect of a 30 cm thick reflector made from different, more exotic materials on the criticality of the studied 2D test core.

Based on the finding of the very strong influence of silicon on the effect of the reflector, some existing typical high-silicon materials were investigated in the last step of the materials study, with very positive results for cast iron with high (GJS-XSiMo 5.1, https://www.brechmann-guss.de/wp-content/uploads/2016/07/Datenblatt-SiMo.pdf (accessed on 1 April 2021) or very high silicon content (Hi Si cast, https://inis.iaea.org/collection/NCLCollectionStore/_Public/35/066/35066186.pdf (accessed on 1 April 2021), and a high Si content aluminium alloy (AlMgSi; https://batz-burgel.com/en/metal-trading/aluminium-product-range/en-aw-6082/ (accessed on 1 April 2021); see Figure 6. For comparison, two artificial materials were added: SS304 with an additional 10% of Si and an artificial ferrocarbon replacing boron by carbon while using the other data from FeBo [12]. Note that the data for SS304 is given on the left end of the figure for comparison. Based on these results, Hi Si cast could be an interesting alternative to stainless steel, but only in the case that it would be financially more attractive; thus, it must be cheaper or on the same level as SS304, which seems to be doubtful, taking into account the amount of stainless steel used in the modern world.

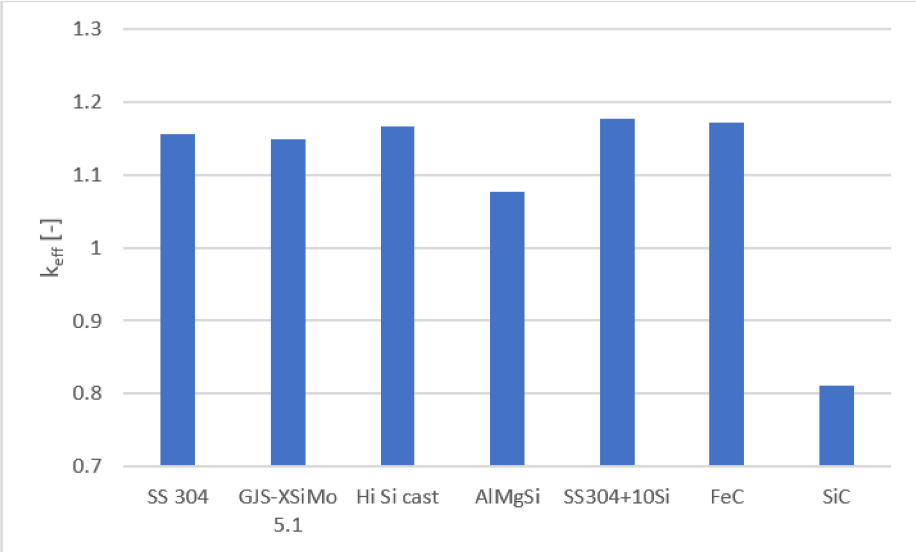

Figure 6. Analysis of the effect of a 30 cm thick reflector made from different silicon- and carbon-rich materials on the criticality of the studied 2D test core.

Finally, it is important to understand the effect of the reflector temperature on the efficiency of the reflector, since, most probably, a zero-power reactor experiment will be operating at room temperature in the first stage of the tests, while, in the longer term, it could be of interest to operate it at higher temperatures up to the potential maximum operation temperature of ~800 K to see the operational conditions and behaviour in real molten salt instead of solid salt. Even if the reflector itself will not be directly in contact with the salt, there will be an elevated temperature level in the whole system. It is important to understand that a potential material should work properly for the first stage of the test on room temperature as well as for the later hot tests. In Figure 7, a systematic final check for the effect of materials is given for scoping for different materials at room temperature as well as at the standard investigation temperature, based on a maximum temperature of 800 K for the reflector. The results show only a very weak dependence of the reflector's effect on the criticality of the operating temperature of the reflector for the metal-based materials. A more pronounced effect was only visible in the case of a hydrogen-rich reflector such as PE.

After the analysis of the effect of the reflector material on criticality, the study focused on another key point for the down-selection of potential reflector candidates for a zero-power reactor physics experiment supporting molten salt fast reactors. The point is the effect of the reflector on the neutron flux distribution in the core of the fast system. Experiments like YALINA have shown that fast reactors can be very sensitive to thermal neutrons entering into the fast system, leading to a massive and absolutely undesirable distortion of the detector readings [17,23] and thus of the power distribution.

The radial power distribution was calculated for a chosen set of attractive materials and some reference cases using the model given on the right side of Figure 2. Figure 8 demonstrates the massive influence of the choice of the reflector material on the radial power distribution in the analysed core. The use of highly reflective light materials, e.g., BeO, H_2O, or graphite, led to a very strong power increase in the outer area, which completely disturbed the natural power distribution in the core, as given by the green curve for the pseudo-unreflected system. Thus, these materials would not be a good choice as a reflector in a fast system. However, it should be kept in mind that this decision may have to be revised when a thermal system is analysed, since in that case, the effect is expected to be irrelevant; thus materials like BeO, H_2O, or graphite are very attractive choices due to their high efficiency in neutron reflection (a strong increase in the k_{eff} of the system), and they should be analysed in more detail for their application in an experimental setup for the investigation of a thermal core.

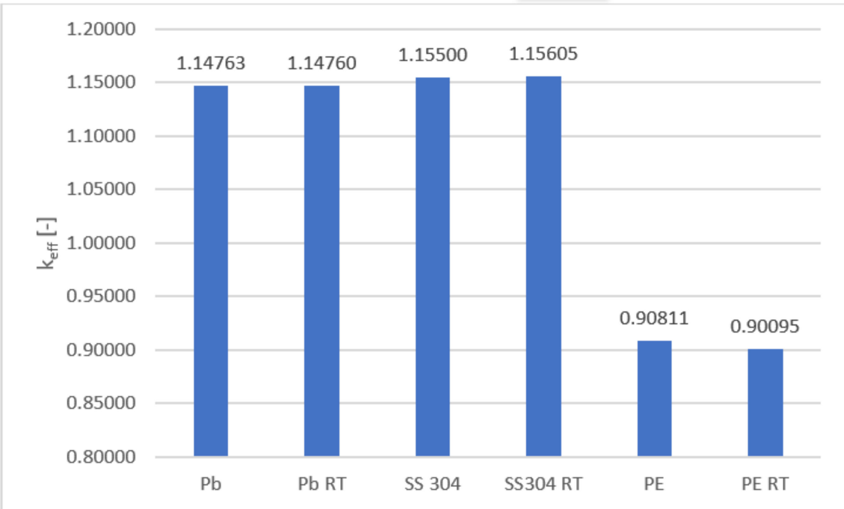

Figure 7. Scoping analysis of the effect of the operational temperature (800 K versus room temperature, RT) of the 30 cm thick reflector using metal-based as well as hydrogen-based materials on the criticality of the studied 2D test core.

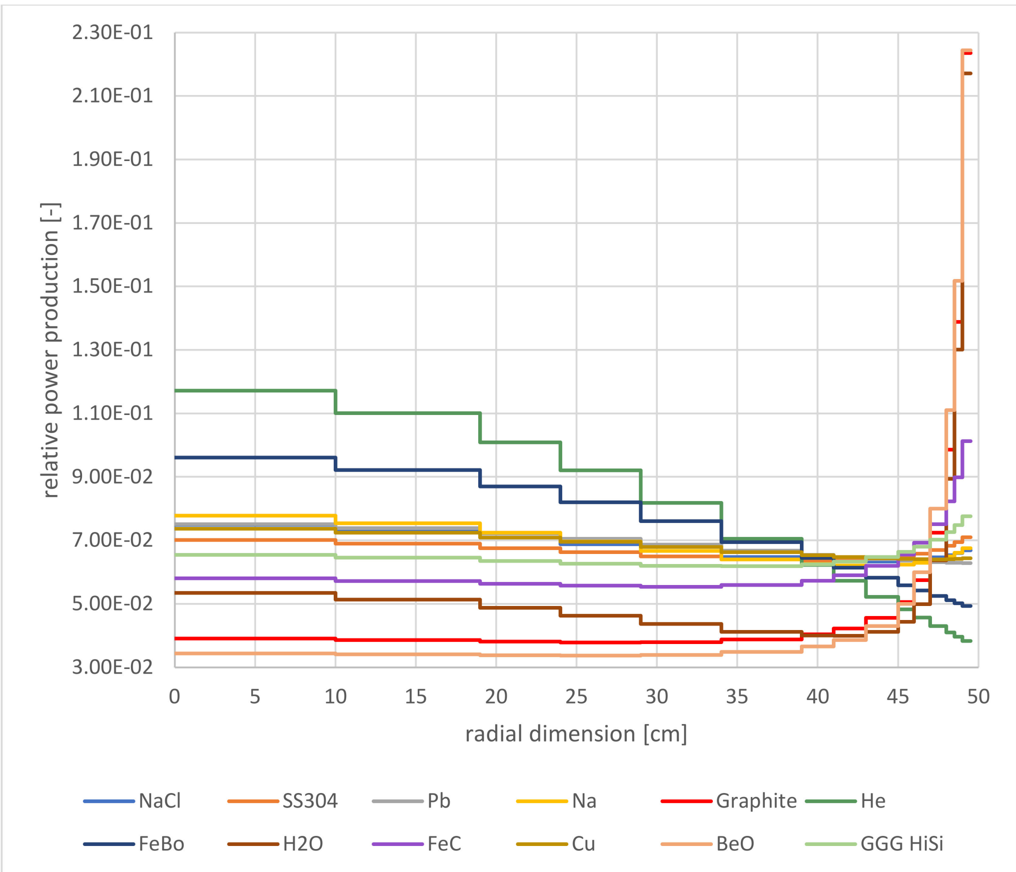

Figure 8. Radial power distribution investigated in a 2D system for different reflector materials for a zero-power experimental core.

If we compare the heavier materials, even here, it is clear that each of these reflectors had a strong influence on the power distribution when compared with the helium case, even with the use of a shielding material with a strong neutron absorption potential such as ferroboron (dark blue versus green). However, even in all heavy reflector material cases, the power distribution will be massively flattened due to the reflector, but, in the ideal case, the spatial form of the power distribution (cosine-like) is kept as natural as possible with a clear peak in the centre of the system and, ideally, only a very limited increase in the power at the boundary.

For a more detailed insight, Figure 9 shows a narrowed-down selection of the most interesting materials, which all showed a natural (cosine-like) power distribution in the inner part of the core while delivering a reasonable increase in the system k_{eff} in the study above. In this figure, it is obvious that all reflectors led to an increase in the power in the outermost ring, but while this increase was stronger for the silicon-containing materials (Hi Si cast and SS304), it was moderate for the sodium-containing materials (pure Na and NaCl), and it was very limited for heavy materials such as lead and copper. In addition, lead and copper showed a very nice power distribution, with a clear peak in the centre, which was slightly lower than for the unreflected system but with a comparable shape.

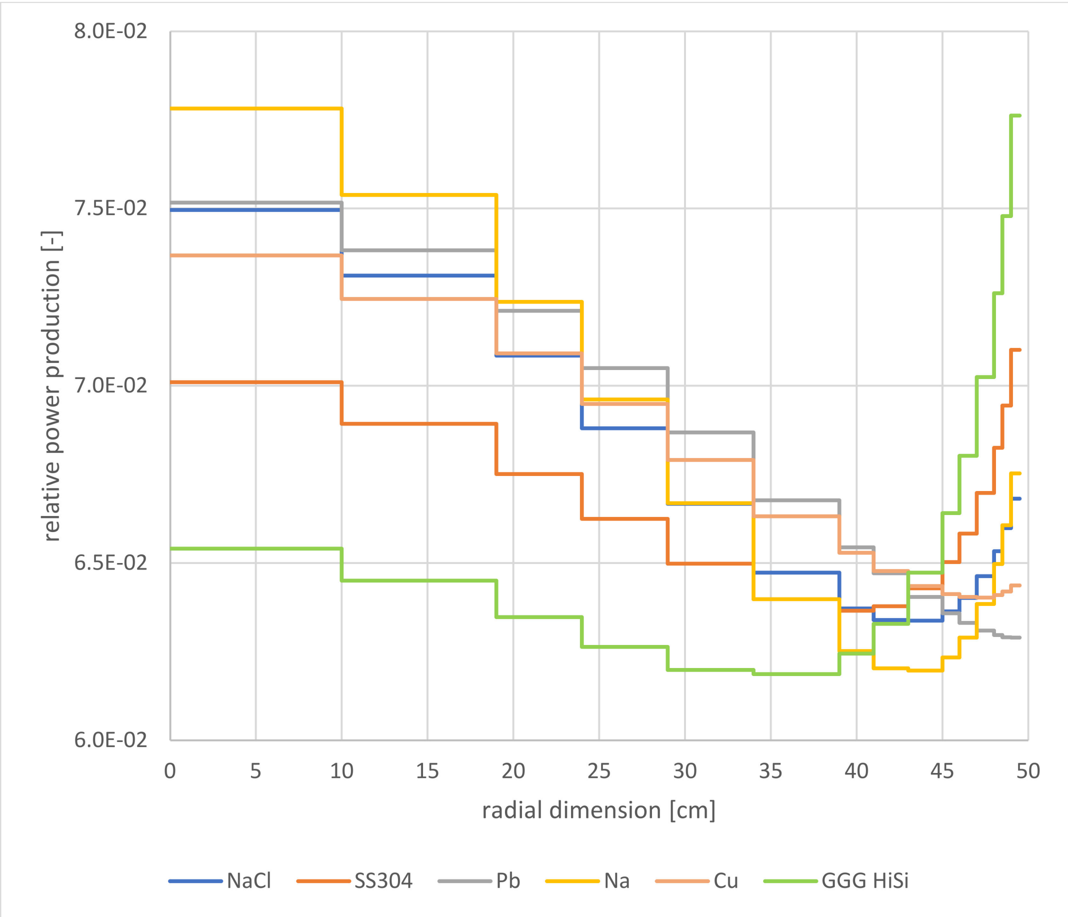

Figure 9. Narrowed-down choice of materials for a deeper investigation of the radial power distribution investigated in a 2D system for different reflector materials for a zero-power experimental core.

The results up to now favoured the use of a copper or lead reflector. For further investigation, these two materials will be compared with the original NaCl reference, with stainless steel, and partly with graphite.

5. Reflector Dimension

In this section, the effect of the reflector on the critical size of the core and the efficiency of the reflector depending on its thickness were investigated to obtain a better understanding of the potential reduction of the demand on fissile material. This will also allow the determination of the ideal reflector thickness, depending on the chosen reflector material.

The core dimension, and thus the required amount of fissile material, is strongly dependent on the choice of the reflector material; see Figure 10. The first comparison was between the heavy-metal-rich core and the eutectic core. The eutectic core required a ~15% larger radius to achieve criticality when the same dimension of reflector was chosen. However, compared with the required heavy metal amount in the analysed 2D core, the eutectic composition required about 9% less heavy metal, which meant that the additional core volume or even a slightly greater volume was filled by NaCl only. Thus, in the case where the core dimension itself is not a limiting value, the choice of the eutectic composition could be favourable, even if the demand on the infrastructure (reflector material, potential control system [6], and the core housing) depends on the absolute core size. Therefore, this opportunity should be recognized and investigated in a future optimization process required for the design of a new type of zero-power reactor. The use of the chosen reflectors reduced, in all cases, the core dimension: the use of a 30 cm reflector consisting of lead reduced the radius by 23%; the use of the SS304 reflector, by 26%; the copper reflector, by 27%; and the graphite reflector, by 35%. The second case with the lead reflector demonstrated that the same reduction in the required core size could be achieved by a 50 cm thick lead reflector, but at the cost of a larger overall system size. Thus, all the investigated metal reflectors which delivered a reasonable power distribution had strong potential to reduce the required core size for a critical system, but the gain was only weakly dependent on the material. This opens a wide opportunity for choosing and analysing different optimization parameters in future core designs.

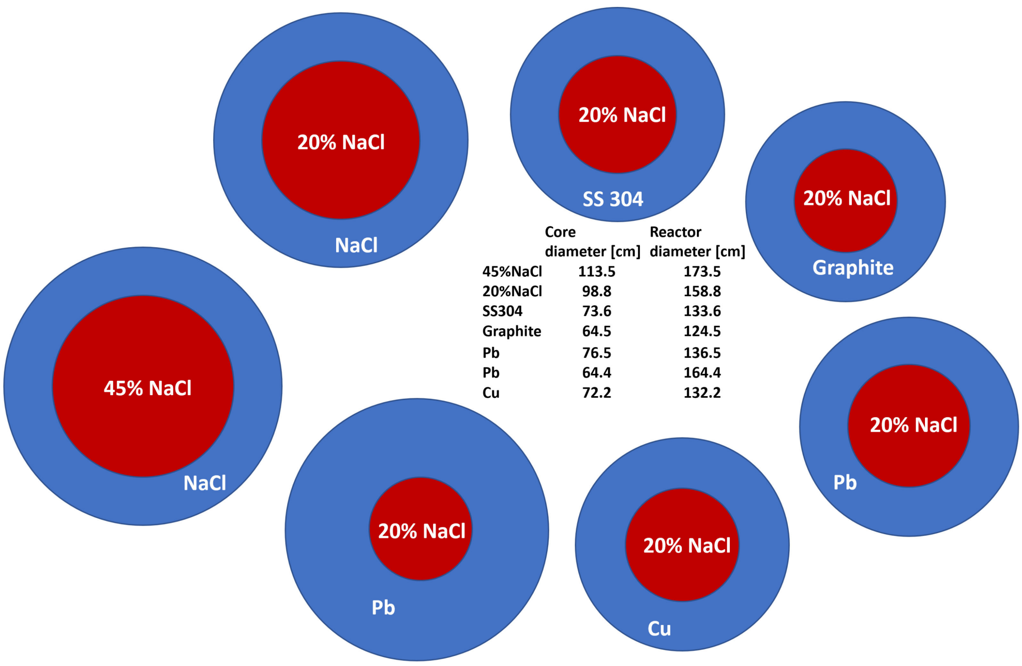

Figure 10. To-scale variation of the 2D core dimension: reflector thicknesses and resulting system dimensions required to achieve a critical configuration for a zero-power system.

With recognition of the great potential that the right choice of the reflector has in reducing the amount of fuel required to form a critical system, the next step was to obtain a deeper understanding of the options. Is there a saturation effect and is the applied first guess of using a 30 cm thick reflector really the ideal choice? The analysis was based on a comparison of the core criticality curves depending on the thickness of the reflector and the different reflector materials, while all cases were normalized on the critical system with the 30 cm thick reference reflector as calculated above.

Figure 11 depicts the variation in k_{eff} with reflector thickness for five reflector materials. For this evaluation, the critical core diameter was determined for each of the different reflector materials for the 30 cm thick reflector. In the following step, the reflector thickness was varied while the critical core size was maintained. This analysis was designed to create a deeper understanding of the trends towards the ideal reflector thickness for different materials, while it showed some different effects. First of all, all reflector arrangements tended to deliver the expected asymptotic behaviour, which confirms that at a certain thickness, the addition of additional reflector has only a very marginal effect. However, it is very interesting to recognize that the asymptotic behaviour set in at very different reflector thicknesses for the different materials, with copper not showing a reasonable gain after increasing the reflector to more than 30 cm, while there was still a reasonable increase in criticality even for 80 to 120 cm in lead. At the other end of the x-axis, the different criticality states with almost no reflector (1 cm) reflected the different core sizes required for the reference solution, while all curves intersected at the reference point 30 cm reflector. The structure of the curves helped to identify the ideal reflector thickness depending on the materials, which tended towards the outcome that for lead, a thicker reflector could be very promising (see the added 50 cm case in Figure 10), while for copper and most probably SS304, a thinner reflector would be sufficient, which, in turn, would provide better value for money.

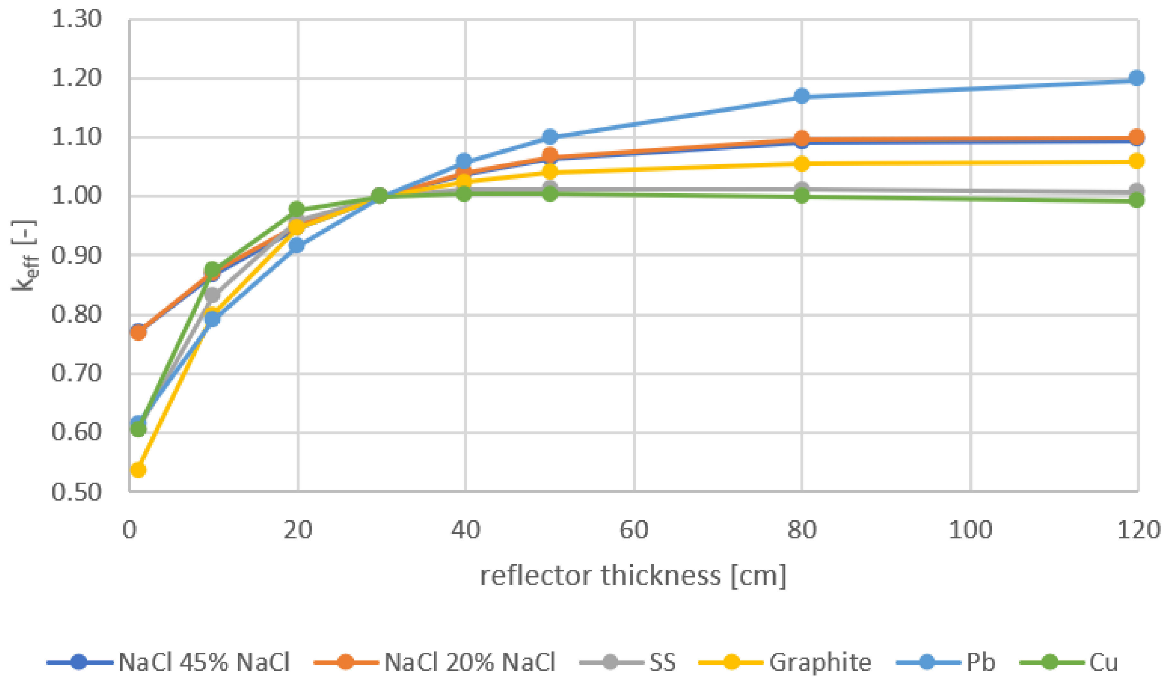

Figure 11. Criticality of the studied 2D system for different reflector thicknesses determined on the basis of the different critical core diameters for each reflector material with a 30 cm reflector and the following variations in the reflector thickness.

The very strong influence of the reflector on the system's criticality, and thus on the required system size and fuel demand, has been demonstrated so far in the current study. In addition, the strong influence of the reflector material on the power distribution was found and an initial optimization of the required 2D core diameter for different reflectors materials was performed. This approach was enriched with a study on the efficiency of the reflector thickness, given in Figure 11. However, all these results were achieved using TRITON/NEWT only. To improve the trust in the results, a comparison using the 2D

KENO VI model given in Figure 3 was performed. For this evaluation, the multi-group approach as well as the continuous energy approach were used, and the results are given in Table 1. The system diameters varied slightly among all three approaches, with the strongest variations for the SS304 reflector, while the results for the Pb and the Cu reflector were much closer. However, it is clear that the dimensional changes were small and were captured with sufficient accuracy for the aim of this study. Further investigations will be required as soon as a reasonable geometry has been designed for a potential core configuration of a zero-power setup.

Table 1. Systematic comparison of the TRITON/NEWT multi-group results with KENO VI in the multi-group approach as well as the continuous energy approach.

Material	System Radius [cm]			Deviation [%]	
Code	**NEWT**	**mg MC**	**ce MC [ref]**	**NEWT**	**mg MC**
SS304	36.8	35.5	37.9	−2.9%	−6.3%
Pb	38.25	37.65	38.1	0.4%	−1.2%
Cu	36.1	35.45	36.05	0.1%	−1.7%

6. Analysis of the Influence of the Reflector Material on the Neutron Flux

6.1. Neutron Spectrum

To create a deeper understanding of the effects of the different reflector materials, the neutron spectrum of the whole system and the spatial neutron flux distribution of five energy groups were analysed. The five energy groups was mainly chosen to reflect the neutron energy distribution of a fast system. The first insight into the global neutron spectrum indicated that the highly reflective materials BeO and graphite led to a neutron spectrum close to a light water reactor spectrum, with a significant thermal peak, while the metal reflectors Cu, Pb, and SS304 led to typical fast reactor spectra, which were similar to the spectrum of the absorber-containing reflector, ferroboron, and the unreflected system using He to fill the reflector region (see Figure 12). This insight into the neutron spectrum for BeO and graphite correlated very well with the observations for the power distributions; see Figure 8. Even if the fuel in the core represents a fast reactor configuration, there is a strong thermal peak which is formed in the strongly moderating reflector. The thermal neutrons then penetrate back into the fast reactor core, having very high importance due to the significantly higher reaction cross-section in the low energy range. Thus, these neutrons very efficiently undergo fission reactions in U-235. This leads to the undesired power peaking at the boundary of the core, caused by a strong self-shielding effect, which limits the depth of the penetration of the thermal neutrons. Thus, these moderating reflectors are not promising for fast reactor investigations, but they would have to be investigated in more detail at a later stage when thermal configurations could be investigated in a multi-purpose facility.

For a more detailed look into the effects of the metallic reflectors, Figure 12 is narrowed down to the energy range that is relevant to the neutron energies expected in a fast reactor. The resulting plot, Figure 13, shows some very important details created by the different metallic reflectors, which correlate once again very well with what is shown for the power distribution in Figure 9. Obviously, SS304, Cu and Pb formed a small low-energy tail in the system as well, and the interesting point is that this low-energy tail exactly coincided with the power increase at the boundary, which was highest for SS304 and lowest for lead. All the metal reflectors tended to soften the neutron spectrum slightly, with an increase in the number of neutrons below ~200 keV and a decrease in the number of neutrons above ~500 keV. In contrast to this, the use of a reflector containing a strong absorber for low energy neutrons, such as ferroboron, tended to harden the neutron spectrum, even compared with an unreflected system, by reducing the leakage of fast neutrons above 1MeV, while there was no effect on the low-energy tail below 10 keV.

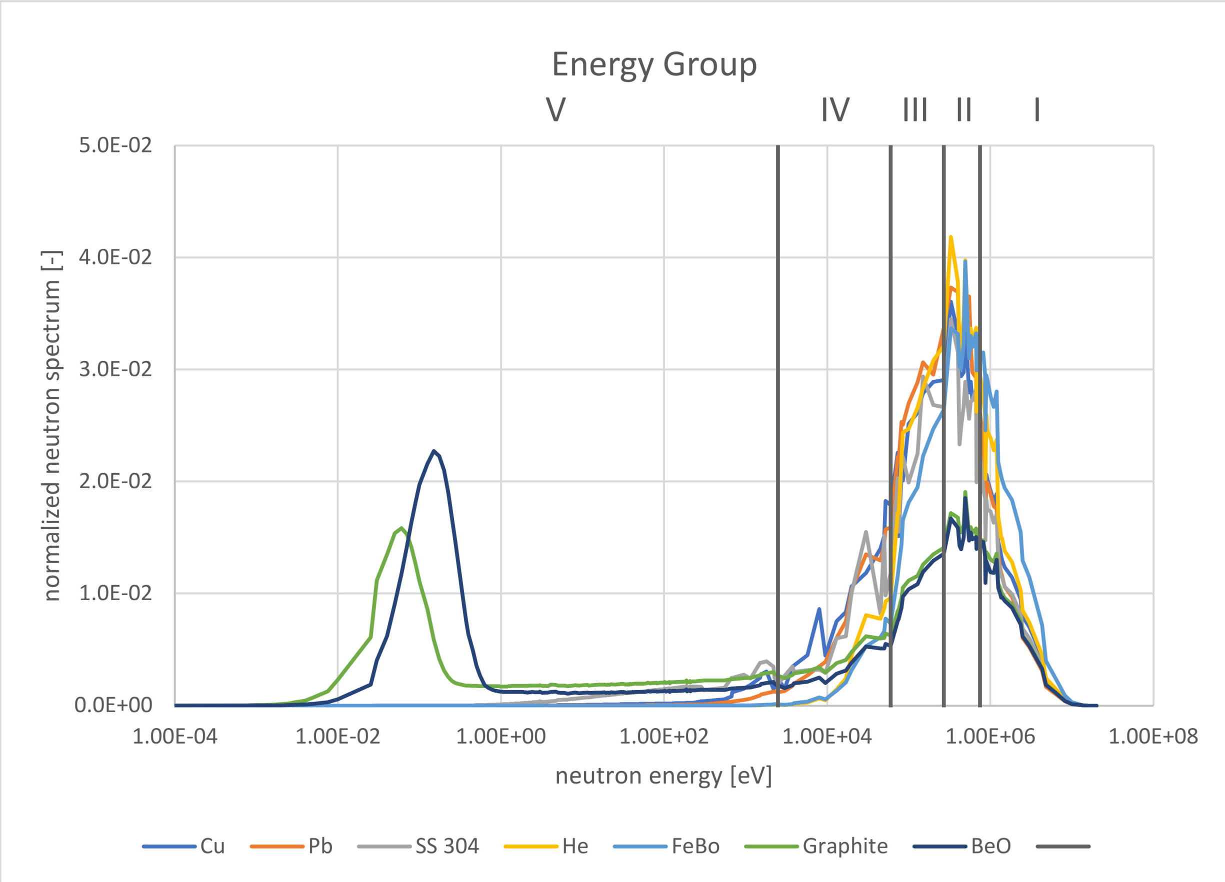

Figure 12. Whole-system integrated 252 energy group neutron spectra in the 2D system, depending on the different reflector materials.

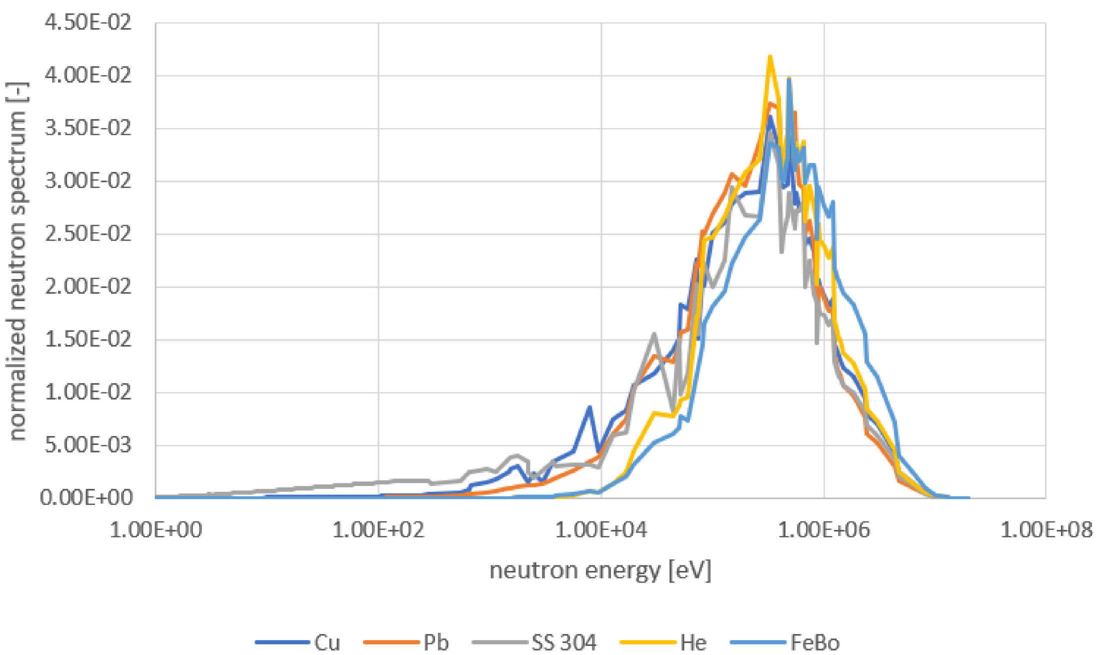

Figure 13. Selected fast reactor neutron spectra in the integrated 2D system, depending on a selection of potential reflector materials.

The spatial and energy resolved neutron flux were investigated through a comparison of two sets of neutron distributions for a five-group neutron flux using the energy boundaries shown in Figure 12. Figures 14 and 15 show the neutron flux distribution for different materials (left to right) with decreasing group energy from top to bottom. At the bottom of the figures, the colour scale based on the normalized neutron flux for each group and each material is given for comparison. To comparing the groupwise spatial flux distribution of the He reflected system, see Figure 14, which represents an unreflected system; with the system using FeBo as an absorbing reflector, the effect of the reflector is visible in each group. In the first three groups, the reflector led to a wider spread of the high flux area in the centre of the core and a very thin area of increased neutron flux outside the steel shell of the core. This effect was more pronounced in Group 4, where an almost flat flux distribution appeared through the whole core, while in Group 5, the flux maximum moved to the outer area of the core, but there are only very few neutrons in this group at all. However, when looking into the absolute values of the neutron flux for the different groups given at the bottom of the figure, it is clear that the absolute number of neutrons in each group has changed only very slightly. All five groups show only a very small penetration depth of the neutron flux into the reflector, which indicates that a much thinner reflector would most probably deliver almost the same result. This is in strong contrast to the case using a lead reflector; here, the penetration depth was already high in the first group and, starting from Group 2, the full reflector was used. Thus, a thicker reflector could be promising in this case. This confirms the results given in Figures 10 and 11, demonstrating that increasing the reflector thickness over the 30 cm standard still has a good influence on the criticality. The lead reflector flattened the spatial neutron flux in Groups 1 to 3 significantly, while it led, compared with the He and FeBo cases, to a decrease in the absolute number of neutrons in the first group and an increase in the second, third, and fourth groups. The maximum neutron flux in the fourth and fifth group appeared in the lead case already in the reflector, leading to an increase in the power production at the core surface. The general tendency in the copper reflector was comparable with the lead reflector, but with a significantly lower penetration depth in the first three groups. The maximum neutron flux in the copper case was slightly lower in Groups 1 to 3, but higher in Groups 4 and 5, as already expected from Figure 13. Groups 4 and 5 indicated a spatial flux maximum in the reflector feeding back into the core and leading to the slight power increase at the core boundary, as shown in Figure 9, with a slightly stronger effect than in the case using the lead reflector.

The groupwise spatial distribution of the neutron flux for the cases with the more moderating reflectors (graphite, BeO, and SS304) are given in Figure 15, with the case of the copper reflector added for comparison. Both the strongly moderating reflectors (graphite and BeO) show that in the first groups, there was a significantly lower penetration of the neutron flux into the reflector when compared with the metal-based reflectors. This indicates that for the BeO reflector especially, there seems to be room for a strong reduction of the reflector thickness. The low penetration depth coincides with the clearly reduced maximum neutron flux in these three groups in the moderating reflectors. The real effect of the moderating reflector is seen in Group 4 and even more in Group 5. In Group 4 the neutron flux peak has already completely moved into the reflector, but in contrast to the metal reflectors, there was only a very thin outer core layer which was boosted by the lower energy neutrons from the reflector. On the one hand, this explains the increase in the neutron flux in Groups 1 and 2 of the moderating layer cases, leading to a flatter neutron flux distribution. On the other hand, it may cause a rim effect, which could be problematic in the first phase of the zero-power reactor's operation, as long as the core is in a solid state. In addition, it will increase the fluence on the core vessel. The configuration was much more pronounced in Group 5, with a significant increase in the absolute number of neutrons in this group; see the bottom row of the figure (with the normalized neutron flux per group and per material), which indicates that the neutron flux in the graphite moderator in this group was approximately a factor of 18 higher than in the copper case and a factor of

280 higher than in the nonreflected system. In the BeO case, it was even worse, with the flux increased by a factor of 28 compared with the copper case and 440 compared with the unreflected case. These two results show that there is a significant number of neutrons "stored" in the reflector that do not significantly take part in the fission reaction cycle; this could lead to problematic behaviour in future zero-power reactor experiments such as rod drop or source pulse experiments [23,24] to determine the core criticality. The comparison of the SS304 case and the copper case showed only minor differences in the neutron flux distribution, a slightly higher penetration depth of the neutron flux into the reflector in Groups 1 to 3, and a slightly higher penetration depth of the neutron into the core when the neutron flux in the reflector was higher in Group 5. In this group, the major difference is shown in the number of neutrons appearing in the group (see the bar chart at the bottom of Figure 15).

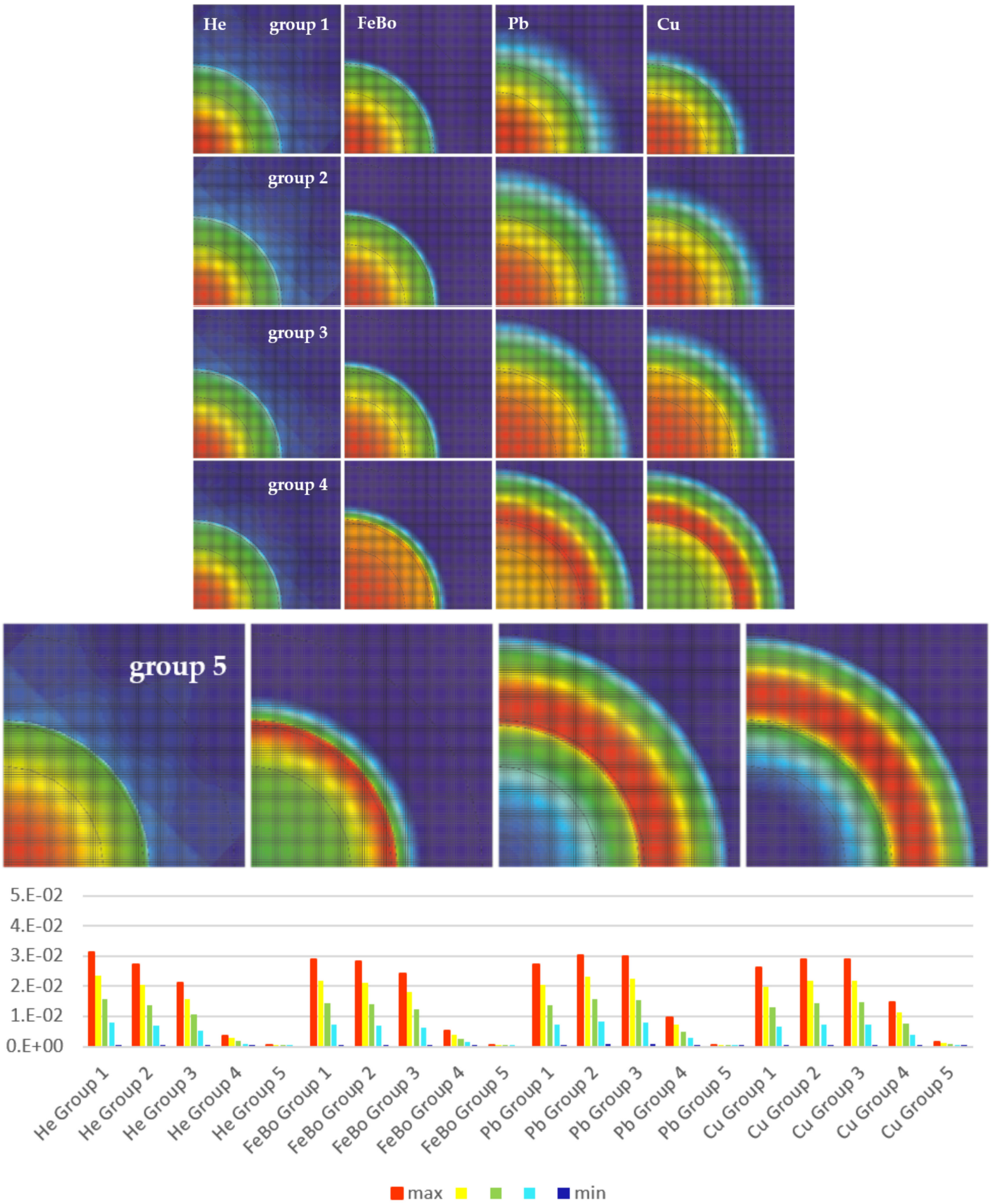

Figure 14. Groupwise 2D spatial neutron flux distribution in the core for four different weakly reflecting materials.

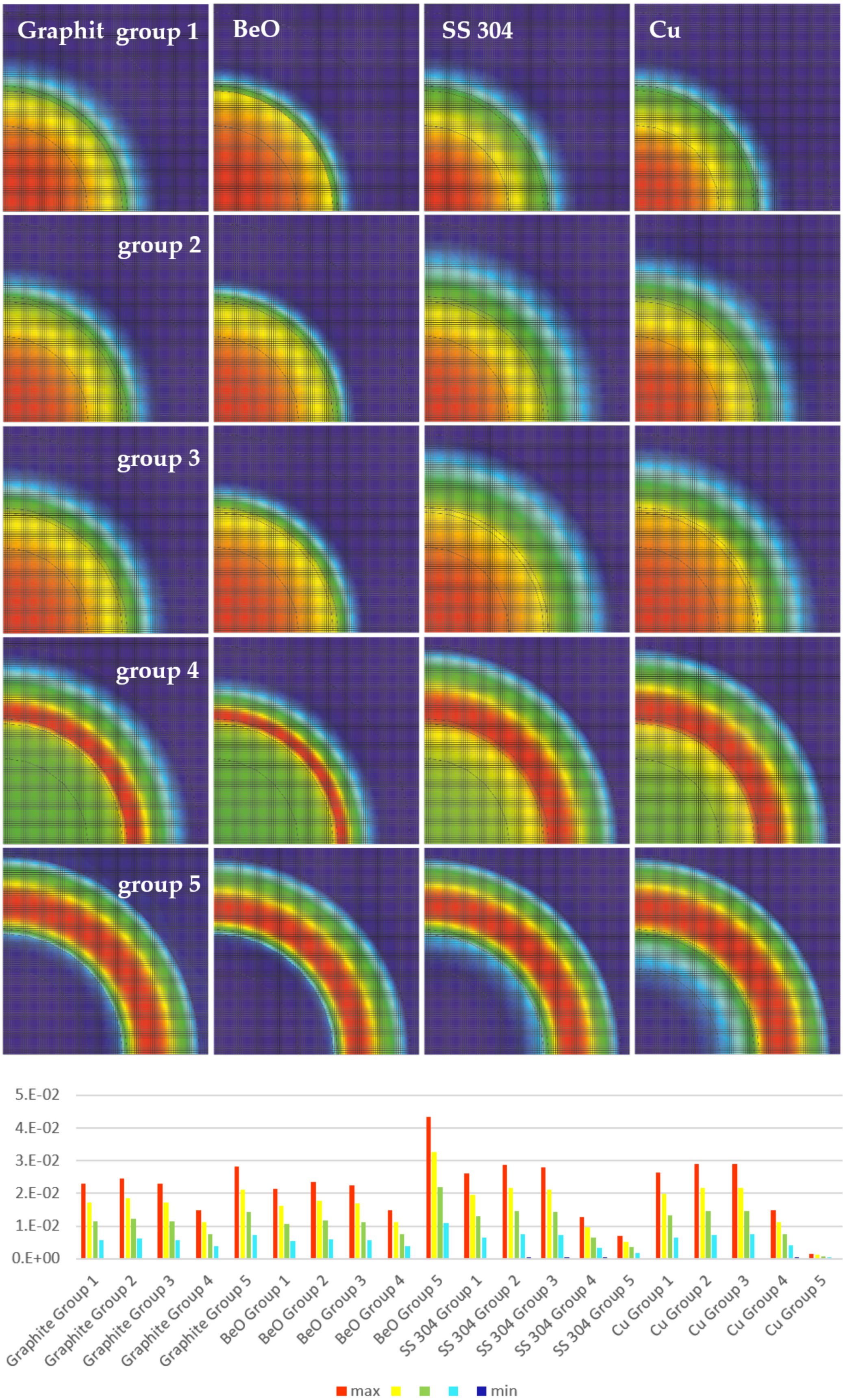

Figure 15. Groupwise 2D spatial neutron flux distributions in the core for four different strongly reflecting materials.

6.2. 3D Monte Carlo Study

The numerical study of the effect of different reflector materials was closed with a 3D Monte Carlo evaluation of the required volume for a critical core, depending on the chosen reflector material. The massive reduction in the required core volume for the different chosen reflectors, compared with the NaCl reflector used in previous studies [5,6], is given in Figure 16. While a core with a 30 cm reflector made from NaCl requires almost 2 m^3 of fuel to achieve a critical configuration, in this study, the chosen metallic reflectors can ensure core criticality with less than 1 m^3 of fuel. The exact result is a matter of optimization, with the SS304 reflector and the copper reflector requiring ~0.85 m^3. However, the study has shown that the copper reflector could most probably be reduced in thickness to achieve the best result, while the lead reflector could deliver better performance with a higher thickness. For confirmation of the results, an additional continuous energy Monte Carlo calculation was performed (see the right-hand bar in Figure 16). This test indicated a difference of about 5% between the multi-group approach and the continuous energy approach, which seems to be acceptable for this kind of broad optimization study. However, for a more detailed analysis, the use of a continuous energy Monte Carlo code seems to be more appropriate.

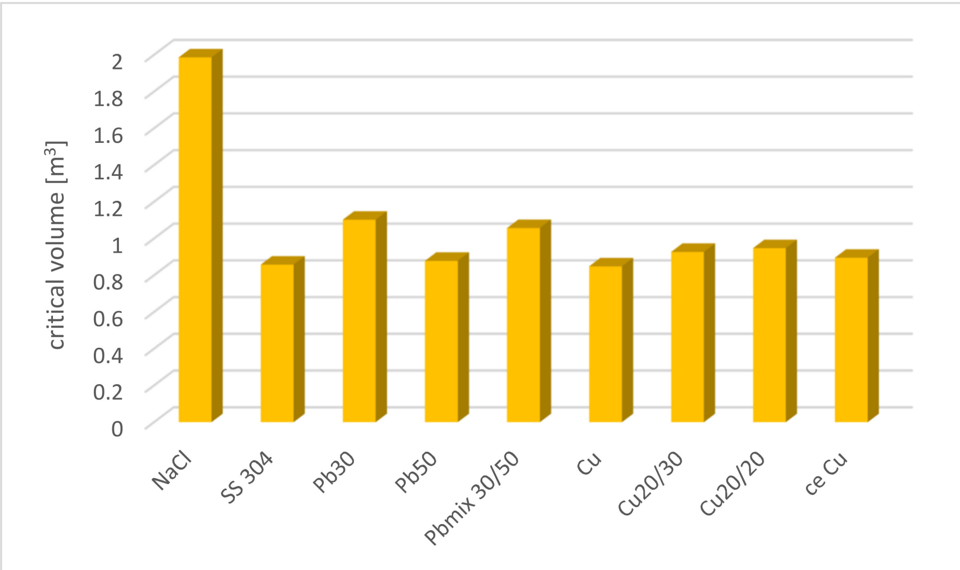

Figure 16. Evaluation of the required core volume to achieve a critical core, depending on the chosen reflector material.

An initial cost analysis of different reflector approaches identified the SS304 reflector as the cheapest solution based on the pure reflector cost; see Table 2 with the data source in the footnote. In general, there is still some optimization potential considering the cost of the fuel, the cost of the reflector, and, potentially, the cost of the required core and reflector support, especially in the case of applying the approach of using a moving reflector for reactivity control. In addition, the effect of the reflector on the quality of the experiments should be added to the consideration.

An initial step to obtain a deeper understanding of the potential savings in core volume and the role of the changes in the axial as well as in the radial reflector, some cases have been investigated for the copper- and the lead-reflected core. From Table 3, it is obvious that increasing the size of the radial reflector was much more efficient than increasing the size of the axial reflector. The effect can be observed with both materials independently.

Table 2. Cost comparison for different reflector configurations.

Reflector	Cost [$/ton]	Density [ton/m^3]	Cost [$/m^3]	Cost Estimate [$]
SS304 30 cm (https://www.stindia.com/stainless-steel-304-316l-price-per-kg-india.html#price_per_kg, accessed on 1 April 2021)	4380	7.390	34,733	88,372
Lead 50 cm (https://markets.businessinsider.com, accessed on 1 April 2021)	2026	11.343	22,980	132,728
Copper 20 cm (https://markets.businessinsider.com, accessed on 1 April 2021)	7735	8.94	69,150	105,458

Table 3. Study of potential volume savings resulting from an increase in the reflector thickness at different places.

	Volume Saving	Case
All reflectors	20.3%	Pb 30 cm to 50 cm
	10.4%	Cu 20 cm to 30 cm
Axial reflector	4.1%	Pb 30 cm to 50 cm
	2.2%	Cu 20 cm to 30 cm
Radial reflector	16.9%	Pb 30 cm to 50 cm
	8.5%	Cu 20 cm to 30 cm

6.3. Control Curve and Shutdown

In a final step, the consequences of the change in the reflector for the reactor control and shutdown system as developed in [6] had to be evaluated to ensure that the changed reflector still allows the application of the envisaged control and shutdown approach. The use of the smaller core with the copper reflector led to a significant increase in the control span compared with the original larger core with the NaCl reflector (see Figure 17). The increase in the control span can be explained by the significantly stronger effect of the reflector on core criticality, which was finally reflected through the opportunity to decrease the size of the core while the core still stayed critical. Thus, the control approach cannot only be kept when using the copper reflector: the approach will even become more efficient and the control span will become wider, which allows the higher flexibility of the reflector control and the core design.

The evaluation of the consequences of changing to a significantly more effective reflector material on the shutdown system is given in Figure 18. The splitting of 30 cm in this layer of the core, including the reflector, delivers a significantly higher shutdown reactivity with the smaller core than in the reference case with the NaCl reflector. Thus, the envisaged shutdown approach would not be negatively influenced by the change to a much more efficient reflector material. It would even allow a potential reduction of the core layer which has to be split away. This optimization should be carried out when a definitive decision has been taken regarding the reflector material and the final core design.

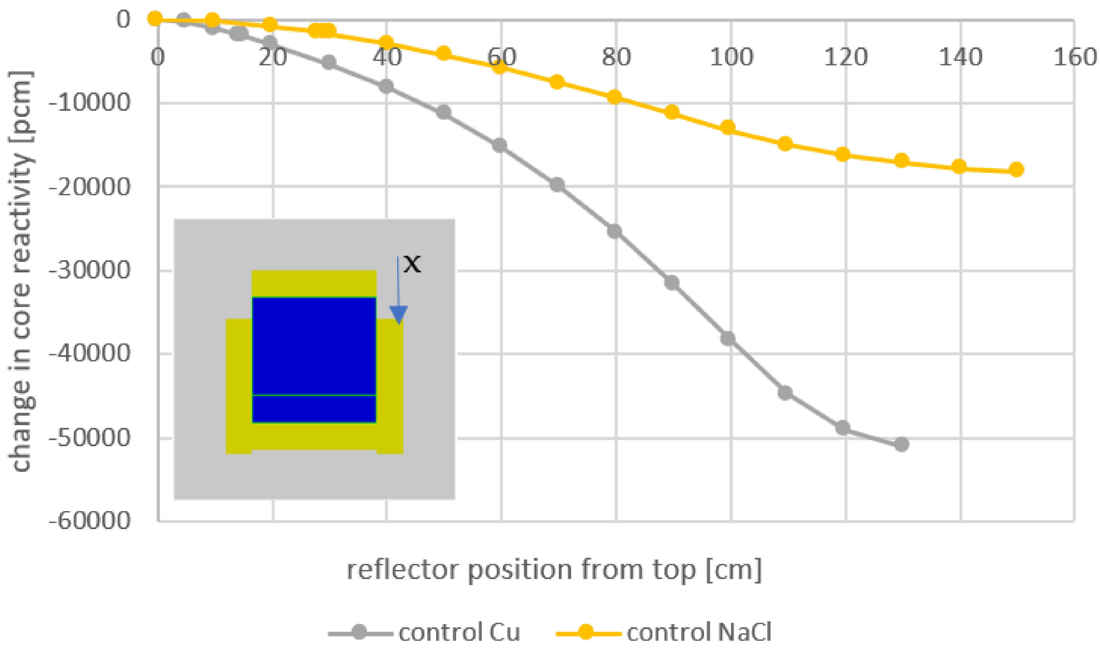

Figure 17. Comparison of the control curve caused by moving the reflector made of NaCl and copper, with the systematics of the study described in the insert.

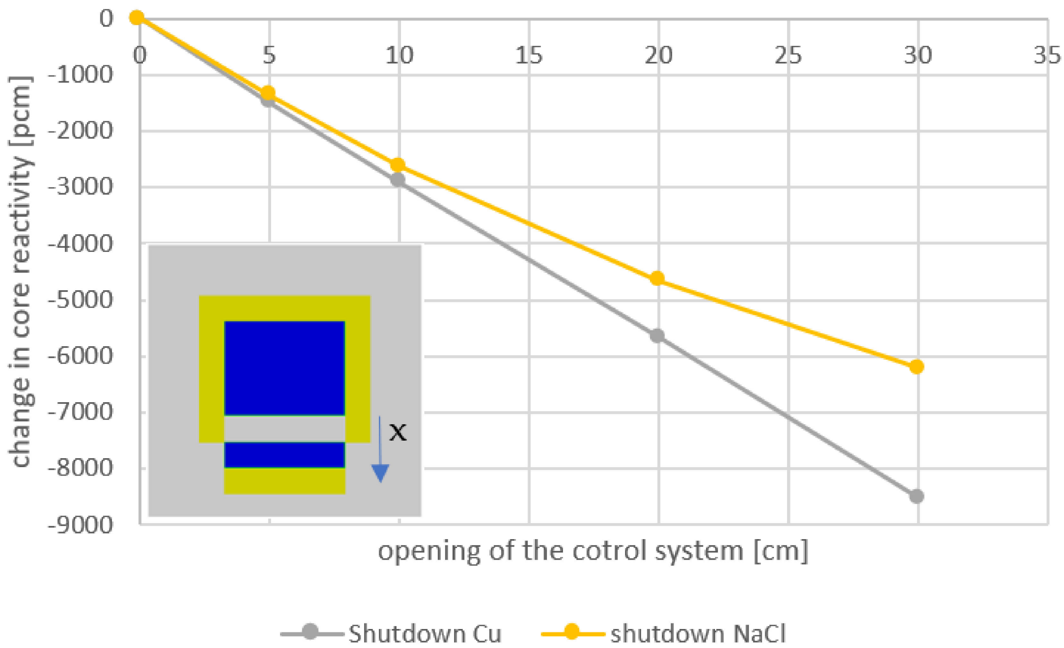

Figure 18. Comparison of the shutdown curve caused by moving the bottom part of the core for the reflectors made of NaCl and copper, with the systematics of the study described in the insert.

7. Conclusions and Next Steps

The relevance of the neutron reflector in the core design was discussed in the introduction with the view of extending it into power reactors as well as into neutronic experiments, where the role of the reflector has a much higher importance. In the following, the theoretical roles of the reflector for any kind of physical neutron installation are discussed. The investigation of the effect of different reflector materials regarding the achievable k_{eff} and power distribution for a given reference configuration was performed. The study of a set of classical reactor materials and more exotic choices led to a first down-selection based on the gain in k_{eff}, with SS304 (as the representative for stainless steel), lead, copper, graphite, beryllium oxide, and iron-based material with a high Si content identified as promising. The following investigation of the power distribution highlighted that the strongly moderating reflectors based on graphite and beryllium oxide had a strong influence on the power distribution within the core and will deliver a non-natural power distribution with a peak at the reactor boundary instead of the reactor centre.

Based on this first down-selection, the 2- critical core dimension was evaluated for the chosen reflector materials, identifying stainless steel and copper as the most attractive solutions, with lead as a potential backup and graphite as an attractive candidate in the case of a future thermal system. The study of the optimal reflector dimension identified that the reference approach of a reflector thickness of 30 cm was a good approach but, especially in the case of copper, a thinner reflector could be sufficient, while in the case of lead, a thicker reflector could be more promising.

The analysis of the influence of the reflector material on the neutron flux spectrum confirmed the expected effect of the moderating reflectors BeO and graphite, while the difference in the neutron spectrum in the cases of the metal-based reflectors was found to be very small. The investigation of the 2D flux distributions split into five energy groups confirmed the expectation that there was a significant number of neutrons stored in the moderating reflectors, which led to a number of very well thermalized neutrons streaming back into the core, explaining the power increase at the core boundary observed in the study of the 2D power distribution. In addition, this insight highlighted the results that the penetration depth in the lead reflector was very high, while the penetration depth in the copper reflector was very low, confirming the result that a thicker lead reflector could be promising, while a thinner copper reflector could be sufficient.

Following all the 2D studies, a 3D Monte Carlo study to investigate fuel volume savings was performed, which highlighted the potential fuel savings possible through a good choice of reflector. There is a potential for a reduction of up to 60% in the fuel volume compared with the reference case using a NaCl reflector, with the best results for stainless steel and copper, or a thicker lead reflector.

The final cost comparison for different reflector configurations identified that the stainless steel reflector was the most cost efficient solution. However, this reflector has the strongest influence on the power distribution. In general, there is some additional optimization needed to make a final choice between the three most promising reflector materials: SS304, lead, and copper.

The study closed with a test confirming that the control curve and shutdown approach developed earlier was not influenced or even partly improved through the choice of efficient reflector material.

For more detailed future studies, investigations at room temperature would be the next step required. For these studies, an urgent need for data for the fuel in the solid state at RT has been identified, which will definitively be required. The next step should be to look into a multi-purpose machine. The current study concentrated on the fast system, but many conclusions can be drawn for the thermal system as well. However, the thermal system would be worth an independent study, possibly for different published core configurations (e.g., Terrestrial Energy and the Chinese TMSR project).

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