On the dimensions required for a molten salt zero power reactor operating on chloride salts

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, United Kingdom
2 Scientific Computing Department, Science and Technology Facilities Council, Daresbury Laboratory, SciTech Daresbury, Cheshire WA4 4AD, United Kingdom
* 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 operation for massive net-zero energy production. The importance of a zero-power reactor for the process of developing a new, innovative rector concept like molten salt fast reactor is described here. It is based on historical developments as well as the current demand for experimental results and key factors that are relevant to the success of the next step in the development process of all innovative reactor types.

In the systematic modelling & simulation of a zero-power molten salt reactor, the radius and the feedback effects are studied for a eutectic based system, while a heavy metal rich chloride-based system are studied depending on the uranium enrichment accompanied with the effects on neutron flux spectrum and spatial distribution. These results are used to support the relevant decision for the narrowing down of the configurations supported by considerations on cost and proliferation for the follow up 3D analysis to provide for the first time a systematic modelling & simulation approach for a new reactor physics experiment. The expected core volumes for these configurations have been studied using multi-group and continuous energy Monte-Carlo simulations identifying the 35% enriched systems as the most attractive and finally leading to the choice of the heavy metal rich compositions 35% enrichment as the reference system for future studies of the next steps in the zero power reactor investigation. The inter-comparison of the different applied codes and approaches available in the SCALE package has delivered a very good agreement between the results creating trust into the developed and used models and methods.

Keywords:

Nuclear; Nuclear Reactors; Reactor Physics; Nuclear Experiments; Zero-Power Reactors; Modelling & Simulation; Molten Salt Reactors

Introduction

Historically, zero or very low power experiments have been seen as the first step into a new reactor program or a new technology [1]. The key requirements were to test new configurations in safe settings and to use the opportunity of these highly flexible experiments to assure effective learning at the beginning off a new technology.

Figure 1 shows the timeline of the MAGNOX development with several zero or very low power facilities Gleep in 1947, BEPO in 1948 to Windscale-1 in 1952 at the beginning of the UK nuclear programme.

At that early point of development, the major arguments for the zero power experiments were the comparably low cost and the opportunity of flexible, well instrumented tests to demonstrate and improve the understanding of the system behaviour, to support the theoretical models, and to investigate a multitude of promising solutions in a short time period promising rapid and effective learning. More recent ideas demonstrate that building a zero-power offers a multi-fold opportunity to support the start up of an innovative reactor program [2].

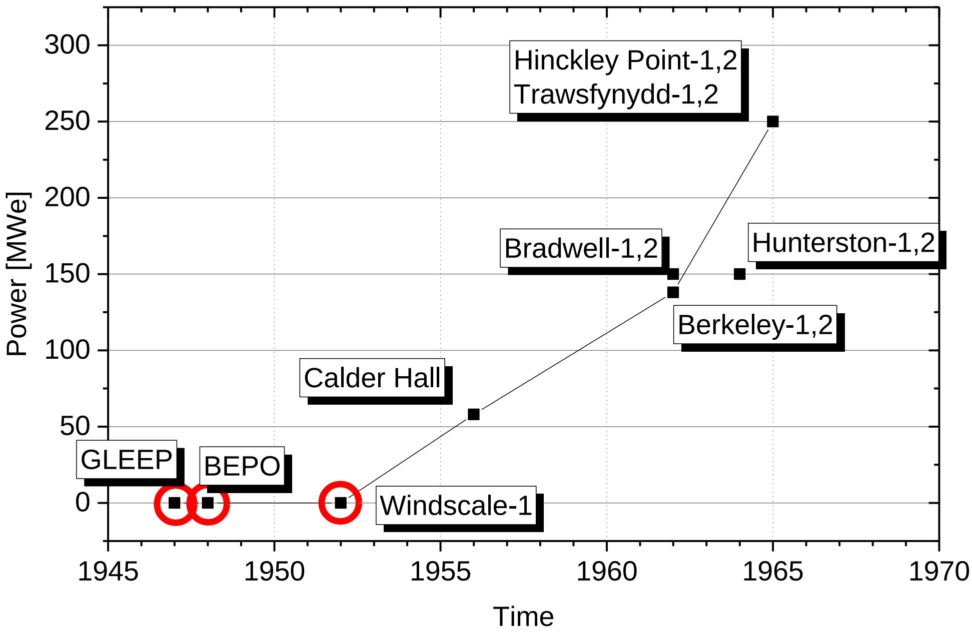

Figure 1: Development timeline of the MAGNOX technology following the data of [1]

At the first glance zero power experiments have lost this high priority in more modern times, e. g. when observing the timeline of the German HTR programme [3] starting with the highly successful AVR experiment. However, looking deeper into the development of the programme, the importance of zero power experiments is even more highlighted due to the decision for the demand of a zero-power facility as basis to provide the more hands on testing leading to the KAHTER facility in 1973 [3]. The developers of the HTR programme confirmed that zero power tests have been essential for the optimization of the system and the confirmation of theoretical models [4]. Nowadays, scientists claim that it is possible to design a new reactor based on modelling & simulation only, which maybe be true for a known technology like light water reactors with a very broad validation base and a wide variety of specially developed codes. However, for any really new technology, these specialized modelling & simulation tools either do not exist or there is a strong demand for code validation on experimental results either demanded by the developers or in the next stage by the regulator in the design assessment process. Typically, validations are required for tools relevant for determination of

- core criticality and reactivity effects
- neutron flux distribution in space and energy as well as the resulting power distribution
- changes in reactivity and neutron flux resulting from density and temperature changes

where zero power experiments can deliver the first validation level. This first level of experiments is the basis for any next step in the process of developing a new, innovative reactor system as given in Figure 2, where the validation request is only a part of the reasoning for the zero power experiment besides:

- the formation of a team of specialists which is able to develop the project

- the development and production of the first key components, e. g. the fuel
- the establishment of a supply chain
- the close interaction with the regulator to get the experiment licensed [3]

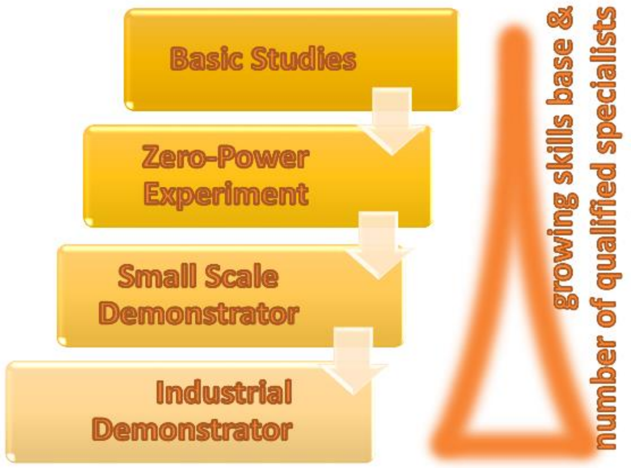

Figure 2: Process steps for the development of a new, innovative reactor system following [3]

The typical zero power experiments kind are almost impossible to implement in power producing systems with high operational temperature and high neutron flux as well as the levels of radiation due to fission products. In contrast to this, a major point in the zero power experiments is the significantly larger operational envelop of a zero-power facility and the higher flexibility than in power producing systems, while not requiring an energy removal system due to low or at least moderate operation temperature and very low power. The low flux and power levels allow accessibility (reduced radiation level due to the absence of large amounts of fission products). These properties, widen the space of available instrumentation significantly and allow rapid changes of the setup to investigate different configurations, allow for almost immediate accessibility to the experiments after shut down and assure extremely fast take up of a relevant set of experimental results.

Following these arguments, the last, new established technology, accelerator driven systems and lead cooled reactors have been accompanied by two different zero power experiments, YALINA [5, 6] and GUINEVERE [7, 8] to create understanding of the interaction between the accelerator and the sub-critical core as well as to deliver validation for lead cooled reactor systems. Looking into molten salt reactor technologies completely new approaches for operating reactors on spent fuel have come up [9, 3], and many companies like TERRESTRIAL Energy [10], TERRAPOWER [11], Elysium industries [12] and others are planning reactors which will have demand for code and design validations. However, due to the homogeneous core composition (unity of coolant and fuel) of a molten salt reactor, a zero power reactor experiment is significantly different to existing, heterogeneous experiments. Thus, novel approaches for design, operation, control, and experimental setup must be designed, developed and invented beginning with this series of publications while Russia has already announced to develop their own research reference facility for their partitioning and transmutation molten salt reactor programme [13].

The focus of this publication will be on answering the questions on the salt compositions and the dimensions required of a potential experimental setup to narrow down the choices for a zero power experiment for a molten salt fast reactor based on a multitude of modelling and simulation results using different tools of the SCALE package.

Codes & General Modelling

The salt system is based on detailed data on the density versus temperature curve from Russian literature [14], see table 1. The data is used for the analysis based on a reference temperature of 980 K with changes by ± 50K for the analysis of feedback effects. Nevertheless, while being a good starting point, the data is limited to a very narrow temperature window and for a temperature range which will not be the first choice for initial experiments in a zero-power environment. Especially, for a detailed study of a future zero-power experiment the temperature range has to be extended down to room temperature to be able to judge the system behaviour under cold conditions which would be the perfect setting for first experiments.

Table 1: Concentration dependent densities for the system NaCl-UCl_3-UCl_4 with the Uranium salt composition 30% UCl_3+70% UCl_4 and varying NaCl concentrations part reprinted form [1]. The experimental error in the density measurements is given with max ± 1.5%

Concentration % NaCl	ΔT [K]	a	b 10^3	std dev 10^3
20.0	934 – 1018	5.3995	1.8646	4
30.0	934 – 1020	4.9360	1.5276	2
45.0	939 – 1029	4.2368	1.0256	3
60.0	872 – 1037	3.8237	0.8774	2
80.0	985 – 1119	3.2382	0.8012	2

Based on the coefficients given in Table 1, the temperature dependent density is calculated based on the following formula:

$$\rho\left[\frac{g}{cm^3}\right] = a - bT[K] \qquad (1)$$

Based on the given salt system investigation [15], the applied standard salt composition for the study for the nominal case, is the eutectic 42.5% NaCl- 40.5 UCl_4- 17% UCl_3. This composition is close enough to the third row of Table 1 to provide a reasonable density estimation. In addition, a heavy metal rich case is investigated with 20%NaCl-56.35%UCl_4-23.65%UCl_3.

The simulations for this initial study of zero-power reactor configurations have been performed using the POLARIS module of the SCALE code system [16]. Polaris is a new module for SCALE 6.2 that provides a 2D lattice physics analysis capability that uses a multigroup self-shielding method called the Embedded Self Shielding Method (ESSM) and a transport solver based on the Method of Characteristics (MoC). In general, POLARIS and its cross-section library has been developed and validated for light water reactors, thus we have provided in a recent publication [17] a first step verification/validation against the Monte-Carlo code SERPENT [18]. This will be extended here by comparisons to the multi-group deterministic S_n transport calculation sequence TRITION/NEWT and multi-group as well as continuous energy Monte-Carlo code Keno VI, all parts of the of the SCALE package [19].

Polaris uses the v7-252 cross section set of the SCALE package, based on ENDF/B 7.1, which is also the basis for the TRITON/NEWT as well as the multi-group (MG) Keno VI calculations while the continuous energy version uses the ce_v7.1_endf library of the SCALE package

For the study, a very specific 2-D and 3D models of a fast molten salt reactor have been built for the simulation. First, the POLARIS model, see Figure 3, consisting of 2D discretized ring core surrounded by a steel vessel and a reflector region with a large amount of absorbing material around the core. Second the NEWT model, reflects a 2D quarter of the core with x-y discretization consisting of the ring core, the steel vessel surrounded by reflector while the rest of the cell is filled with vacuum using reflective boundaries at the bottom and the right side and vacuum boundaries at the other two sides, see Figure 4. Third, the 2D and 3D Keno VI models in Figure 5, reflecting a cylindrical core surrounded by a vessel and a reflector on all sides for the 3D model and reflective boundary conditions at top and bottom for the 2D model.

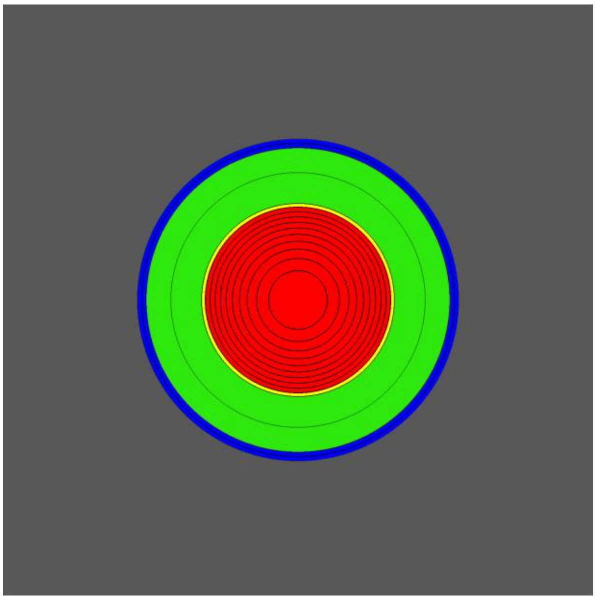

Figure 3: 2D SCALE/POLARIS model (molten salt fuel core – red, stainless steel – yellow, NaCl reflector – light green, vacuum – blue, absorber material – dark grey) used for the general analysis

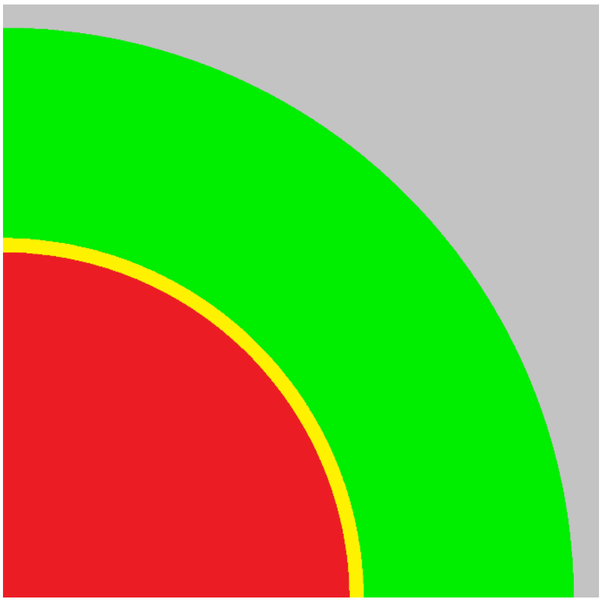

Figure 4: 2D SCALE/TRITON/NEWT model (molten salt fuel core – red, stainless steel – yellow, NaCl reflector – light green, vacuum – grey) used for the analysis of the neutron flux distribution

Figure 5: 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 molten salt fuel core – blue, stainless steel vessel – light green, reflector – yellow, and vacuum - grey used for the validation of the results and the 3D studies

The limit for the dimensional iterations in POLARIS, NEWT, and KENO VI has been set to ±100 pcm. For the Monte-Carlo simulations a setting of 1000 generations with 10000 particles each has been used for the iteration and for the final evaluation 5000 generations with 50000 particles have been used. This setting leads to an accuracy of ±12 pcm and below at 95% confidence, which is more than sufficient in comparison to the spatial dimension iteration limit.

Results and Discussion

The first important information for designing a small scale zero-power core is the demanded size, the required salt amount, and the related amount of nuclear material. The required core size is studied through the variation of the enrichment followed by the determination of the radius required to achieve a critical configuration in the 2D system with an iteration accuracy of ± 100 pcm. The mentioned size of the core is strongly dependent on the salt composition – eutectic composition versus heavy metal rich composition, and on the fissile enrichment in the uranium chloride salt. The system radius and thus the required amount of salt is, as to be expected continuously decreasing with increasing U-235 enrichment showing a kind of asymptotic behaviour for very high enrichment, see Figure 6.

The observation holds for the reflected and the unreflected system (modelled through replacing the reflector material though vacuum) as well as for the eutectic and the heavy metal rich system. The volume gain

$$volume\ gain = \frac{vol_{HMR} - vol_{ET}}{vol_{HMR}}\ [\%]$$

for the heavy metal rich (HMR) system stays almost constant with a volumetric reduction of ~30% compared to the eutectic system (ET), only for the 20% enriched system the volume gain is slightly higher. The slight variation in the curves seem to be a result of the iteration limit for the dimensional iteration. From the point of the required salt volume a good gain can be achieved by increasing the U-235 enrichment to 35% - thus a value higher than the LEU level of 20%, the effect of going to higher enrichments doesn't seem to give the required significant improvement to justify moving to a highly enriched fissile material.

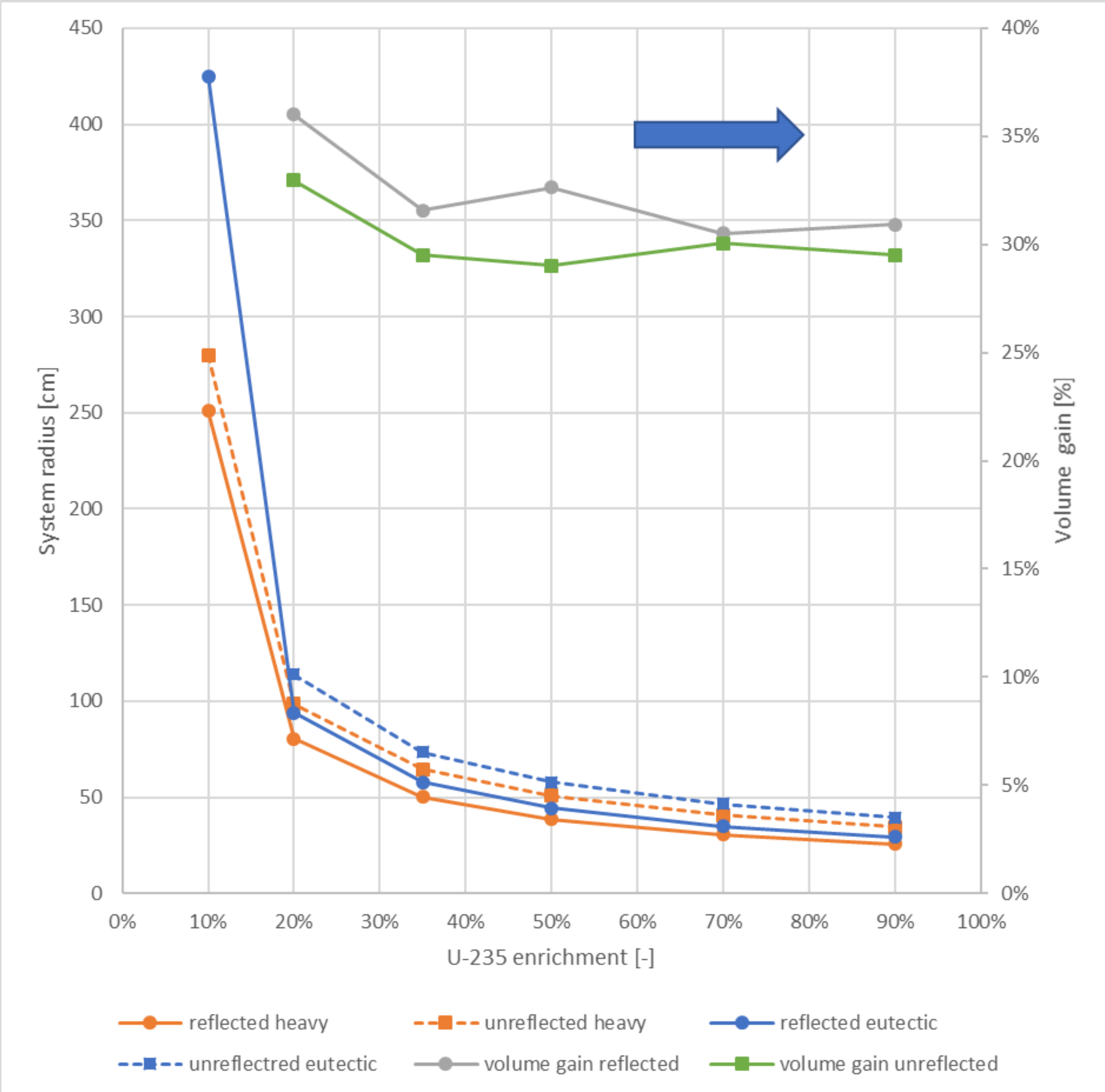

Figure 6: 2D system radius for the eutectic and the heavy metal rich system depending on uranium enrichment for the reflected and the unreflected systems as well as the volume gain per step archived by changing form the eutectic to the heavy metal rich system

The second step of the study analyses the efficiency of the reflector dependent on the U-235 enrichment and the two different salt configurations, Figure 7. For this step all reflected critical configurations of the last step have been recalculated with the reflector region filled with vacuum. The figure indicates a clear change in the effect of the reflector with the expected growing effect of the reflector with increasing U-235 enrichment and the correlated decrease of the size of the critical system. The k_{eff} of the drop caused by eliminating the reflector reaches up to more than 20000 pcm for the highest enrichment while the effect starts to saturate at high enrichments. The effect of removing the reflector is slightly stronger for the heavy metal rich system for lower enrichments while this difference disappears for higher enrichment. The results of this step indicate a good opportunity to use the reflector as a future control system for a zero-power reactor in the case the enrichment is sufficiently high, at least 35% or higher. The control- and shut-down system will be discussed and analysed deeper in a second part of this study [20] and the effects of the use of different reflector materials in a third part [].

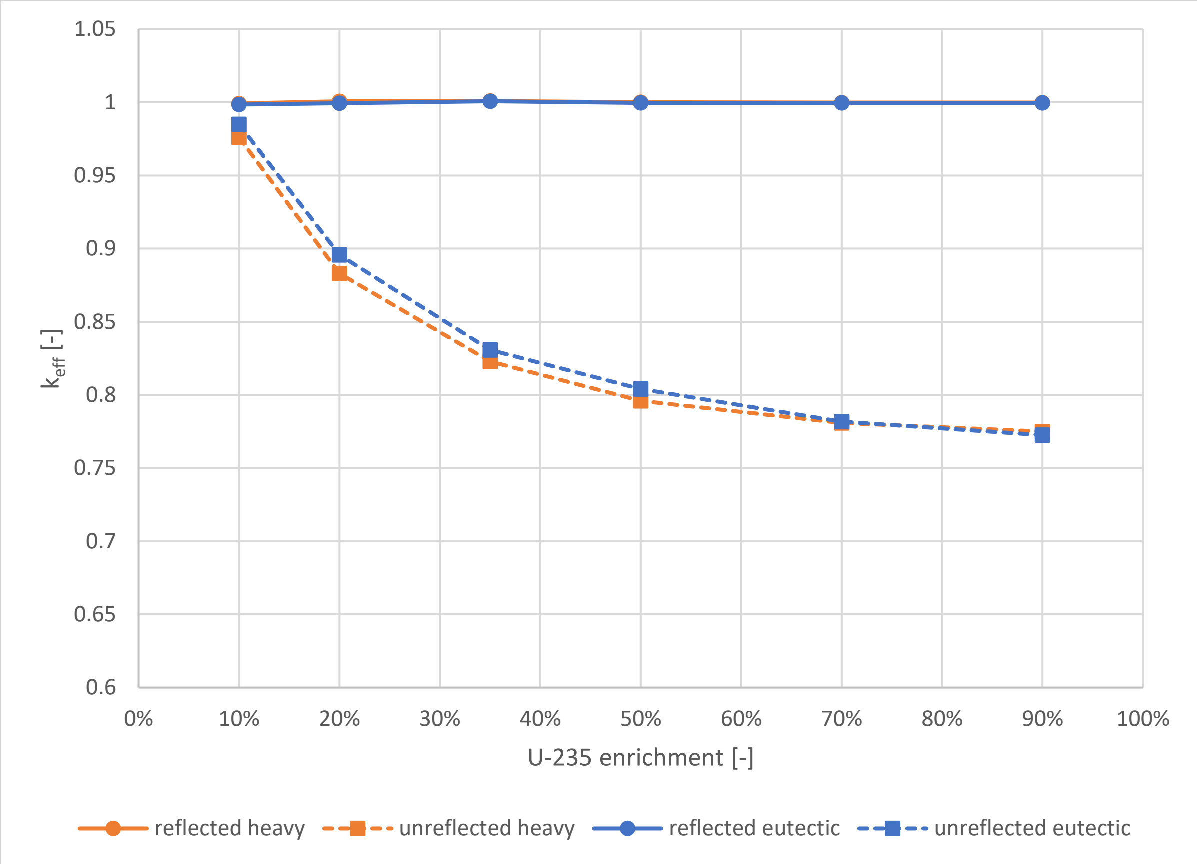

Figure 7: 2D system criticality reduction by eliminating the reflector for the eutectic and the heavy metal rich system depending on uranium enrichment

Another important feature for the control of the reactor is its stability due to the inherent temperature feedback effect. This feedback effect is combined out of two major components in a molten salt reactor, one is the density change of the molten salt which acts in unity as coolant as well as fuel. The other effect is the Doppler or fuel temperature effect which leads to a higher level of neutron absorption in the reactor fuel due to resonance broadening. The feedback effect is determined through the change in density using Eq. 1 to provide new number densities combined with the change of the temperature of the molten salt applied for the cross-section correction due the Doppler effect. In general, molten salt reactors possess a very strong negative feedback behaviour. The effect of the density changes in the salt leads to a reduction of the density of fissile atoms in the salt volume of the core thus the criticality will be strongly reduced when the salt expands, while the classical Doppler effect is in a comparable range to other reactors operating over a comparable temperature level. However, there are two things which are of interest: How much dependence does the temperature feedback effect show with regards to the variation of the uranium enrichment and thus the core dimension? The second point would be the feedback effects at low operational temperature around room temperature with solid salt, but the density over temperature data is currently not available for this high importance temperature window.

The temperature feedback increases with increasing U-235 enrichment, but it shows the same style of saturation as already seen in the dimensional study and the reflector study. Thus, the effect of increasing the enrichment is stronger at lower enrichment than for very high enrichment, see Figure 8. In general the effect grows for ~-3 pcm/°C to -20 pcm/°C for the eutectic system and ~-7.5 pcm/°C to -34 pcm/°C for the heavy metal rich system. The growing effect due the increased enrichment as well as for the heavy metal rich case can be explained through the higher amount of fissile material which is pushed out of the core in the case of a reduction of the density due to temperature increase.

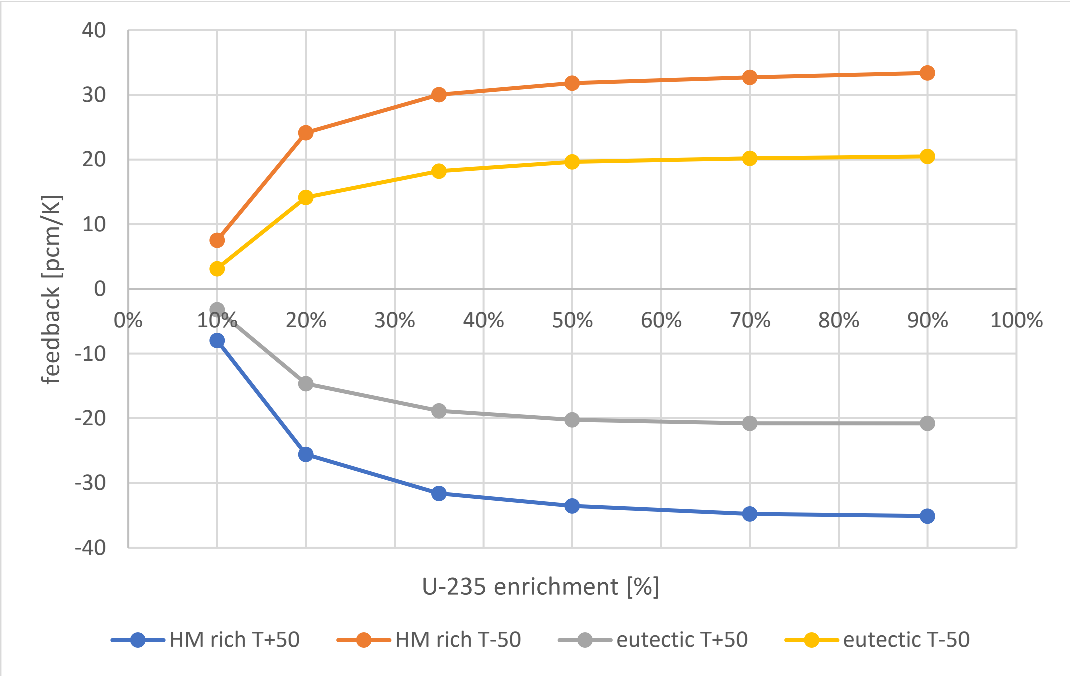

Figure 8: 2D system thermal feedback effects (salt density and fuel temperature) for the eutectic and the heavy metal rich system depending on uranium enrichment

The next part shows an investigation of the influence of different system alternations: heavy metal content of the salt, the use of the reflector and the enrichment on the neutron spectrum in the system. The general neutron spectrum in the NaCl-UCl system is highly comparable with a fast reactor where almost no neutron flux below 100 eV is observed and there is a clear peak between 200 keV and 1 MeV. The spectrum is slightly harder than in a classical sodium cooled fast reactor fuel assembly of EFR type [22], see the grey line in Figure 9. The molten salt reactor spectrum is characterized by a much smaller but still visible low energy tail formed by the sodium, a clearly lower number of neutrons below 100 keV and a higher number of neutrons above this value.

The change from the eutectic to the heavy metal rich system leads to a slightly harder neutron spectrum with a decrease of the number of neutrons below ~ 100keV and a slight increase of the number of neutrons around 1MeV, see Figure 9. However, the change in the neutron spectrum is only very limited, the general spectral distribution stays almost constant.

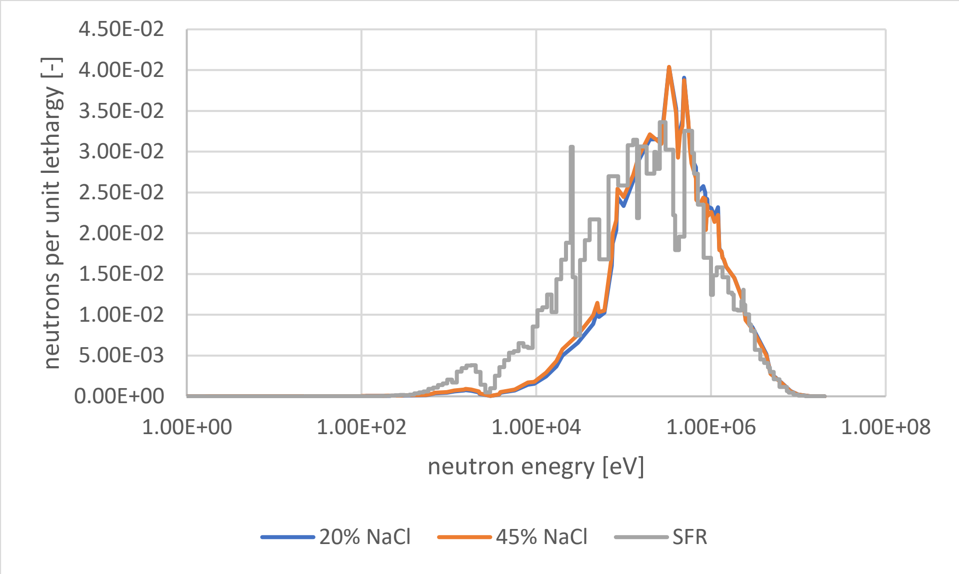

Figure 9: Neutron spectrum 35% enriched for the eutectic and the heavy metal rich system in comparison with the neutron spectrum in a classical sodium cooled fast reactor (SFR) fuel assembly of EFR type

The influence of the NaCl reflector on the neutron flux spectrum is much stronger than the influence of the salt composition, see Figure 10. The reflector creates a new peak around 1 keV which disappears when the reflector is removed. This low energy peak reflects neutrons which are undergoing several collisions without leading to neutron reactions, which happens mainly in the reflector. Besides this, the neutron spectrum of the system is clearly softened by the reflector creating a higher neutron flux below ~200 keV and a lower neutron flux around 1 MeV.

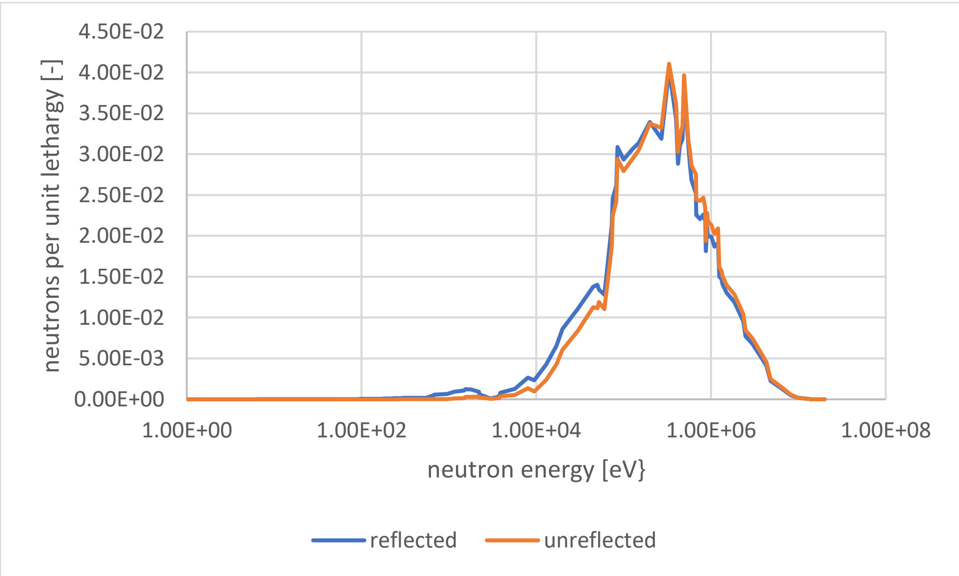

Figure 10: Neutron spectrum 20% enriched for the reflected and reflected eutectic system

The strongest change in the neutron spectrum is caused by the change in the U-235 enrichment, see Figure 10. The use of highly enriched uranium leads to a clear reduction of the system size, see Figure 6. The small system size leads on the one hand to a significantly higher neutron leakage and less collisions, on the other hand the strong reduction of the U-238 amount diminishes the parasitic absorption of neutrons in the system since most of the heavy metal is in the 90% enriched system fissile material. Overall, these changes lead to a decrease of the number of neutrons in the energy range below 200 keV and an increase of the number of neutrons above 500 keV. The neutron spectrum of the 90% enriched system is much closer to the fission neutron spectrum.

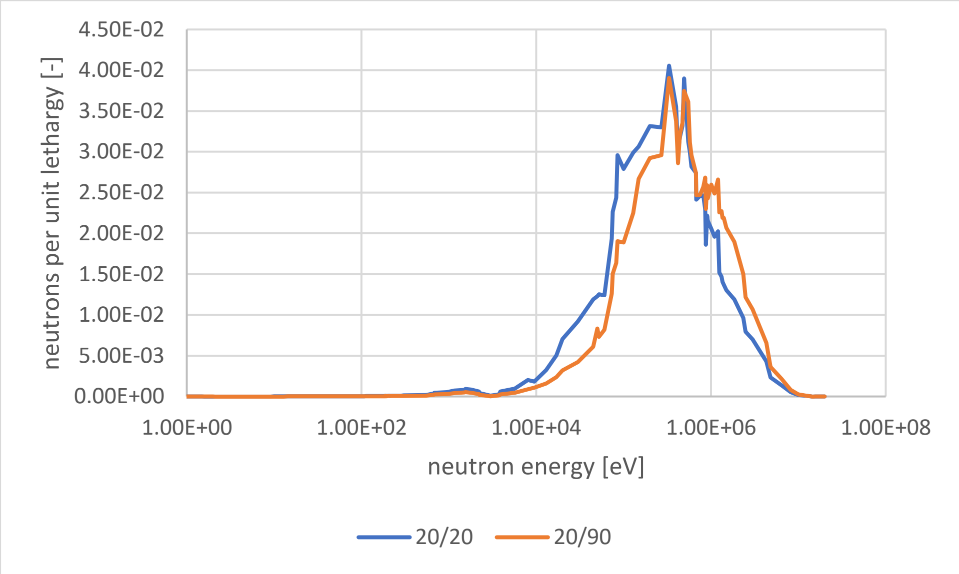

Figure 11: Neutron spectrum for the heavy metal rich system (20% NaCl) with 20% enrichment (20/20) compared to the 90% enriched system (20/90)

All results presented and discussed up to now have been based on the described POLARIS model and the application of POLARIS, a code which has been developed originally for lattice calculations for light water reactors modelling infinite grids of unit cells and fuel assemblies by applying reflective boundary conditions. This effect has been eliminated by a very elaborate model using a large amount of absorber. The reliability of the results using this model and the POLARIS code is investigated in Table 2. The aim of this comparison is to assure that the results of POLARIS are robust regarding the used model, the method, and the cross-section basis. The method of characteristic model is evaluated against another transport code applying the S_n method on an unstructured mesh using the TRITON/NEWT sequence and the identical cross section set but another procedure for the self-shielding. The results show a good agreement too within one centimetre in core radius for all three tested cases with POLARIS being for all cases on the conservative side. The quality of the two deterministic results is evaluated by a comparison to the results gained with the Monte-Carlo code Keno 6 of the SCALE package using the multi-group self-shielded cross section set produced with the identical procedure as for the deterministic NEWT transport solver. The Keno 6 multi-group results show only a very small deviation (less than 1.5 cm in radius) to the NEWT results and to the POLARIS results – thus the results of both significantly different transport methods agree very well. Finally, the last approximation, the use of the multi group library relying on the 252-group master library traditionally weighted for light water reactor application is investigated. This task is accomplished by a comparison to the application of the Keno 6 code using a continuous energy approach based on the ENDF-B VII.1 library to evaluate the potential bias of the multi-group master library. The Keno 6 continuous energy results once more coincide very well with all other results, thus all results stay in less than ± 1 cm form the highest level as well as highest complexity results provided by the continuous energy Monte-Carlo calculation which confirms the quality of the significantly faster operating models using a higher level of approximation. The quality of all results is definitively sufficient for this kind of first step study for the analysis of the potential dimensions of a zero-power chloride based molten salt reactor experiment.

Table 2: Comparison and evaluation of different relevant results for the expected core radius of the 2D system using deterministic and stochastic simulation methods based on multi-group and continuous cross section sets

		42.5% NaCl	20% NaCl	20% NaCl
		35% enr	20% enr	35% enr
Scale/Polaris	core radius [cm]	**57.7**	**80.6**	**50.3**
Scale/Trition/NEWT	core radius [cm]	56.9	80.5	49.3
Scale/Keno 6 multi-group	core radius [cm]	56.3	79.63	49.1
Scale/Keno6 continuous	core radius [cm]	56.84	80.26	49.54

After the test on the reliability of the different codes, a first glance will be taken into the spatial effects on the spectrum caused through the third dimension leakage which can be evaluated through the TRITON/NEWT sequence and the spatial distribution of the neutrons of a set of defined neutron groups characteristic for the neutron spectrum of the system. The comparison of the different settings for the spectral analysis, Figure 12. The spectrum of the 2D system without leakage in axial direction is the softest with the highest amount of lower energy neutrons. As soon as an axial leakage is taken into account the spectrum starts to harden with decreasing axial dimensions. However, the strongest hardening of the spectrum appears to happen in the case when the radial reflector is eliminated, see grey line in Figure 12. In addition, to the spectral information, the energy groups for the 2D spatial analysis of few group neutron flux distribution are given in this figure with the energy groups I to V separated by the blue vertical lines to get a higher fidelity of the spatial neutron flux distribution which will allow to understand where each of the groups have their highs and lows in the spatial distribution.

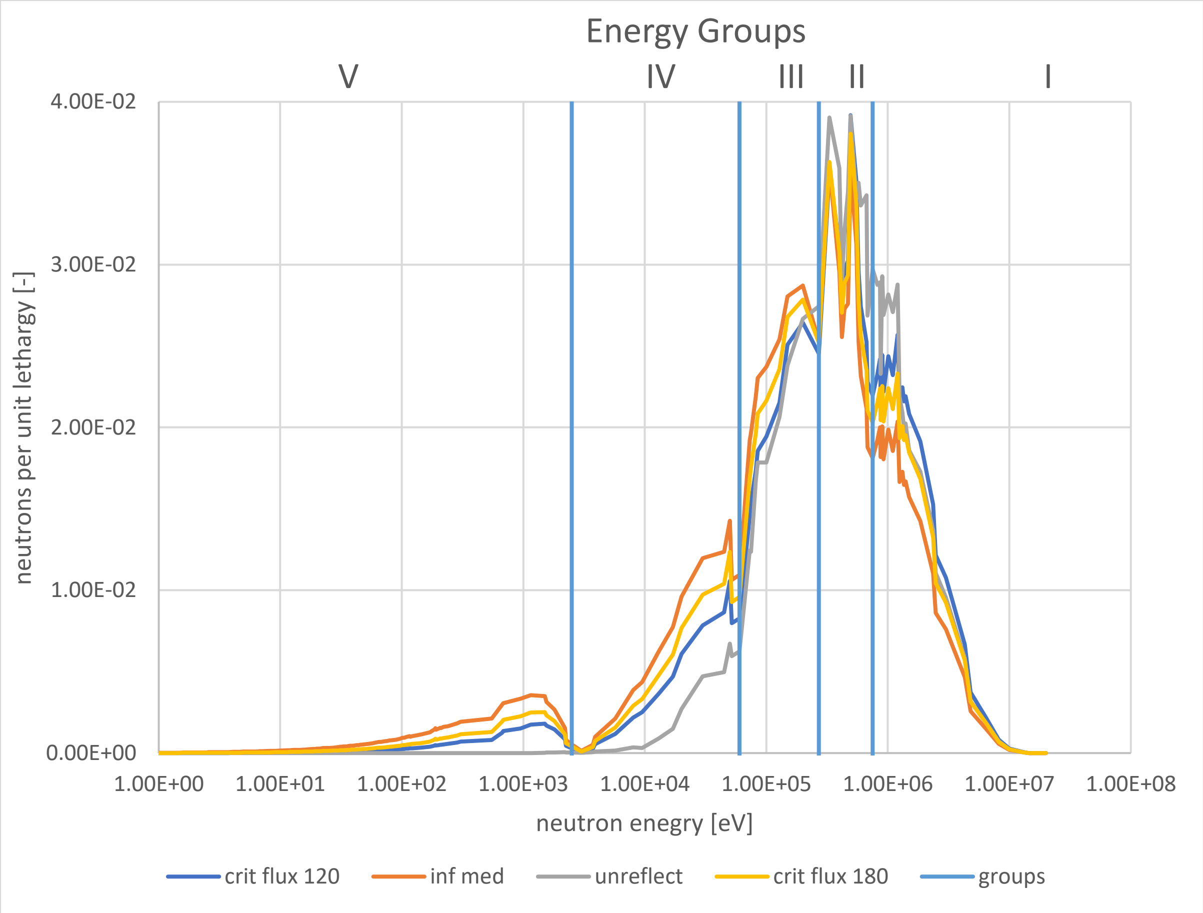

Figure 12: Neutron flux spectrum for the reflected and the unreflected core as well as for different axial leakage approximation (infinite medium, 120 cm core height, and 180 cm core height) using different core heights with added neutron group structure for the spatial flux distribution analysis

The group wise 2D spatial neutron flux distribution for the extra defined 5 group scheme given in Figure 12 is shown in Figure 13. In the three higher energy groups, the highest neutron flux (red) is concentrated in an inner core ring, see mark at 40 cm radius while the rest of the core up to 57 cm radius is covered by lower flux with intermediate intensity. All three groups have almost the same intensity of neutron flux, see scale at bottom, right. While the neutron flux in the reflector is already very low in group one (left, top), there is an increased flux visible in the reflector in group 2 (top, right), which is getting again stronger in group 3 (centre left). Thus, it becomes apparent that the flux distribution flattens out with lower energies. Group 4 has an overall much lower intensity and an almost flat profile from the centre until about half of the reflector followed by a rather sharp decrease in the outer half of the reflector. Group 5 has an overall very low intensity with a peak in the reflector and a small neutron flux increase at the outer boundary of the core which indicated that the lower energy neutrons slowed down in the reflector penetrate only to a small depth into the core due to the self-shielding caused by the high importance of the low energy neutrons. However, it is expected that the influence is very limited due to the low over all intensity. Nevertheless, this behaviour should be kept in mind when investigating different reflector materials since the use of more efficient reflector materials like polyethylene or graphite could enhance this effect strongly due to the high neutron thermalization power of these materials. A comparable effect has been discovered in the YALIA-booster experiments where a fast system was surrounded by a system thermalized by polyethylene.

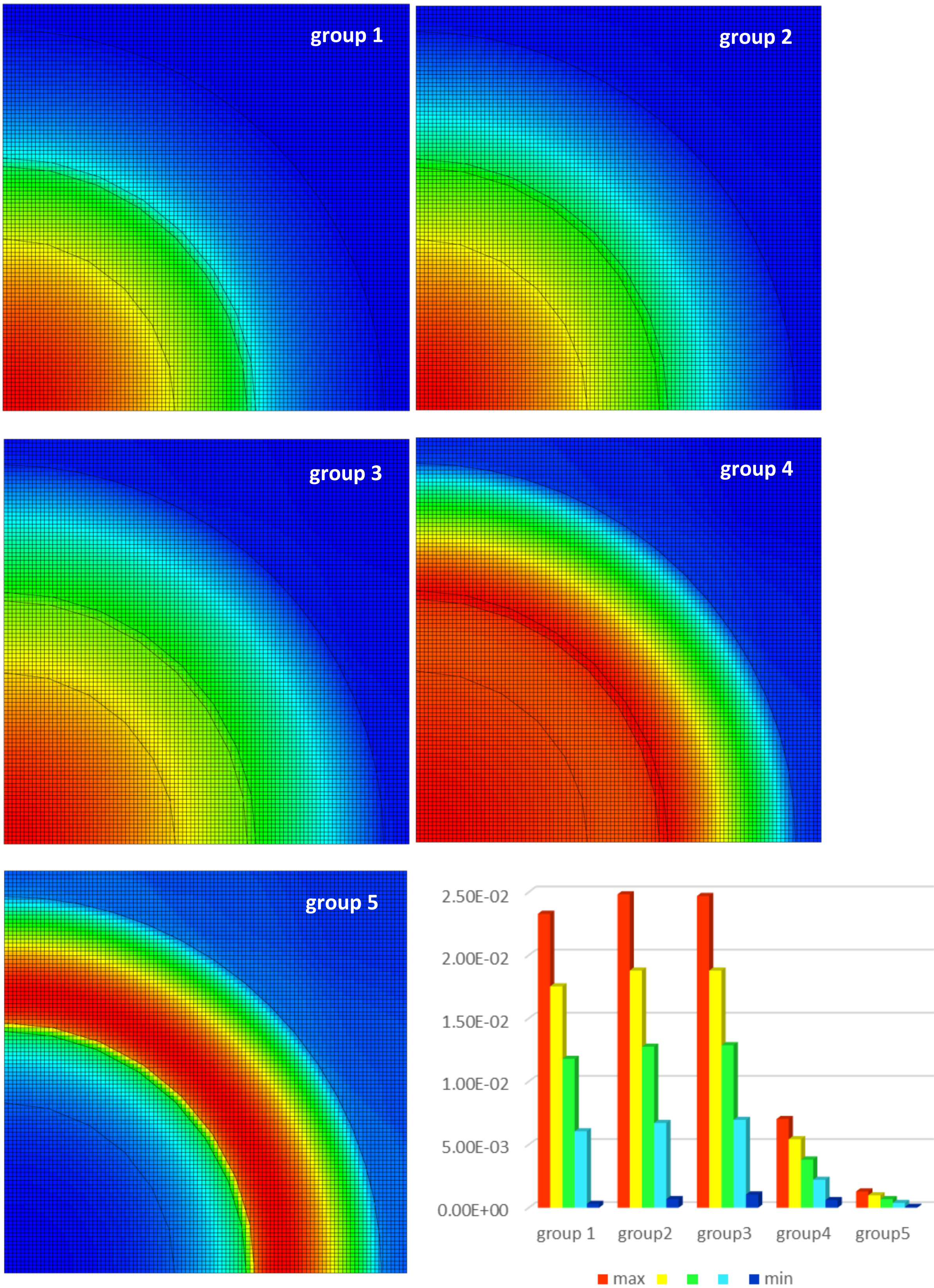

Figure 13: Spatial neutron flux distribution in the 5 defined energy groups and related neutron flux values in each group

Following the extensive 2D analysis, the potential configurations are narrowed down to 3 different compositions for the 3D analysis to create a first guess on the amount/volume of fuel which will be required to achieve a critical configuration. The three compositions are:

- A eutectic composition with 35% enriched Uranium
- A heavy metal rich composition with 35% enriched Uranium
- A heavy metal rich composition with 20% enriched Uranium

The choice for these compositions has been taken to get a deeper understanding of the advantage in reducing the core size and consequently to the cost of the system achievable through the use of the heavy metal rich composition instead of the eutectic composition on the one hand, while on the other hand the extra volume is analyzed, which would be required if the aim is to create a core based on low enriched uranium. The calculations performed are based on the 3D model given in Figure 5 using for the primary investigation, the multi-group Monte Carlo code Keno-VI and for a later cross check the continuous energy version of the same code.

Table 3 indicates the expected results with the lowest core volume of less than 1.8 m^3 for the heavy metal rich system and an U-235 enrichment of 35% which seems in the current state of the study the most promising combination. The change to the eutectic salt compositions would increase the required volume to achieve a critical system by almost 50%, while the switch to the more proliferation resistant fuel system with only 20% enrichment would increase the volume by almost a factor of 4 which would be a hardly acceptable size and volume of the core for a zero power experiment.

The cross comparision with the continuous energy solution indicate only a small difference below 3% regarding the system voume. This results confirm the quality and usability of the 252 goup set used not only for the 3D, but als for the 2D Monte-Carlo and the 2D deterministic S_n transport solutions. Table 3: Studied cases for the 3D Monte-Carlo analysis to determine the minimum volume required to achieve a critical configuration

	42.5% NaCl, 35% enr.			20% NaCl, 20% enr			20% NaCl, 35%enr		
	Radius [cm]	Height [cm]	Volume [m^3]	Radius [cm]	Height [cm]	Volume [m^3]	Radius [cm]	Height [cm]	Volume [m^3]
Multigroup	67.2	100	2.84	104.25	100	**6.83**	65.6	65	**1.76**
	64.2	120	3.11						
	74.25	75	**2.60**						
Continuous Energy	75.25	75	2.67	105.55	100	7.00	66.55	65	1.81

The detailed results given in Table 3 are depicted in Figure 14. From the visualization, it is clear that there is very good agreement of the results of both different Monte-Carlo calculations (multi-group versus continuous energy). In addition, the clear advantage of the heavy metal rich system and the massive advantage of use of 35% enriched Uranium is highlighted. Based on this outcome a first recommendation for further investigation is to concentrate on the heavy metal rich system with an enrichment of 35% which seems to be a reasonable value when compared to other recent reactor physics experiments like GUINEVERE [24] with 30% enrichment and YALINA-Booster with an enrichment of 36% in the leading lead fast zone [25].

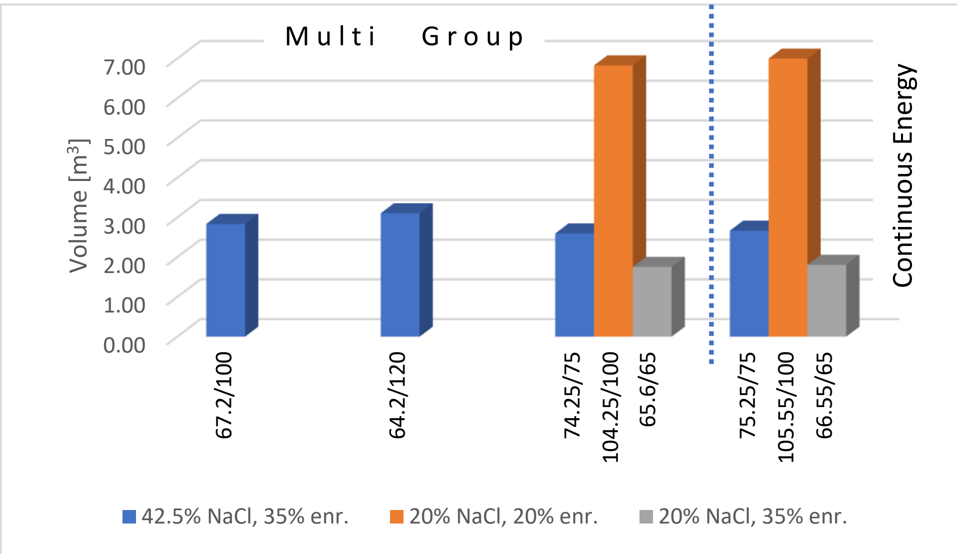

Figure 14: Expected core volumes for the different studied cases using multi-group and continuous energy Monte-Carlo simulations

Summary and Conclusions

The investigation topic is introduced by making the case for the importance of a zero power reactor for the process of developing a new, innovative rector concept like molten salt fast reactor. This is based on historic developments as well as the current demand for experimental results and relevant key factors for the success of the next step in the development process.

The focus of the modelling & simulation work in this publication is on answering the questions on salt compositions and required dimensions of a potential experimental setup to narrow down the choices for a zero power experiment for a molten salt fast reactor. A multitude of modelling and simulation results using different tools of the SCALE package is delivered studying two different salt systems, the eutectic and the heavy metal rich system. The studies on the 2D system radius show the volume reduction to be strongest in the step form 20% enrichment to 35% enrichment and the reflector effect to be continuously increasing with enrichment. This results in reductions of the system radius, while the heavy metal rich system requires in all cases a smaller volume. The study of the thermal feedback effects (salt density and fuel temperature) shows a strong increase of the feedback effect with increasing enrichment and decreasing system radius with some indication of saturation at very high uranium enrichment.

The study of the neutron spectrum indicates that for the systems have a slightly harder neutron spectrum than in a typical sodium cooled fast reactor with some limited spectral hardening in the heavy metal rich system, increased spectral hardening in the case of the absence of the reflector and significant spectral hardening in the cases with very high uranium enrichment. The analysis of the spatial neutron flux distribution of the reflected system using 5 specifically defined energy groups demonstrates that the major part of the lower energy flux is created in the reflector through collisions which will lead to a slight increase of the power production in the outermost core region while the majority of the fast neutron flux follows a distribution with a strong central neutron flux peak.

Based on the results and considerations on cost and proliferation three configurations have been chosen for the follow up 3D analysis – the eutectic composition with 35% uranium-235 enrichment and the heavy metal rich compositions with 20% and 35% enrichment. The expected core volumes for these configurations have been studied using multi-group and continuous energy Monte-Carlo simulations identifying the 35% enriched systems as the most attractive and finally leading to the choice of the heavy metal rich compositions 35% enrichment as the reference system for future studies of the next steps in the zero power reactor investigation. The inter-comparison of the different applied codes and approaches available in the SCALE package has delivered a very good agreement between the results creating trust into the developed and applied models and methods. However, this will not be sufficient to avoid the need for validation experiments to assure the best possible results for future modelling and simulation of molten salt reactor systems.

The current analysis is only applied for a very narrow window of operational temperature in molten salt, which is related to the limited data availability. Thus, a much more comprehensive study will be required as soon as the relevant thermo-physical properties are available down to room temperature.

References

1. Government and Industry Roles in the Research, Development, Demonstration, and Deployment of Commercial Nuclear Reactors: Historical Review and Analysis. EPRI 2017. 3002010478

2. B. Merk et al: A zero-power facility as multi-fold opportunity to support quick progress in innovative reactor development, atw 66 (3) 2021

3. "iMAGINE - A disruptive change to nuclear or how can we make more out of the existing spent nuclear fuel and what has to be done to make it possible in the UK?", atw 6/7 2019

4. V. Drüke, D. Filges (1987) The Critical HTGR Test Facility KAHTER–An Experimental Program for Verification of Theoretical Models, Codes, and Nuclear Data Bases, Nuclear Science and Engineering, 97:1, 30-36, DOI: 10.13182/NSE87-A23493

5. A. I. Kievitskaya et al., "Experimental and theoretical research on transmutation of long-lived fission products and minor actinides in a subcritical assembly driven by a neutron generator," in Proceedings of the 3rd International Conference on ADTTA, Praha, Czech Republic, 1999.

6. Kiyavitskaya, H., Bournos, V., Fokov, Y., Martsynkevich, B., Routkovskaia, C., Gohar, Y., Persson, C.-M., Gudowski, W., 2007. YALINA-Booster Benchmark Specifications for the IAEA Coordinated Research Projects on Analytical and Experimental Benchmark Analysis on Accelerator Driven Systems and Low Enriched Uranium Fuel Utilization in Accelerator Driven Sub-Critical Assembly Systems, IAEA.

7. GUINEVERE: Generator of Uninterrupted Intense Neutron at the lead VEnus REactor, available: https://science.sckcen.be/en/Projects/Project/GUINEVERE, accessed 25/11/2020

8. H. Aït Abderrahim and P. Baeten, "The GUINEVERE-project at VENUS, project status," in ECATS Meeting, Cadarache, France, January 2008.

9. B. Merk, D. Litskevich, K. R. Whittle, M. Bankhead, R. Taylor, D. Mathers: "On a Long Term Strategy for the Success of Nuclear Power", ENERGIES, 8(11), 12557-12572. doi:10.3390/en81112328.

10. https://www.terrestrialenergy.com/technology/sustainable-clean-energy/, accessed 25/11/2020
11. https://www.energy.gov/ne/articles/southern-company-and-terrapower-prep-testing-molten-salt-reactor, accessed 25/11/2020
12. http://www.elysiumindustries.com/technology, accessed 25/11/2020

13. https://www.sibghk.ru/news/9068-na-gkhk-proshlo-rabochee-soveshchanie-po-voprosu-sozdaniya-zhidkosolevogo-reaktora.html, accessed 25/11/2020

14. Desyatnik, V.N., & Katyshev, S.F. (1980). Volumetric and surface properties of the NaCl-UCl3-UCl4 melts. Zhurnal Fizicheskoj Khimii, 54(6), 1606-1610.

15. Merk, B.; Detkina, A.; Litskevich, D.; Atkinson, S.; Cartland-Glover, G. The Interplay between Breeding and Thermal Feedback in a Molten Chlorine Fast Reactor. Energies 2020, 13, 1609.

16. M. A. Jessee, J. J. Jarrell, W. A. Wieselquist, M. L. Williams, K. S. Kim, T. M. Evans, S. P. Hamilton, C. A. Gentry: POLARIS - 2D LIGHT WATER REACTOR LATTICE PHYSICS MODULE, in SCALE Code System edited by B.T. Rearden, M.A. Jessee, February 2017

17. B. Merk, A. Detkina, S. Atkinson, D. Litskevich, G. Cartland-Glover: Evaluation of the Breeding Performance of a NaCl-UCl-Based Reactor System, Energies 2019, 12(20), 3853; https://doi.org/10.3390/en12203853

18. J. LEPPÄNEN et. al. "The Serpent Monte Carlo code: Status, development and applications in 2013." Ann. Nucl. Energy, 82 (2015) 142-150.

19. B. T. Rearden, M. A. Jessee, Ed.: SCALE CODE SYSTEM, ORNL/TM-2005/39 Version 6.2.2, February 2017

20. B. Merk, A. Detkina, S. Atkinson, D. Litskevich, G. Cartland-Glover: Evaluating reactivity control options for a Chloride-Salt based molten salt zero power reactor, Applied Science special edition Nuclear Waste Management 2020

21. B. Merk, A. Detkina, S. Atkinson, D. Litskevich, G. Cartland-Glover: Innovative investigation of reflector options for the control of a Chloride-Salt based molten salt zero power reactor, Applied Science special edition Nuclear Waste Management 2020

22. Merk, Bruno & Rohde, Ulrich & Glivici-Cotruţă, Varvara, Litskevich, Dzianis & Scholl, Susanne. (2014). On the Use of a Molten Salt Fast Reactor to Apply an Idealized Transmutation Scenario for the Nuclear Phase Out. PloS one. 9. e92776. 10.1371/journal.pone.0092776.

23. B.Merk, V.Glivici-Cotruţă, F.P.Weiß (2012) On the use of different analytical solutions for recalculation of the YALINA-Booster experiment SC3A, Progress in Nuclear Energy, Volume 58, July 2012, Pages 11-20

24. W.Uyttenhove, P.Baeten, G.Van den Eynde, A.Kochetkov, D.Lathouwers, M.Carta (2011) The neutronic design of a critical lead reflected zero-power reference core for on-line subcriticality measurements in Accelerator Driven Systems, Annals of Nuclear Energy Volume 38, Issue 7, July 2011, Pages 1519-1526

25. B.Merk, V.Glivici-Cotruţă, F.P.Weiß (2012) On the use of different analytical solutions for recalculation of the YALINA-Booster experiment SC3A, Progress in Nuclear Energy, Volume 58, July 2012, Pages 11-20