A Physics Study on Moderated SiC Block for High-Temperature Gas-Cooled Reactor

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1. Introduction

In recent years, there has been a growing interest in High-Temperature Gas-cooled Reactors (HTGR) due to their remarkable advantages. These include the intrinsic safety and proliferation-resistance potentials of TRISO-based fuels, along with the outstanding fuel utilization capability offered by HTGRs. Nonetheless, to achieve such high fuel utilization, the moderator and structural materials must withstand huge fluence values. Commonly, isotropic graphite is used, however it shows limitations in this regard [1].

In this work, a novel approach for compact-based HTGRs by introducing a Silicon Carbide (SiC) block as a substitute of graphite (C) is proposed. The use of SiC allows greater safety qualities due to the improved mechanical properties, thermal resistance and enhanced fission products confinement in case of TRISOs rupture [2].

TRistructural ISOtropic (TRISO) fuels are well known for their stability and intrinsic safety. They are composed of different layers, surrounding the fuel at the center (referred hereafter as the "kernel"); there are several options of fuel suitable as kernel materials, from the traditional oxides (UO_2) to more innovative ones like carbides (UCO, UC_2) or nitrides (UN). In addition**,** coating layers have been added, comprised of porous and pyrolytic graphite, followed by a SiC layer to improve the mechanical strength, and finally one additional sealing layer of pyrolytic graphite [3].

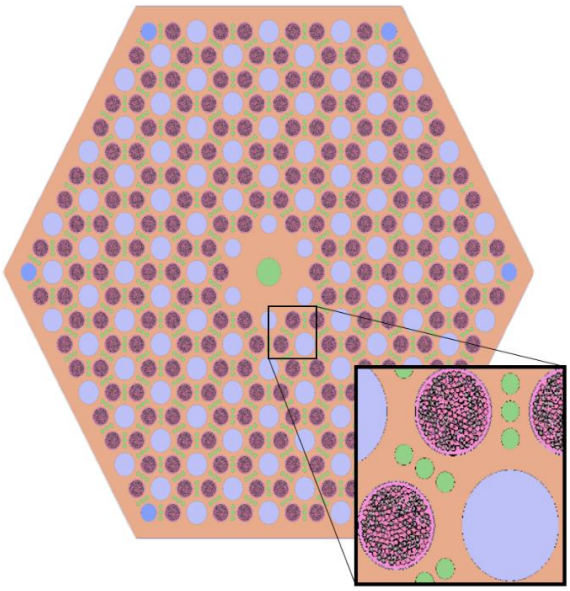

Fig. 1 Whole fuel assembly structure with 3 moderating channels

Regarding the Bistructural ISOtropic (BISO) technology, these particles are an earler version of TRISO particles. Mainly, they consist of a single kernel with two additional layers – distinct from TRISOs. In this study, they are employed as moderator particles, randomly dispersed in the fuel. Further elaboration on this approach will be provided in the "Model Description" Section.

2. Methodology

2.1. *Model description*

The proposed layout is inspired from previous work of *Kim, Yonghee et al*. [4] and it is concisely summed up for ease of reference; Fig. 1 provides a proper visualization of the geometry, while Table I presents a comprehensive overview of the model. The structure is hexagonal – hence the triangular pitch is chosen – within a SiC block. The penalty in moderation caused by the introduction of silicon must be solved through the inclusion of some additional moderator; furthermore, it is evident the energetic spectrum cannot be as soft as conventional HTGRs, otherwise the absorption contribution will strongly affect the multiplication factor k.

Since a more effective moderator must be introduced, the selection process has identified yttrium hydride ($YH_{1.85}$) as a prime candidate, due to the well-known moderation properties of hydrogen (H). This choice was taken based on the available data, the stability of the molecule, and the moderating ratio [5]. The assembly consists of 210 fuel channels along with 102 cooling channels. These channels are divided into two distinct types – large ones, predominant in the assembly, and small channels, solely located in the center. At the edges

Table I Geometry details of the fuel assembly in Fig. 1

Material	Dimension [cm]	Color
Coolant (He)	(Large) R=0.7940 (Small) R=0.6350	
FCM Compact	R=0.6225, gap=0.0125	
Moderating channels	(Small) R=0.150 (Large) R=1.786	
BA slot (Graphite-filled)	R=0.6225, gap=0.0125	
Structure block material (SiC)	(apothem) d=18.0	

there is a dedicated channel for burnable absorbers, to control the possible reactivity swing, and it has been filled with graphite. No hexcan is present around the assembly, and a central handling hole is modelled. As per [6], the handling hole is supposed to be filled except for the extremities; in the current design it was filled with SiC and some moderator, while in the extremity holes no material is present – these parts of the reactor however have not been modelled, as well as the dowels. For more in-depth insights into the layout, the reference [4] could be consulted.

The proposed innovative layout introduces two new features, which are the incorporation of the moderator through the use of BISO and the insertion of moderation channels strategically positioned only between two fuel channels.

Although the utilization of BISO particles decreases the overall maximum amount of loaded fuel, it allows a very efficient use of the moderating material. Due to the small dimensions, the thermalized neutrons are more likely to escape the interaction with ^{89}Y, as the mean free path is at least ten times larger than the diameter of the BISOs. Moreover, the uniform distribution within the fuel pellet leads to a flatter thermalization profile, thereby decreasing the possibility of ^{89}Y absorption because of the average high energy of the neutrons. In the study the additional manufacturing procedures wanted to be minimized, thus the external diameter of the BISO particles is equal to that of the TRISOs. The BISO particles considered in this study consist of an inner $YH_{1.85}$ kernel, an intermediate layer of porous graphite designed to accommodate possible dissociated hydrogen – and to promote the recombination among individual hydrogen atoms – and an external layer of SiC (matching the materials of the TRISO particles as described in Table II.

As mentioned before, the yttrium hydride is also inserted inside the block through moderating channels designed as solid cylinders. The insertion of this advanced moderator leads to a degradation of the whole system thermal properties; this behavior is caused by the intrinsic properties of the hydrides, which possess lower conductivity compared to SiC. Therefore, by placing these moderator channels between the coolant and fuel channel would hamper the heat transfer. Consequently, these channels are not uniformly distributed; instead, they are placed exclusively between pairs of distinct fuel

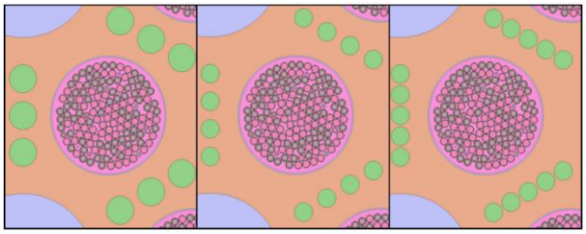

Fig. 2 Different layouts proposed. The maximum dimensions are shown.

Table II Particles data

Particle	TRISO	BISO
Kernel material (enrichment)	UCO (19.75%)	$YH_{1.85}$ (nat.)
Kernel radius [μm]	215	355
Buffer thickness [μm]	100	40
iPy thickness [μm]	40	/
SiC thickness [μm]	35	35
oPy thickness [μm]	40	/

channels, and not between fuel and coolant channels. The current work presents the outcomes for three different configurations – 3, 4 and 5 moderating channels between two fuel element positions, as shown in Fig. 2 – and it explores the impact of varying radii.

Since the material to enclose the $YH_{1.85}$ is the same of the assembly, no additional volume is needed for its implementation. The rationale behind proposing three different layouts is linked to the required amount of $YH_{1.85}$: the larger the number of moderating channels, the lower the mass of $YH_{1.85}$ in the core, facilitating a more uniform moderation. Furthermore, increasing the total number of moderating channels necessitates a reduction in the maximum radius, allowing a reduction of the heterogeneity effects.

In this study, the considered temperature is 900°C, and all the properties have been modified accordingly. The densities are adjusted adhere to the general law based on the linear temperature expansion coefficients (LTE) [7], while the neutronics properties are interpolated [10] from the mother library ENDF/B VII.1. For each compact, the average power density is uniformly set to 30 [W/cc], a prevalent value for compact based HTGRs.

2.2. *Moderator*

The selection of the moderating material is driven by the moderation efficiency; the motivation lies in the deterioration of mechanical properties with the replacement of SiC, limiting the available volume. Hydrogen (H) is well-known as the best moderator, thus the hydrides are the most desirable material to use H in a solid phase. However, this choice raises concerns about the overall molecule stability, due to two primary factors: firstly, in terms of the reactor operation conditions, it is crucial to avoid the H gas formation, considering the additional stresses exerted on the fuel assembly (and consequently the whole reactor core) due to gaseous H accumulation. The second concern pertains to the manufacturing process, particularly focusing on H dissociation issues and effective H concentration.

Among the potential candidates, $YH_{1.85}$ stands out due to its remarkable high-temperature stability, making this option the first-choice despite of the relatively large ^{89}Y absorption cross section. These properties have driven a growing interest in $YH_{1.85}$, leading to the availability of more data in recent times.

As mentioned, $YH_{1.85}$ has a high dissociation temperature, that means the amount of H dissociated during normal operations is minimum [8]. Due to the potential threat H poses to nuclear reactors, it is imperative to employ suitable materials that effectively impede the H releases both in nominal and accidental scenarios. As mentioned in [9], ceramics based on Nitrogen (N) or Carbon (C) based are well-regarded choices for hydrogen containment, with SiC being a prominent option among them. No documented instances of particularly detrimental reaction exist between Y and Si, thus the $YH_{1.85}$ molecule is perceived as the most promising candidate for fulfilling this role.

2.3. *Simulation details*

The characterization and optimization study were conducted utilizing the depletion feature of the Monte Carlo code Serpent, version 2.20 [10]. The overall problem was modelled with 1/6-th symmetry, imposing reflective boundary conditions – hence the model is based on the infinite lattice – and the number of histories and active cycles was adapted to achieve a reasonably low uncertainty – on average, the k_∞ values exhibit a standard deviation of approximately ±50 [pcm].

A range of different radii is investigated, spanning from a minimum of R_{min}=0.5 [mm] to a maximum of R_{max}=1.5 [mm] – however for the 4- and 5- moderating channels layout, the maximum radius is fixed at R_{max}=1.0 [mm] – and the upper bound in all the cases is imposed by steric constraints.

Given the non-linear relationship with the volume fraction of the TRISO (and BISO) within the compact, an optimum search is conducted. This search involves varying the relative fraction of fuel particles while maintaining a constant overall volume fraction of VF=60%.

The primary criteria employed to judge the configuration are mainly the k_∞ value magnitude and the energetic spectrum. In case of a more refined distinction, the priority lies in minimizing the quantity of $YH_{1.85}$. Upcoming studies will delve deeper into the burnup behaviour.

3. Results

The results of the optimization are shown below, and for the optimal cases, the energetic spectra are also available. Upon examining various charts, it is apparent that optima are present for both VF_{fuel} and R variables. The most important ones are the optima in function of R, when the VF_{fuel} is fixed, because these optimal points indicate the optimal moderation amount, due to the aforementioned competitive reactions of ^{235}U fission and ^{89}Y absorption. Since an optimum with respect to the VF_{fuel} highlights the optimal balance between amount of fuel and moderator quantities, it is important to recognize that this alignment is not necessarily coincident with the optimal amount of moderation requirements, as it can be neatly seen in Section 3.3.

3.1. *Optima in function of the moderating channels radius*

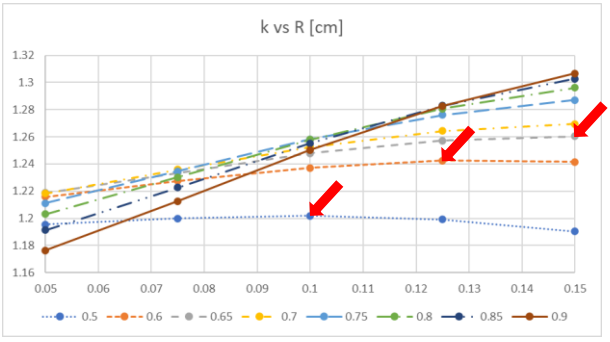

Fig. 3a) k_∞ in function of radius of the three moderating channels. The optima selected are highlighted by the arrows.

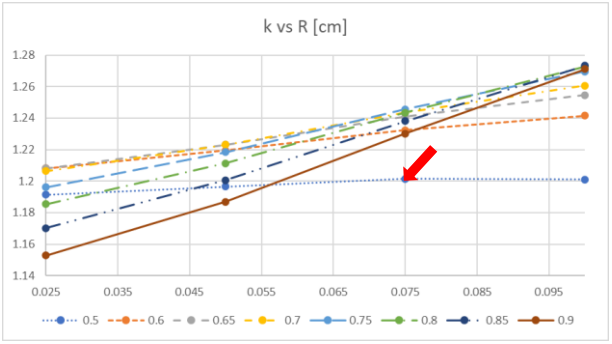

Fig. 3b) k_∞ in function of radius of the four moderating channels. The optima selected are highlighted by the arrows.

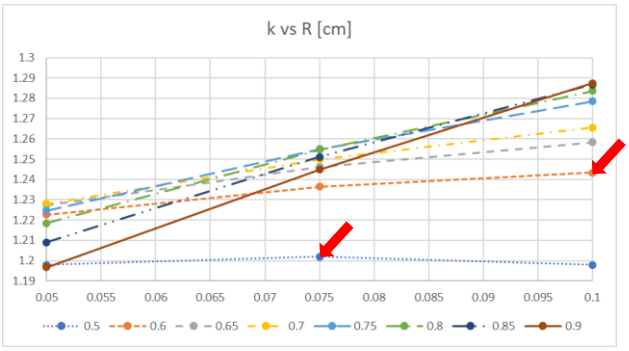

Fig. 3c). k_∞ in function of radius of the five moderating channels. The optima selected are highlighted by the arrows.

As shown in Fig. 3a), it is apparent that the optimal points for the three moderating channels are correspondent to with the three lowest fractions – actually, VF=65% is not granted to be the optimum, but the slope of the connection of the two points is close

enough to 0. Analyzing in the same fashion the other two configurations, it can be inferred that only one point is an optimum – strictly speaking, however for the case with five moderating channels also the rightmost point could be considered as optimal candidate. The summarized outcomes for all the three cases are summarized in Table III.

3.2. *Optima in function of the TRISO volume fraction*

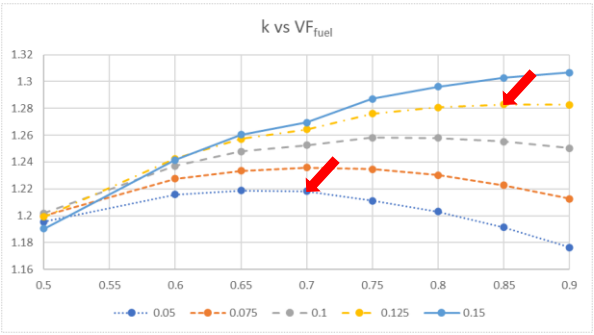

Fig. 4a) k_∞ in function of the VF_{fuel} for different radii for the 3-channel layout. The optima are highlighted by the arrows.

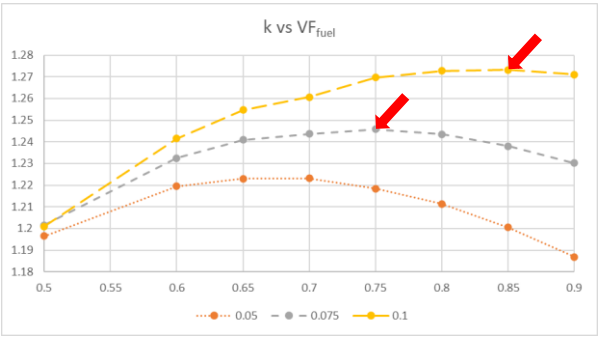

Fig. 4b) k_∞ in function of the VF_{fuel} for different radii for the 4-channel layout. The optima are highlighted by the arrows.

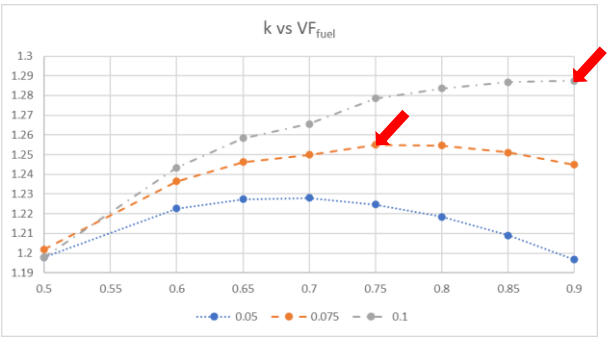

Fig. 4c) k_∞ in function of the VF_{fuel} for different radii for the 5-channel layout. The optima are highlighted by the arrows.

In regards of the packing fraction, the optima are many, and easier to observe. Yet, the current focus is centered on attaining an optimum balance between fission and absorption. The results are summed up in Table III for all the previous cases. The selected points chosen are the mathematical optima – where the derivative is close

Table III Selected optimal points for spectrum analysis. All the radii are in cm.

Characteristics	k_∞	Optimized variable
3 channels		
R = 0.100, VF = 50%	1.20190	R
R = 0.125, VF = 60%	1.24262	R
R = 0.150, VF = 65%	1.26050	R
R = 0.050, VF = 70%	1.22806	VF_{fuel}
R = 0.125, VF = 85%	1.28287	VF_{fuel}
4 channels		
R=0.075, VF=50%	1.20152	R
R=0.075, VF = 75%	1.24573	VF_{fuel}
R=0.100, VF =85%	1.27323	VF_{fuel}
5 channels		
R = 0.075, VF = 50%	1.20188	R
R = 0.100, VF = 60%	1.24329	R
R = 0.050, VF = 70%	1.22806	VF_{fuel}
R = 0.100, VF = 90%	1.28748	VF_{fuel}

enough to zero – in the case of the fixed VF_{fuel} (Fig. 3 a, b, c) while for the fixed R_{mod} (Fig. 4 a, b, c) a different logic has been followed: for the three-moderating channel layout the two extreme values have been analyzed, while for the four- and five- moderating channels layouts only the configurations with the highest VF_{fuel} have been considered.

3.3. *Energy spectra*

The energy spectra of the flux are illustrated utilizing the 238 groups-based SCALE format [11]. Thus, it can be easily compared among the different layouts.

As introduced earlier in the beginning of the section, the difference between the 2 kinds of optima is evident. Based on the k_∞ values, the best choices seem to lean towards VF_{fuel} optima, however, a notable observation emerges when assessing the energy spectra where the spectra are not thermal enough. This highlights the preferences for radius optima, and the best candidate is the 3 moderating channels layout, with large radius.

Additionally, the candidate with the largest k_∞ value and optimized for the radius (which is the third case in Table III) has the largest VF_{fuel}. This implies that the $YH_{1.85}$ content is minimized, aligning the total fuel fraction to the conventional graphite-based HTGRs ($VF_{fuel,YH1.85} = 0.6*0.65 = 0.39$ vs $VF_{fuel,C} \approx 0.4$).

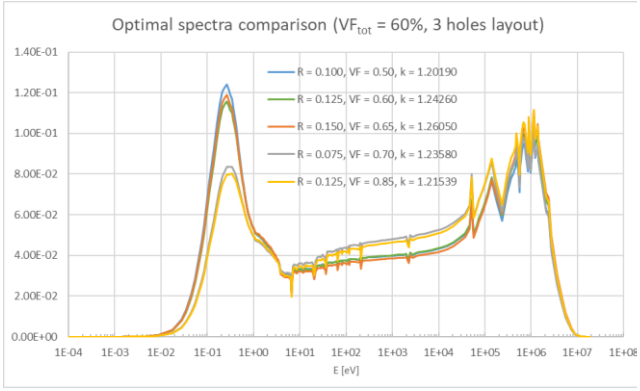

Fig. 5a) Energetic spectra for the 3 moderating channels candidates

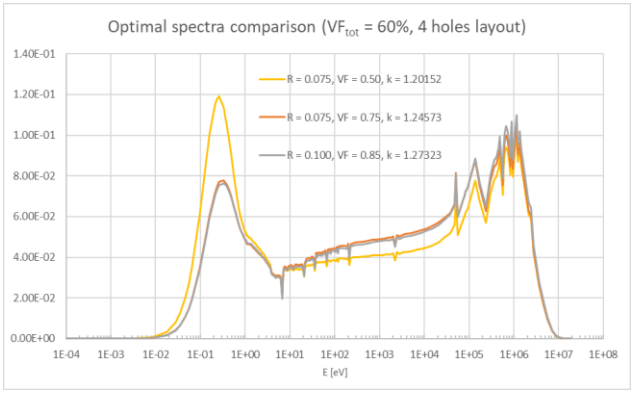

Fig. 5b) Energetic spectra for the 4 moderating channels candidates

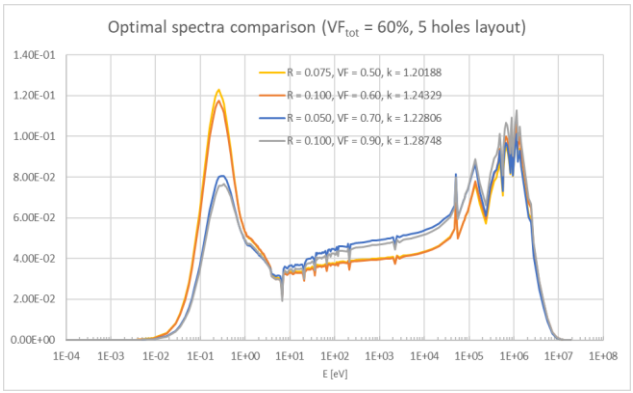

Fig. 5c) Energetic spectra for the 5 moderating channels candidates

3.4. *Discharge burnup estimation*

Employing the linear reactivity model, through the burnup calculation, different batches configurations were evaluated to estimate the discharge burnup. The initial reactivity being considered was the reactivity after the xenon equilibrium – roughly after the first seven days of full power operation – and a penalty of 4000 pcm due to parasitic capture and leakage has been assumed, leading to an initial reactivity around ρ_0=0.16195. The outcomes, presented in Table IV, are an undeniable showcase of the strengths of HTGRs, as highlighted in the introduction: extensive fuel utilization.

The results are compared to the conventional graphite moderated HTGR modelled as [3]; the only differences lie in the fuel type: UO_2 fuel kernels 19.75% enriched were used, and a coherent fuel loading as well, incrementing the volume fraction mentioned in the reference up to VF=0.39.

Despite the drawback in the overall cycle length, the substitution of C with SiC and $YH_{1.85}$ still gives nearly one and a half years of operation for the two-batch scheme, without the embrittlement problem caused by the graphite exposure to large neutronic fluxes [1]. A similar assessment can be done for the three-batch fuel management, where the discharge burnup is prioritized; overall, it can be appreciated a 23% of degradation in performances, despite the benefit of using SiC.

Comparing the discharge burnup, the proposed layout performs as expected, exhibiting values comparable to the conventional C-based fuel assemblies. Particularly, the two- and three- batch schemes are considered suitable tradeoffs, and the choice between these two is dependent on economic aspects.

Table IV Comparison of the performances of the case study and the reference through the linear reactivity model

Assembly type	# of batches	Discharge Bu [MWd/kg$_U$]	Cycle Length [days]
3 holes, R=0.125 [cm]	1	63.68	810
	2	84.91	540
	3	95.53	405
	4	101.89	324
Reference	1	82.51	945
	2	110.01	630
	3	123.76	472.5
	4	132.01	378

4. Conclusion

An innovative assembly for compact-based HTGRs has been introduced. A comprehensive characterization of the entire assembly has been done, followed by the lattice optimization. The optimization process has revealed the presence of optimal points in all the proposed layouts, and the optimal configuration for the required criteria has been found. In addition, by using the linear reactivity model, the optimal case shows a great potential for multi-batch fuel management. Through the implementation of this novel fuel assembly, it is feasible to load the same fuel content of graphite-based compacts while entirely eliminating the graphite, granting the potential to extend the cycle length.

For forthcoming research, a broader perspective could consider overall fuel utilization as the main criterion for optimization, looking at the maximum burnup, or at the fuel cycle length, investigating the Effective Full Power Days (EFPD). In addition, a comprehensive analysis for

the whole-core calculation will be performed. Furthermore, supplementary work can be done assessing the mechanical stresses the assembly can undergo before failure. Moreover, the hypothesis regarding the nominal average temperature of the assembly, set at 900°C, needs to be validated.

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