

Neutronic analysis of accident tolerant fuel concepts in spectral shift regulation conditions

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Abstract. The study of Accident Tolerant Fuels (ATFs) has gained significant attention due to their potential to enhance the safety and reliability of nuclear reactors, especially under severe accident conditions. This work investigates the neutron-physical performance of ATF concepts in Light Water Reactor (LWR) using spectral shift regulation (SSR). The SSR mechanism, which adjusts the moderator-to-fuel ratio, by means of mechanical displacers that run in the guide tubes, enables spectral hardening during the initial cycle and softening toward the end, optimizing fuel utilization and reactor safety. Using collision probability method with the GETERA simulation tool and BNAB library, this study evaluates various ATF designs, including chromium-coated zirconium (CrZry), FeCrAl alloys, and SiC composites, combined with uranium silicide (U_3Si_2) and uranium nitride (UN) high density fuels. Key metrics such as infinite multiplication factor, nuclide inventory, and plutonium buildup are analyzed. Results demonstrate that SiC cladding paired with UO_2 or U_3Si_2 fuels offers the best neutronic characteristics, requiring slightly lower uranium enrichment. Thin FeCrAl cladding, on the other hand, shows higher enrichment needs but still around enrichment level of the fuel in Light Water Reactors, when paired with combination with U_3Si_2 . The integration of SSR in the LWR reactor improves burn-up efficiency while burning produced plutonium and lower natural uranium consumption, resulting in reduced waste. Among the ATF options studied, SiC cladding shows good promise for guide tube and displacer applications, due to their neutron transparency and thermal stability.

1 Introduction

In search of improved safety and performance in nuclear power generation, the development of accident tolerant fuel (ATF) systems, particularly for light water reactors (LWRs), has accelerated in the last decade. The total station blackout (SBO) leading to beyond-design-basis accident (BDBA) at Fukushima-Daiichi in 2011 reignited concerns over the integrity of conventional zirconium-based fuel cladding under high-temperature steam conditions. In response, research efforts have prioritized advanced fuel and cladding materials capable of improving core resilience during normal operations, power ramps and accident scenarios such as SBO, loss of coolant accidents (LOCA), reactivity insertion accidents (RIA), etc. [1]. Improved accident performance is generally interpreted as increased coping time for operators to respond, for example, fuels and claddings that resist oxidation and overheating longer, delaying core

damage in the event of BDBA as described as black swan events by reference [2]. Over the 2011–2025 period, numerous experimental and computational studies have evaluated candidate ATF materials, from enhanced Zr alloys and coatings to novel ceramics and composites, to quantify their neutronic behavior and safety benefits [3–7]. The concept of ATFs combines high-performance ceramic or metallic claddings, such as FeCrAl, SiC, and chromium-coated zirconium with advanced fuels such as doped UO_2 , uranium carbide (UC), high-density fuels like uranium silicide (U_3Si_2) and uranium nitride (UN) [8,9].

In parallel, reactor operation strategies aimed at improving fuel utilization and reducing nuclear waste have reintroduced interest in spectral shift regulation (SSR). SSR enables a controlled hardening of the neutron spectrum over the fuel cycle by varying the moderator-to-fuel ratio, either through mechanical means such as displacers, or chemical methods involving D_2O/H_2O moderator adjustments [10,11]. Spectral hardening increases the resonance absorption in fertile isotopes like U-238, producing

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plutonium breeding and increasing the conversion ratio. Recent studies [12–14] have also demonstrated that SSR can optimize fuel cycle length, increase plutonium production, and reduce reliance on soluble boron or burnable absorbers. Similarly, use of ATFs in small modular reactors (SMR), which have close neutronic environment as that of SSR reactors, is evaluated and shows further optimization of above-mentioned parameters [15,16].

Merging these two advancements, ATF materials and spectral shift core design, presents an opportunity to improve reactor safety and economics simultaneously. The literature suggests that ATF materials offer improved safety margins but often come with neutronic trade-offs (e.g. FeCrAl's absorption penalty) [17]. Meanwhile, spectral shift reactors like VVER-S [18] promise better fuel economy by design. However, there is limited published work on how ATF fuels would perform in such spectral shift LWR cores. This paper addresses that gap by analyzing various ATF fuel and cladding combinations in the SSR environment, building on prior knowledge of both domains. The objective of this work is to evaluate key neutronic parameters (multiplication factor, isotopic inventories, plutonium production, etc.) for advanced ATFs in a representative region of the VVER-S reactor core [18]. We focus on polycell calculations, which model a group of unit cells (fuel rods with surrounding coolant and structures) to represent the heterogeneity of a full fuel assembly. By comparing the traditional UO_2 /Zircaloy fuel system with various ATF candidates under identical spectral shift operating conditions, we can identify the most promising configurations and any design adjustments needed to accommodate them. In the following, we present selected ATF combinations and spectral shift reactor polycell structure, then describe the methodology and tools used, before presenting detailed results of the comparative analysis.

2 Materials and methodology

2.1 Selected ATF candidates

By reviewing the literature, including references [7–9], three advanced cladding materials, silicon carbide (SiC), chromium-coated zirconium alloy (CrZry), and FeCrAl alloy (APMT) with the composition Fe–21Cr–5Al–3Mo (wt.%), and two high density fuels, U_3Si_2 and UN, are selected for neutronic evaluations. Chromium-coated Zircaloy is a near-term ATF cladding option where a thin ($\sim 5\text{--}20\ \mu\text{m}$) chrome layer on the conventional Zr alloy significantly improves high-temperature oxidation resistance. Experiments have shown order-of-magnitude reductions in oxidation rate and hydrogen production for Cr-coated cladding compared to uncoated Zircaloy [9]. FeCrAl alloys (high-Cr, Al-bearing steels) are another promising cladding, its excellent corrosion resistance in steam and maintained strength at elevated temperatures has already been proven. FeCrAl cladding forms a protective Al_2O_3 layer that dramatically slows oxidation (at the cost of a higher neutron absorption cross-

section due to iron and chromium content). For instance, reference [19] demonstrated very good oxidation resistance of FeCrAl under steam conditions up to 1400°C . SiC fiber-reinforced composites represent a long-term cladding solution with very high temperature capability (melting point $> 2700^\circ\text{C}$) and low neutron absorption. SiC is essentially immune to rapid steam oxidation, and it is seen as a long-term ATF candidate, since its brittleness, irradiation-assisted swelling and thermal conductivity behavior are active research topics [20].

The standard UO_2 fuel is suggested to be replaced or mixed with higher uranium density compounds to extend fuel burnup or enable smaller fuel volume [8,9]. Leading candidates are uranium silicide (U_3Si_2) and uranium mononitride (UN). U_3Si_2 has a uranium density of 11.3 gU/cm^3 (about $1.2\times$ that of UO_2) and thermal conductivity of $5\times$ higher than UO_2 , which can reduce fuel operating temperature. It has been under active investigation, including in-reactor tests, for example, Westinghouse's EnCore fuel program is loading test rods with U_3Si_2 pellets encased in coated cladding [21]. One challenge for U_3Si_2 that has been stated is its reaction with water at high temperatures. Studies indicate it oxidizes in steam above 300°C unless additives or protective measures are used [22]. UN fuel has even higher uranium density (13.5 gU/cm^3) and excellent thermal properties, but it reacts readily with water/steam and thus it is believed that it must be paired with isolation barriers. Reference [23] reported that UN pellets exposed to 500°C steam at 0.5 bar completely converted to UO_2 and ammonia within an hour, highlighting the need for flawless cladding to use UN in LWRs. Additionally, the use of enriched nitrogen (^{15}N) suggested to be a requirement to avoid excessive absorption by ^{14}N . Despite these challenges, UN's high fissile density could allow very long cycles or compact cores if the neutronic design is optimized.

2.2 Computational tool

Neutronic calculations are carried out using the GETERA code (version 93), a deterministic reactor physics code based on the first collision probability method for cell and polycell calculations. GETERA is well-suited for lattice physics analysis of thermal reactors and can model burnup with spectral history effects using BNAB nuclear data library, which stores 135 nuclide data in 299 energy groups [24–26]. It treats a unit cell (fuel rod with surrounding coolant and structural material) in a cylindrical or hexagonal geometry and can also solve multiple interacting cells (a polycell) to approximate full assembly behavior. Key features of GETERA include solving the neutron transport equation in 22 energy groups using collision probabilities, computing the neutron spectra, and iteratively burning the fuel over time. In this study, we utilize GETERA's polycell capability and cylindric geometry to model an entire VVER-S fuel assembly containing both fuel rods and displacer channels (Fig. 1). Input parameter optimization and graphical analysis is done using Python programming language.

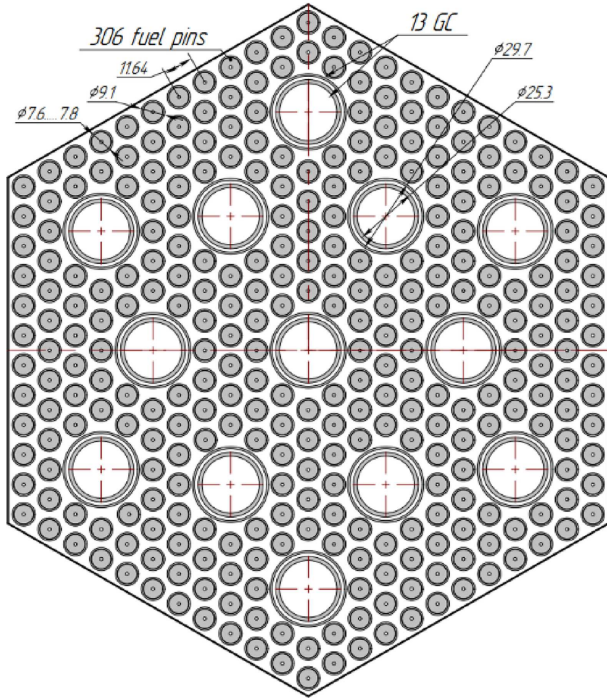


Fig. 1. Reference fuel assembly model. (Authors own solid drawing motivated by and based on Ref. [18]).

2.3 Reactor model

Reference [18] proposed the VVER-S (Super-VVER) design, an evolution of the 1500 MWe VVER with spectral shift rods, and reported key characteristics at the PHYSOR 2014 conference. In VVER-S, arrays of zirconium hydride or hollow Zr displacer rods are inserted in specially designed fuel assemblies; these displacers can be gradually withdrawn during operation to vary the water volume fraction. This approach eliminates the need for boron in the coolant and increases the conversion of U-238 to Pu-239, allowing the core to sustain power for longer on the same initial fissile loading. The reference design modeled is an equilibrium cycle of the VVER-S core, based on published VVER-S parameters [18]. Each fuel assembly (FA) has a hexagonal lattice, containing 306 fuel rods and 13 displacer rods (guide tubes for movable displacers) in a symmetric arrangement. The fuel pellet geometry has pellet outer diameter 7.6 mm with a 1.2 mm central hole (typical for VVER), and the pin pitch fixed by the assembly design (Fig. 1). The cladding thicknesses are the same 650 μm for all the claddings (SiC, Zry, CrZry) except FeCrAl which is evaluated at two thicknesses, 330 μm (AS-thin) and 650 μm (AS-thick). The displacers are hollow zirconium alloy tubes that can be filled with water or removed to change moderation. At beginning of cycle (BOC), all displacers are inserted (filled with Zr and helium gas inside, displacing water) to create an under moderated lattice. Throughout burnup, the displacers are sequentially withdrawn to introduce more water and thermalize the spectrum, maintaining reactivity. The range of moderator-to-fuel ($\text{H}_2\text{O}/\text{U}$) ratio thus varies from an initial low value with displacers-in to a higher

value with displacers-out. Based on the FA geometry, the Water-Uranium Ratios (WUR) in our model is 1.5 with displacers in (BOC) and 2.0 with displacers out (end of cycle, EOC) for the standard UO_2 fuel, consistent with design targets [18].

2.4 Simulation procedure

For each fuel/cladding combination, a burnup simulation is run in GETERA for multiple cycles. The reactor operates with spectral shift, we model this by adjusting the moderator content stepwise as burnup proceeds' (i.e., accounting for displacer withdrawal). Key neutron physics outputs, including the infinite multiplication factor k_∞ as a function of burnup/time, and isotopic concentrations (U-235, U-238, Pu-239, Pu-240, Pu-241, Xe-135, Sm-149, etc.), are recorded. First, a single-cycle (fresh fuel) run is done to observe initial reactivity and isotope generation. Then, a multi-cycle equilibrium simulation is performed for the baseline case to determine the natural uranium utilization and to calibrate the spectral shift reactivity gains.

In our previous works [27], we demonstrated the impact of spectral shift regulation on a traditional fuel system, uranium dioxide encased in Zircaloy cladding for the one-cycle and conducted a preliminary evaluation of the necessary enrichments for several ATF combinations. For the latter we iteratively adjusted the enrichment for each variant in a multi-cycle mode until the infinite multiplication factor (k_∞) at the end-of-cycle met the criterion for a full cycle length (approximately six effective full-power years). For this evaluation, we first calculated 17 sets of polycell burnup scenarios, separately, corresponding to different partial displacement intervals, ranging from zero days to a condition with displacers always present, with each interval lasting 20 days longer than the previous one. Next, we averaged the isotope inventories from these scenarios and used the resulting values as input for a cylindrical polycell burnup calculation. Using a linear approximation, we then determined the necessary enrichment for a reference six-year cycle. This provided the minimum enrichment required for each fuel system to achieve the same cycle length, which is a practical metric for comparing fuel efficiency. Although a truly realistic simulation would require a 3D dynamic tool that can continuously model changes in core geometry during displacer withdrawal/insertion, this remains a topic for future work.

In the present study, we present the results for advanced ATF combinations using an identical lattice, enrichment, and burnup time. All comparisons between variants assume the same core spectral shift strategy (same number and schedule of displacers withdrawn). The selected assembly-level polycell structure undergoes burnup calculations under constant power mode for both with and without mechanical displacers over specified time intervals (Fig. 2). We note that kinetics and thermal-hydraulic performance are beyond the scope of this neutronics study.

Initially we compare results for selected claddings with Zirconium alloy cladding all having UO_2 fuel. Then com-

Table 1. Corresponding density, thermal conductivity, melting temperature and WURs for selected ATF fuels. (*Ref. [28] is the source of numbers given by *. WURs are authors own calculations*).

Fuel type (g/cm ³)	U density conductivity	Thermal temperature (W/m · K)	Melting displacers (°C)	WUR with displacers	WUR without
UO ₂	9.6*	4*	2840*	1.51	1.98
U ₃ Si ₂	11.3*	15*	1665*	1.2	1.68
UN	13.5*	20*	2762*	1.07	1.41

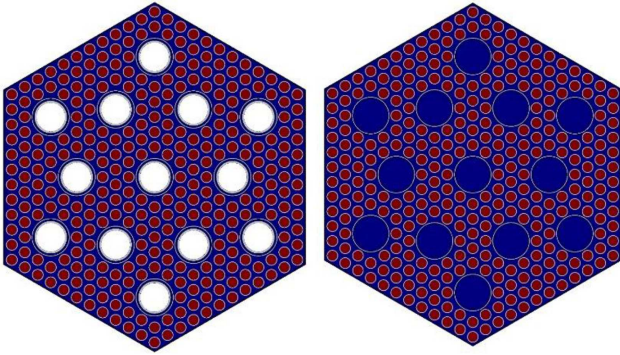


Fig. 2. Calculation model for burning with and without displacers (white gaps and right: blue-water, respectively). (*Authors own drawing*).

parison of ATF claddings performance with high density fuels, UN and U₃Si₂, is done. Each variant is simulated under the same geometric and operating conditions, which represents burning under the influence of mechanical displacers during the first 160 days, followed by operation without displacers thereafter. As expected, the higher-density fuels result in a significantly lower moderator-to-fuel ratio in the given geometry, particularly for UN. For all simulations, the displacer and guide tube material are the same as cladding material, except in the FeCrAl cladding case where we also explore using SiC for the displacers and guide tubes (another ATF concept for non-fuel components) to improve neutronic performance. All fuel variants are set to 4.6% ²³⁵U enrichment (a typical value for PWR fuel) to compare their reactivity behavior on an equal basis. The water uranium ratios (WUR) are given in Table 1.

3 Results and discussions

3.1 Impact of cladding materials (with UO₂ Fuel)

The infinite multiplication factors (k_{∞}) evolution is given in Figure 3. The ranking of these materials by decreasing k_{∞} is primarily explained by their respective neutron absorption cross-sections. SiC yielded the highest k_{∞} at all points in the cycle among the cladding cases considered. It is because Si and C have smaller neutron absorption cross-section than Nb and some isotopes

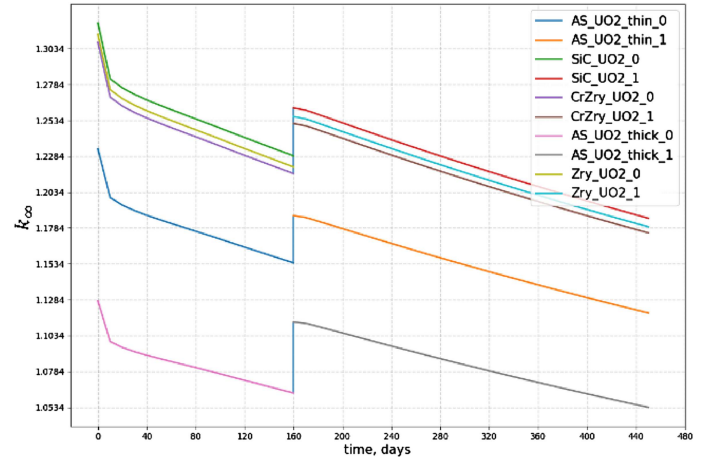


Fig. 3. Dependency of k_{∞} against time for Zry, CrZry, FeCrAl, SiC/UO₂.

of Zr [29]. Thus, the better neutron property of SiC cladding allows for lower enrichment and deeper burnup. Chromium-coated zircaloy cladding has slightly less k_{∞} than zircaloy cladding, because of the higher absorption cross-section for Cr. By a negligible increase in enrichment or by enjoying a marginally shorter cycle, Cr coating provides safety benefits without significant disruption of core neutronics and altering its design. The FeCrAl alloy shows the most notable effect on reactivity. Standard-thickness FeCrAl cladding (650 μ), the same material guide tubes and displacers cause a heavy k_{∞} depression. This is due to the higher thermal neutron absorption of Fe and Cr elements in the cladding, which act as strong parasitic absorbers. However, the figure improved in the case of a thinner FeCrAl cladding (330 μ m) and with SiC the displacers/guide tubes.

Two key trends emerge from Figure 4. First, ²³⁹Pu accumulates more rapidly when displacers are used, which results in harder neutron spectrum, compared to when they are not. Second, claddings with higher thermal neutron absorption cross sections, such as advanced steel, produce a harder neutron spectrum, which in turn increases resonance absorption in ²³⁸U (Fig. 5) and thus leads to greater ²³⁹Pu buildup, that indicates FeCrAl-hardening of the spectrum. Also, the equilibrium concentrations of fission products of higher importance like ¹³⁵Xe and ¹⁴⁹Sm (Figs. 6 and 7, respectively) are higher in FeCrAl cases, as

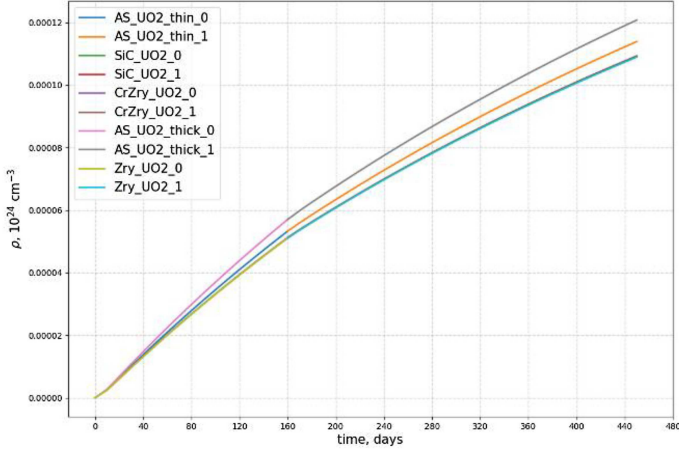


Fig. 4. Change in ^{239}Pu concentration against time for Zry, CrZry, FeCrAl, SiC/ VO_2 .

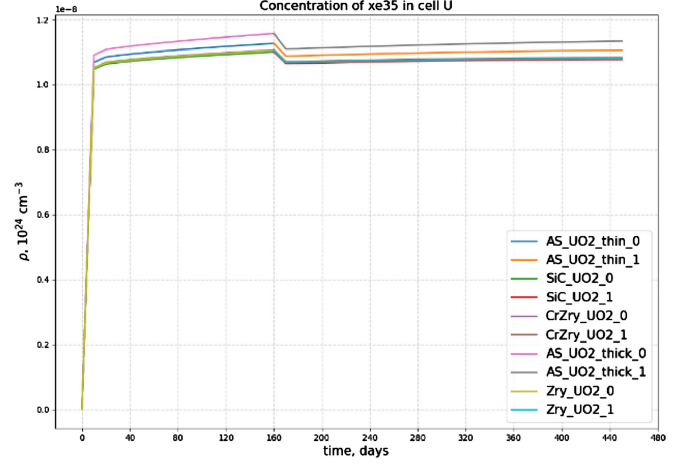


Fig. 6. Change in ^{135}Xe concentration against time for Zry, CrZry, FeCrAl, SiC/ VO_2 .

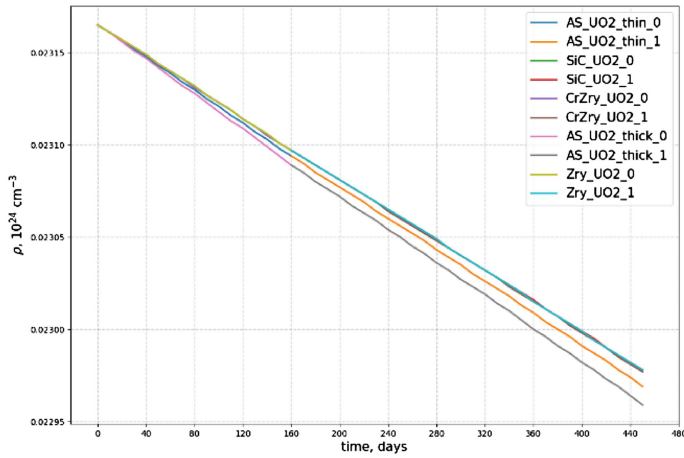


Fig. 5. Change in ^{238}U concentration against time for Zry, CrZry, FeCrAl, SiC/ VO_2 .

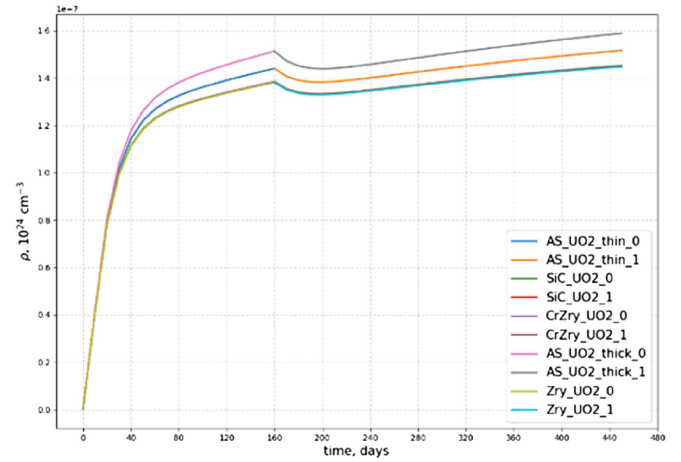


Fig. 7. Change in ^{149}Sm concentration against time for Zry, CrZry, FeCrAl, SiC/ VO_2 .

fewer thermal neutrons are available to burn them out during operation. These effects show that FeCrAl changes the neutron economy appreciably. The positive view is that FeCrAl-clad fuel can still be utilized in PWRs, provided enrichment is increased into the 5–6% range and design optimization (e.g. reducing the thickness and/or lattice dimensions for high density fuels) is implemented. In summary, for VO_2 fuel the rank of cladding neutronic performance is in the following order, SiC best (even better than Zircaloy) > Zircaloy $\approx$ Cr-coated Zry > FeCrAl (with penalties).

3.2 Impact of fuel type in various claddings

Change in the k_∞ and ^{239}Pu buildup by time for CrZry cladding with U_3Si_2 , VO_2 , UN fuels are given in Figures 8 and 9, respectively. Here the cladding effect is minimal (nearly identical to Zircaloy), so differences are primarily due to the fuel. With all fuels at the same enrichment and identical geometry, the VO_2 fuel have the highest initial k_∞ , U_3Si_2 is slightly lower, and UN is the

lowest. U_3Si_2 's k_∞ declines more slowly than VO_2 's, whereas UN's remains low, under constant power. Trend can be explained by several factors, that are the relatively low parasitic absorption of silicon (its capture cross section is only marginally higher than that of oxygen) and U_3Si_2 fuel contains more heavy metal per volume, which tends to improve reactivity, but because this VVER-S geometry was originally optimized for VO_2 , the higher fuel density of U_3Si_2 makes the lattice a bit under moderated. Under ideal conditions, these factors would yield a higher k_∞ . However, the harder spectrum slightly reduces the reactivity gain one would expect from the higher fissile atoms count. Better still, the slower decrease in k_∞ for U_3Si_2 indicates that it could achieve the necessary performance parameters within 5 wt.% enrichment limits.

Similar trends are seen in k_∞ for FeCrAl (thin, with SiC structure) and SiC claddings (see Figs. 10 and 11, respectively). At the end of one effective year (330 days total), modeled as 160 days with displacers followed by 170 days without, the infinite multiplication factors k_∞ for FeCrAl, CrZry, and SiC cladding with U_3Si_2 fuel

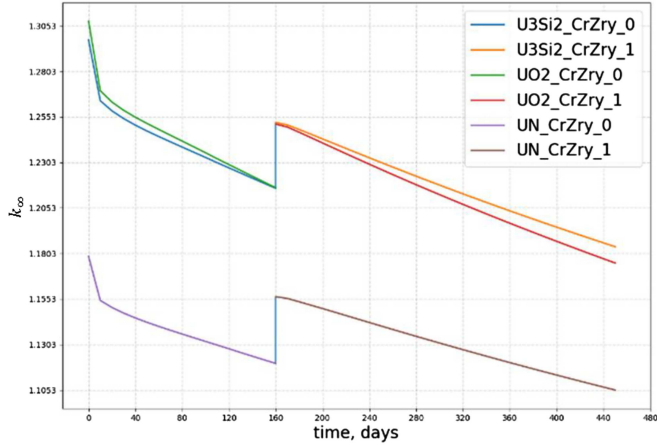


Fig. 8. Change in the k_{∞} against time for CrZry/UO₂, U₃Si₂ and UN.

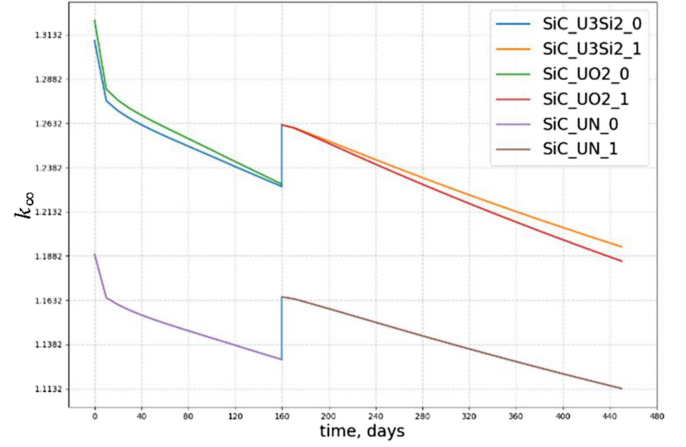


Fig. 10. Change in the k_{∞} against time for SiC/UO₂, U₃Si₂ and UN.

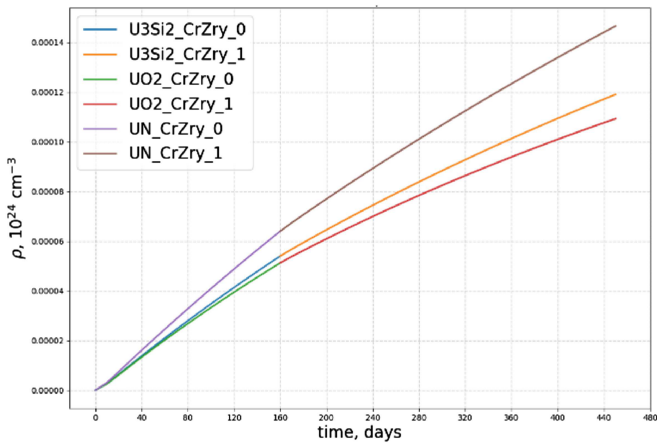


Fig. 9. Change in the ^{239}Pu concentration against time for CrZry/UO₂, U₃Si₂ and UN.

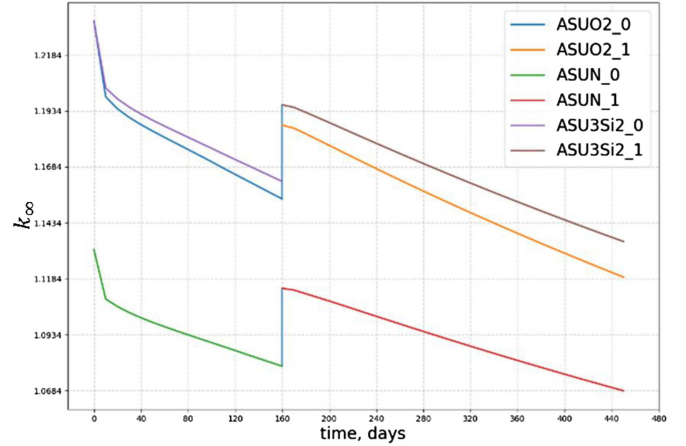


Fig. 11. Change in the k_{∞} against time for FeCrAl/UO₂, U₃Si₂ and UN.

is 1.16, 1.21, and 1.23, respectively. The k_{∞} of uranium nitride (UN) fuel is lower than that of other fuels due to several factors. First, nitrogen exhibits higher parasitic absorption. Second, the water-to-uranium ratio (WUR) for UN is 1.07 with displacers and 1.41 without, which is significantly lower than the optimal value of approximately 3. Third, the fuel rod radius is not optimized for this high-density fuel, leading to a noticeable self-shielding effect. These factors are even stronger in UN with FeCrAl case (Fig. 11), in which k_{∞} is doubly penalized by both the cladding absorption and the under moderation. Parasitic absorptions, in combination with the suboptimal WUR and geometry, shifts the neutron spectrum to higher energies, which in turn increases fissile plutonium production rates in high-density fuels. Moreover, lowest k_{∞} for UN as it has the most uranium, highlights that simply loading a denser fuel in an unmodified geometry is not enough without adjusted moderation.

Figure 12 shows plutonium accumulation for SiC/U₃Si₂ Fuel. The lowest curve represents continuous operation without displacers, while the highest

curve shows operation with displacers for the entire 6-year reference cycle. Intermediate curves correspond to different partial displacement intervals, each lasting 20 days longer than previous one, illustrating how varying the duration of displacement affects plutonium buildup. The graph shows that, over the 6-year cycle, burning with displacers leads to a 19% higher plutonium buildup compared to burning without displacers in this particular case.

4 Conclusion

This work presents a detailed neutronic evaluation of various Accident Tolerant Fuel candidates in the context of a VVER-S spectral shift reactor design. Focusing on a polycell model of the core with spectral reactivity control, we compare combinations of ATF fuel and cladding. Calculations show that SiC cladding is an excellent candidate for ATF. It allows using slightly less enriched uranium, especially, in combination with U₃Si₂ fuel with slow rate of decrease in k_{∞} due to the higher

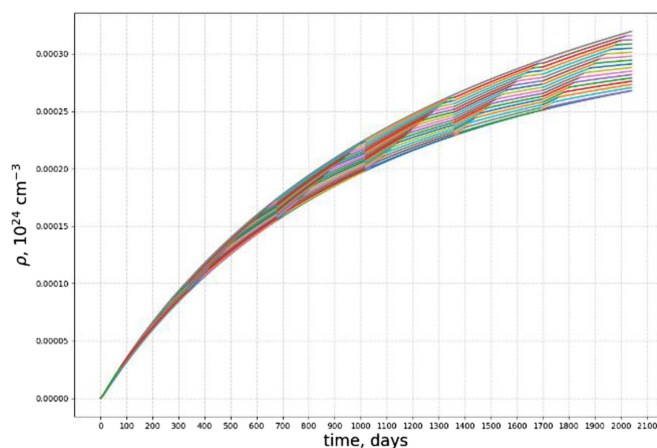


Fig. 12. Change in the ^{239}Pu concentration against time for CrZry/ U_3Si_2 for 6 cycles.

concentration of fissile material. Uranium silicide (U_3Si_2) fuel demonstrates better characteristics compared to UO_2 in spectral shift operation. Despite a slightly harder neutron spectrum due to higher uranium density, U_3Si_2 's greater fissile inventory leads to a slower drop in reactivity and ultimately requires noticeably lower enrichment to reach target burnup. k_∞ for UN fuel is lower than other fuels in combination of all selected cladding candidates. It is because of parasitic absorption of nitrogen, the lower water-uranium ratio, the radius of fuel rods is not optimum for this type of high-density fuel, so the self-shielding effect is high. SiC/ UO_2 , SiC/ U_3Si_2 , CrZry/ U_3Si_2 and FeCrAl/ U_3Si_2 fuel systems have shown good characteristics. The reference cladding thickness of 650 μm for FeCrAl exhibits a notably low k_∞ . However, due to its better mechanical properties, for FeCrAl can be fabricated at half the thickness of traditional zirconium alloy claddings. In the case of FeCrAl cladding with a feasible thickness of 330 μm , the k_∞ values for all three tested fuels are noticeably lower than those with CrZry and SiC claddings, thus requiring higher enrichment to achieve the desired fuel cycle length. The multiplication factor of chromium-coated Zircaloy is slightly lower than in the case of Zircaloy/uranium fuel and requires a slight increase in the enrichment. This VVER fuel assembly oriented study can be considered complementary neutronics analysis for the EU-supported VVER long-term operation goals [30], as it evaluates feasibility of using advanced materials in a similar structure. Future work will focus on integrating multi-physics reactor level simulations with different tools to further evaluate fuel performance under dynamic operational scenarios.

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Conflicts of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability statement

This article has no associated data generated, but detailed simulation procedure and results are available upon request to the corresponding author.

Author contribution statement

Conceptualization, D.T., G.S. and A.T.; Methodology, D.T., A.T., G.S. and S.A.; Software, D.T., A.T., G.S. and S.A.; Validation, D.T., A.T., and S.A.; Formal Analysis, D.T. and A.T.; Investigation, D.T., A.T., and S.A.; Data Curation, D.T., A.T., and S.A.; Writing – Original Draft Preparation, D.T., A.T., and S.A.; Writing – Review & Editing, A.T., G.S. and S.A.; Visualization, D.T., A.T., and S.A.

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