Journal of Engineering and Technological Sciences

Investigation on Neutronic Parameters of the KLT-40S Reactor Core with U₃Si₂-FeCrAl using SCALE Code

Alif Al Mahfudz, Alexander Agung* & Andang Widi Harto

Department of Nuclear Engineering and Engineering Physics, Faculty of Engineering, Universitas Gadjah Mada, Jalan Grafika 2, Yogyakarta 55281, Indonesia

Corresponding author: a_agung@ugm.ac.id

Abstract

From a safety point of view, the fuel-cladding of the current design of the KLT-40S reactor still carries a potential risk in the event of a loss-of-coolant accident (LOCA) allowing the formation of hydrogen gas. The concept of accident tolerant fuels (ATF) offers a variety of new safer fuel-cladding materials, one of which is U₃Si₂-FeCrAl, a potential fuel-cladding combination according to various research sources. In this research, a study of neutronic parameters (1) cycle length, (2) reactivity feedback coefficient, and (3) reactor proliferation resistance was performed with ATF material U₃Si₂-FeCrAl as fuel-cladding in the KLT-40S reactor core. Modeling and simulation of the ATF-fueled KLT-40S reactor core were performed using KENO-VI and TRITON modules from SCALE code. The results showed that replacement of the fuel-cladding material with the ATF material in the KLT-40S reactor resulted in a shorter cycle length, and the enrichment required to reproduce the original cycle length was above the safeguard limit. The fuel temperature, moderator temperature, and void reactivity coefficient were negative, although not as negative as the original ones. The spent fuel produced at the end of the cycle had good proliferation resistance, although not as good as the original one.

Keywords: accident tolerant fuel; cycle length; FeCrAl; KLT-40S; proliferation; reactivity coefficient; SCALE; U₃Si₂

Introduction

Russia's first floating nuclear power plant, Akademik Lomonosov, uses small modular reactor (SMR) technology and is equipped with two KLT -40S reactor systems with 35 MWe capacity each. It was designed to access hardto-reach areas where it can operate for three to five years without refueling [1]. Because of its modular nature and because it can be used in remote areas, this reactor concept can be applied in archipelagic countries such as Indonesia.

The KLT-40S reactor is a pressurized water reactor (PWR) that works in the thermal neutron spectrum. The core uses fuel elements (FEs) with a cylindrical cladding of zirconium alloy (zircaloy) and fuel with higher uranium content based on uranium dioxide (UO₂) pellets in an inert matrix [2]. UO₂ pellets and zirconium alloys have been the most popular nuclear fuel-cladding materials for decades, thanks to their excellent performance in water reactors [3].

From a safety point of view, the fuel-cladding choice from the KLT-40S reactor design still carries a potential risk in the event of a loss-of-coolant accident (LOCA). Oxidation of the zirconium cladding at high temperatures in the presence of steam produces hydrogen exothermically [4]. This reaction occurred in boiling water reactors 1, 2, and 3 of the Fukushima Daiichi Nuclear Power Plant after the reactor's cooling was interrupted by related earthquake and tsunami events. Hydrogen gas was vented into the reactor maintenance halls and the resulting explosive mixture of hydrogen with air oxygen detonated. The explosions severely damaged external buildings and at least one containment building.

After the Fukushima nuclear disaster, the accident tolerant fuels (ATF) concept was developed, which offers a variety of new safer fuel-cladding materials [3]. Based on various studies on ATF, from several ATF fuel-cladding concept combination candidates, the U₃Si₂-FeCrAl pair is a potential ATF candidate. FeCrAl has better accident tolerant performance than the current zircaloy, because its oxidation rate is at least two orders of magnitude

lower than that of zircaloy [5]. However, FeCrAl has a larger neutron capture cross-section, thus U_3Si_2 fuel is proposed because of its larger density and higher uranium concentration [6].

In this research, the effect of using U₃Si₂-FeCrAl ATF as fuel-cladding in the KLT-40S reactor core was investigated from the neutronic aspect. Neutronic parameters investigated were the cycle length, reactivity feedback coefficient, and reactor proliferation resistance. The cycle length is affected by the fuel enrichment and the presence of burnable poison material. The reactivity coefficient affects the safety aspects of the nuclear reactor design and was investigated from fuel temperature, moderator temperature, and coolant void. Reactor proliferation resistance can be determined by observing plutonium isotopes mass fraction formed during the burnup. A reactor is considered to have good proliferation resistance if the plutonium produced in the spent fuel is identified as reactor-grade plutonium. Thus, the spent fuel produced is resistant to the misuse of nuclear materials.

Previously, similar studies have been performed on the same neutronic parameters in the KLT-40S reactor core by Fajri, et al. [7] to see the feasibility of the KLT-40S reactor design. Referring to the results of the mentioned research, the effect of changing the fuel-cladding material into ATF on the neutronic parameters that have been studied previously were observed in this research.

Methodology

Fuel Assembly and Core Modeling

The KLT-40S reactor core was modeled in SCALE using the GeeWiz graphical interface, starting with the fuel assembly (FA). The FA was modeled as in Figure 1 (left), similar to that performed in the referenced research, but with material changes in the fuel and cladding. The fuel rod consisted of U_3Si_2 fuel with FeCrAl cladding. As for burnable poison rods (BPR), a mixture of Gd_2O_3 and U_3Si_2 was used with FeCrAl cladding. The FeCrAl cladding used had a material composition with a weight percentage (wt%) of Fe/Cr/Al = 75/20/5 [5]. The Gd_2O_3 in the BPR had a mass fraction of 9.607%. Geometry specification details of the modeled FA can be seen in Table 1. The modeled FA was then arranged into a full core configuration as shown in Figure 1 (right), with simplification such that the core contained only one type of FA. The FAs were arranged into a triangular lattice with a pitch of 10 cm [2].



Figure 1 Modeled FA (left) and core (right) of KLT-40S.

Property	Value	Unit
Fuel rod outer radius	0.34	cm
Big BPR outer radius	0.34	cm
Small BPR outer radius	0.238	cm
Cladding thickness (fuel rod & BPR)	0.05	cm
Fuel element pitch	0.995	cm
FA shroud thickness	0.075	cm
FA side-to-side outer diameter	10	cm
FA height	120	cm

Table 1FA geometry specification [2].

The modeled core was then placed inside the reactor vessel, with simplification by eliminating devices other than the core so that only the core remained inside the vessel. The vessel was made of $15Cr_2NiMo$ VA-A steel alloy with composition details shown in Table 2. The reactor core in the vessel was modeled with the model and dimensions as shown in Figure 2.

 Table 2
 15Cr2NiMo VA-A steel alloy composition [8].



Figure 2 Reactor core in the vessel and its dimension.

Parameter Variation and Simulation

The ATF-fueled KLT-40S reactor cycle length and plutonium isotopes distribution were obtained by simulating the modeled ATF-fueled KLT-40S reactor core with the same parameters as the referenced research. This case

was simulated using the TRITON module T6-DEPL depletion sequence in SCALE version 6.2.4. The enrichment used in this case referred to the average enrichment obtained in the results of the referenced research, which considered the average fuel enrichment needed to achieve a cycle length that is close to the official claims of the KLT-40S reactor design, i.e., 18.6% [7].

The uranium enrichment that could produce the original KLT-40S cycle length was obtained by simulating the modeled ATF-fueled KLT-40S reactor core and changing the uranium enrichment until the original cycle length was obtained. In this case, the enrichment that produced the same cycle length obtained in the referenced research was sought. Simulations for this case were also performed using the TRITON module T6-DEPL depletion sequence in SCALE version 6.2.4.

The fuel temperature reactivity coefficient (FTC) was obtained by simulating the model with fuel temperature variation starting from 650 K at HZP (Hot-Zero Power) operating condition to 900 K at HFP (Hot-Full Power) with 50 K increments.

The moderator temperature reactivity coefficient (MTC) was obtained by simulating the model with moderator temperature variation in the range of ± 22 K from the average temperature at operating conditions, i.e., 571 K. The moderator temperature was varied with 11 K increments to obtain five variations. The moderator density was also varied based on its temperature under subcooled conditions at 12.7 MPa reactor operating pressure. The parameter variation in this case can be seen in Table 3.

 Table 3
 Moderator temperature and its density variations.

Variation	Moderator temperature (K)	Moderator density (g/cc)
1	549	0.76710
2	560	0.74711
3	571	0.72509
4	582	0.70036
5	593	0.67175

The void reactivity coefficient (VRC) was obtained by simulating the model with coolant/moderator void fraction variation starting from 0% to 25% with a 5% increment. The coolant/moderator temperature in this case was the water saturation temperature at reactor operating pressure, i.e., 602.04 K. Void fraction was varied by changing the density of water using the following equation:

$$D_{moderator}(\vartheta\vartheta) = \left(D_f \times (1 - \vartheta\vartheta)\right) + \left(D_g \times \vartheta\vartheta\right) \tag{1}$$

where $\Re\theta$ is the void fraction, D_f and D_g are saturated liquid density and saturated vapor density at a reactor operating pressure of 12.7 MPa. The parameter variation in this case is shown in Table 4.

Table 4 Void f		raction variations.	
Variation	Void fraction (%)	Coolant density (g/cc)	
1	0	0.65011	
2	5	0.62139	
3	10	0.59267	
4	15	0.56395	
5	20	0.53523	
6	25	0.50652	

All simulations to obtain the reactivity coefficient were performed at the beginning of the cycle and using the KENO-VI module CSAS6 sequence in SCALE version 6.2.4 with 18.6% fuel enrichment.

Results and Discussion

Cycle Length

Figure 3 shows the effective multiplication factor (k_{eff}) as a function of burn days data obtained from the simulation results of the original KLT-40S reactor core model from the referenced research (represented by Ori

18.6%), the ATF-fueled KLT-40S reactor core model with the same parameters as the referenced research (represented by ATF 18.6%), and the ATF-fueled KLT-40S reactor core model with the fuel enrichment that produces the same cycle length as the model from the referenced research (represented by ATF 21.85%). The cycle length obtained for the ATF-fueled KLT-40S reactor core model was 609.12 days, or 20.01 months, which is shorter than the cycle length for the original KLT-40S reactor core model, i.e., 719.19 days, or 23.63 months. In terms of fuel burnup, the ATF-fueled reactor core had around 15% lower than the original core [2].



Figure 3 The value of k_{eff} as a function of burn days for all models.

Several conclusions can be drawn from the graph comparison between the ATF-fueled core model and the original core model. The more significant k_{eff} decrease in the original fueled core model from the higher peak k_{eff} value indicates that at the beginning of the cycle, the k_{eff} value of the original fueled core model was higher than that of the ATF-fueled model when no burnable poison was present in the reactor core. The addition of burnable poison to the original fueled core model resulted in a more significant k_{eff} decrease at the beginning of the cycle than adding the same amount of burnable poison material to the ATF-fueled core model. Hence, the k_{eff} of the original fueled core model was lower than that of the ATF-fueled core model at the beginning of the cycle. The use of higher fuel density of ATF made the ratio of moderator-to-fuel decrease, leading to a shift in neutron spectrum towards higher energy. Such a spectral-shift makes the burnable poison less effective in decreasing the reactivity at the beginning of the cycle in the ATF-fueled core model.

This also indicates that the larger FeCrAl neutron capture cross-section significantly affects the k_{eff} value. The simulation results performed on SCALE with the KMART feature activated, showed that the neutron absorption reaction rate in FeCrAl is more prominent than in zirconium alloys. It is known that FeCrAl has a neutron capture cross-section that is about ten times higher than that of zirconium alloys [3]. The larger cross-section of FeCrAl causes more thermal neutrons to be absorbed in the cladding, increasing the absorption cross-section of the reactor core system on the ATF-fueled core model, which will then decrease the value of the thermal utilization factors f and k_{eff} according to the six-factor formula.

$$k_{eff} = \eta \varepsilon P_F p P_T f \tag{2}$$

$$\eta = v_T \frac{\Sigma_f^F}{\Sigma_a^F} \tag{3}$$

$$f = \frac{\Sigma_a^F}{\Sigma_a^F + \Sigma_a^M + \Sigma_a^C + \Sigma_a^S + \Sigma_a^P} \tag{4}$$

Superscript F, M, C, S, and P represent fuel, moderator, coolant, structure, and other neutron absorbers, respectively, while subscript f represents fission and subscript a represents neutron absorption.

Additional calculations were conducted using zirconium-niobium alloy as cladding instead of FeCrAl to further investigate the effect of high absorption in FeCrAl. The composition of this alloy was based on M5 cladding [9]. The results showed that the cycle lengths obtained by using zirconium-niobium alloy cladding were 675 days (for 18.6% enrichment) and 782 days (for 21.85% enrichment). These values showed an improvement against FeCrAl cladding, although they were still smaller than for the original UO₂-Zr fuel. In other words, these results emphasize the effect of high absorption in FeCrAl on cycle length.

U₃Si₂ fuel was used to compensate for the larger cross-section of FeCrAl. U₃Si₂ has a higher uranium density by about 16.3% compared to UO₂ [3]. However, the simulation results show that the k_{eff} decreased in the ATF-fueled core model because the larger cross-section of FeCrAl is more significant than the k_{eff} increase caused by the higher uranium density of U₃Si₂.

It can be concluded that the use of ATF U₃Si₂-FeCrAl in the KLT-40S reactor core will significantly reduce the effect of Gd₂O₃ burnable poison and reduce the k_{eff} value as a result of the large cross-section of the FeCrAl, thereby causing a decrease in the reactor cycle length. One way to extend the cycle length is to increase the fuel enrichment. A higher fuel enrichment will enlarge the fission absorption macroscopic cross-section of the fuel and reduce the total absorption macroscopic cross section of the fuel, which will increase the values of η and k_{eff} with the relation shown in Eqs. (2) and (3).

From the simulation results, the fuel enrichment required for the ATF-fueled core model to produce the same cycle length as the original fueled core model is 21.85%. The fuel enrichment obtained is above the limit of the existing safeguard rules. The uranium enrichment limit can be categorized as low enriched uranium (LEU) to meet international proliferation standards of 20%. Thus, the fuel enrichment must be less than 20% to meet the safeguard rules. Therefore, extending the cycle length of the ATF-fueled reactor core model while obeying the safeguard rules cannot be done by only increasing the fuel enrichment.

Other methods that can be used to extend the cycle length of the ATF-fueled core model include: (1) reducing the thickness of the FeCrAl cladding (reducing the effect of significant FeCrAl neutron absorption), (2) replacing the burnable poison material, (3) changing the geometric arrangement (size, number, and/or placement of fuel rod, BPR, and/or FA) in the reactor core, or (4) a combination of these methods.

Reactivity Coefficient

Figures 4, 5, and 6 respectively show the change in reactivity per degree change in the fuel temperature, the moderator temperature, and the per percent change in the void volume obtained from the simulation results of the ATF-fueled reactor core model. The graphs show that the FTC, MTC, and VRC are all negative, i.e., -1.44 pcm/K, -25.83 pcm/K, and -103.98 pcm/%void, respectively. This shows that the ATF-fueled reactor core model has a good inherent safety system.



Figure 4 The core's reactivity as a function of fuel temperature for the ATF-fueled core model.



Figure 5 The core's reactivity as a function of moderator temperature for the ATF-fueled core model.



Figure 6 The core's reactivity as a function of void fraction for the ATF-fueled core model.

The FTC value of the ATF-fueled core model was lower than the FTC of the original fueled core model, i.e., -1.67 pcm/K. This is due to the use of fuel with a higher fissile density in the ATF-fueled core model. The higher fuel mass in the ATF-fueled core model with the same fuel surface area as the original fueled core model resulted in a lower FTC value. This can be understood by reviewing the semi-empirical formula of the resonance integral for low ²³⁵U enrichment UO₂ fuel and ThO₂ fuel and the Doppler temperature reactivity coefficient formula for thermal reactors.

$$I(T_F) = I(300 K) \left[1 + \beta'' \left(\sqrt{T(K)} - \sqrt{300} \right) \right]$$
(5)

where

$$I(300 K) = a + b \left(\frac{S_F}{M_F}\right)$$

$$\beta'' = c + d \left(\frac{S_F}{M_F}\right)$$

$$\alpha_{T_F}^D = -\ln\left[\frac{1}{p(300 K)}\right] \frac{\beta''}{2\sqrt{T_F(K)}}$$
(6)

Eq. (5) is the semi-empirical formula of the resonance integral, where I(300 K) is the resonance integral at a temperature of 300 K, *a*, *b*, *c*, and *d* are constants that depend on the fuel, S_F represents the surface area of the fuel, and M_F represents the mass of the fuel [10]. Eq. (6) is the Doppler temperature reactivity coefficient formula for thermal reactors. A lower S_F/M_F value will result in a lower B'' value and thus the FTC value will also become lower.

The MTC value of the ATF-fueled core model was lower than that of the original fueled core model, i.e., -38.86 pcm/K. The VRC value of the ATF-fueled core model was also lower than that of the original fueled core model, i.e., -144 pcm/%void. Both were due to the use of fuel with a higher fissile density in the ATF-fueled core model. A higher fissile density in the fuel will result in a lower moderator to fuel ratio. It is known that the PWRs, including the KLT-40S, were designed as under-moderated reactors. In this condition, a lower moderator-to-fuel ratio will result in a lower resonance escape probability change and a lower k_{eff} change [11]. As a result, the reactivity coefficient will also become lower.

Plutonium Isotopes Distribution at the End of Cycle

The plutonium isotopes distribution at the end of the cycle for all models are shown in Table 5. It can be seen that the ATF-fueled core model produced a higher percentage of ²³⁹Pu than the original fueled core model at the end of the cycle. This is due to the use of fuel with a higher uranium density in the ATF-fueled core model. The higher the density of uranium in the fuel, the higher the density of ²³⁸U in the core, and more ²³⁹Pu will be produced from the ²³⁸U neutron capture reaction.

Fuel 9 envictment	Plutonium isotopes distribution at the end of the cycle (%mass)				
ruei a enrichment	²³⁸ Pu	²³⁹ Pu	²⁴⁰ Pu	²⁴¹ Pu	²⁴² Pu
Ori 18.6%	4.28	49.20	22.55	16.06	7.91
ATF 18.6%	4.44	59.47	17.54	14.93	3.62
ATF 21.85%	5.46	58.58	17.12	15.14	3.70

Table 5Plutonium isotopes distribution at the end of the cycle for all models.

Both ATF-fueled core models produced ²⁴⁰Pu percentage slightly below 19%, thus the plutonium produced cannot be identified as reactor-grade plutonium based on the percentage of ²⁴⁰Pu produced. However, assessing the percentage of ²³⁹Pu, the plutonium produced can be identified as reactor-grade plutonium, because the ²³⁹Pu produced percentage is in the range of 55-70% [12]. Therefore, it can be concluded that the spent fuel produced by the ATF-fueled core model at the end of the cycle has a good proliferation resistance, although not as good as the original fueled core model, which produces a lower ²³⁹Pu percentage and a higher ²⁴⁰Pu percentage at the end of the cycle.

Conclusions

Using U₃Si₂-FeCrAl ATF as fuel-cladding in the KLT-40S reactor resulted in a shorter cycle length. The use of ATF significantly reduces the effect of Gd₂O₃ burnable poison material, and the effect of a larger FeCrAl cross-section to decrease the k_{eff} is more significant than the effect of U₃Si₂ higher uranium density, resulting in a decrease of k_{eff} and a shorter cycle length. The uranium enrichment required for the ATF-fueled core model to produce the same cycle length as the original fueled core model is 21.85%, which is above the limit of the existing safeguard rules. Therefore, extending the cycle length of the ATF-fueled core model while obeying the safeguard rules cannot be done just by increasing the fuel enrichment.

The use of ATF in the KLT-40S reactor produces negative FTC, MTC, and VRC. This shows that the ATF-fueled reactor core model has a good inherent safety system, although not as good as the original fueled core model, producing more negative FTC, MTC, and VRC. The use of ATF in the KLT-40S reactor produces spent fuel with good proliferation resistance at the end of the cycle, although not as good as the original fueled core model, which produces a lower ²³⁹Pu percentage and a higher ²⁴⁰Pu percentage at the end of the cycle. The ATF-fueled KLT-40S reactor core model produces cycle length, reactivity coefficient, and reactor proliferation resistance that are not as good as those of the original fueled model. Therefore, unless the core configuration is modified, the use of U₃Si₂-FeCrAl ATF material is not recommended as fuel-cladding material in the KLT-40S reactor core.

Acknowledgment

The authors thank the Nuclear Energy Technology Laboratory, Department of Nuclear Engineering and Engineering Physics, UGM, for providing access to the code and computational resources. This research was supported by UGM through the research grant scheme Recognition of Final Project (RTA) year 2022.

References

- [1] Cholteeva, Y., *Is Floating Nuclear Power a Good Idea?*, Power Technology, 2019, https://www.power-technology.com/features/floating-nuclear-power/, (5 April 2021).
- [2] IAEA, Advances in Small Modular Reactor Technology Developments, A Supplement to: IAEA Advanced Reactors Information System (ARIS), 2020 edition, pp. 111–114, 2020.
- [3] Rebak, R.B., Accident-Tolerant Materials for Light Water Reactor Fuels, Elsevier, 2020.

- [4] World Nuclear Association, Fukushima Daiichi Accident, 2021, https://www.world-nuclear.org/information-library/safety-and-security/safety-of-plants/fukushima-daiichi-accident.aspx, (5 May 2021).
- [5] Chen, S. & Yuan, C., Neutronic Analysis on Potential Accident Tolerant Fuel-Cladding Combination U₃Si₂-FeCrAl, Science and Technology of Nuclear Installations, 2017, 3146985, 2017. doi: 10.1155/2017/3146985.
- [6] Chen, S., Yuan, C. & Guo, D., Radial Distributions of Power and Isotopic Concentrations in Candidate Accident Tolerant Fuel U3Si2 and U02/U₃Si₂ Fuel Pins with FeCrAl Cladding, Annals of Nuclear Energy, 124, pp. 460-471, 2019, DOI: 10.1016/j.anucene.2018.10.025.
- [7] Fajri, D.F., Agung, A. & Harto, A.W., The Study of Floating Nuclear Power Plant Reactor Core Neutronic Parameters using SCALE 6.1 Code, International Journal on Advanced Science, Engineering, and Information Technology, 10, pp. 1774-1783, 2020, DOI: 10.18517/ijaseit.10.5.6609.
- Bazaras, Ž., Timofeev, B., Zotova, A. & Skvireckas, R., *Investigation of Ageing of Russian RPV Materials*, Proceedings of the 6th International Scientific Conference TRANSBALTICA, pp. 11–14, 2009.
- [9] Kecek, A., Tuček, K., Holmström, S. & van Uffelen, P., Development of M5 Cladding Material Correlations in the TRANSURANUS Code: Revision 1, EUR 28366 EN, Publications Office of the European Union, Luxembourg, 2016, ISBN 978-92-79-64655-3, doi:10.2789/332093, JRC100644.
- [10] Harto, A.W., *Nuclear Reactor Physics*, Department of Nuclear Engineering and Engineering Physics, Universitas Gadjah Mada, Yogyakarta, 2009. (Text in Indonesian)
- [11] Nuclear Power, Moderator Temperature Coefficient MTC, 2022, https://www.nuclearpower.com/nuclear-power/reactor-physics/nuclear-fission-chain-reaction/reactivity-coefficientsreactivity-feedbacks/moderator-temperature-coefficient-mtc/, (24 February 2022).
- [12] World Nuclear Association, *Plutonium*, 2021, http://www.world-nuclear.org/informationlibrary/nuclear-fuel-cycle/fuel-recycling/plutonium.aspx, (18 January 2022).