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Model Comparison of Passive Compact-Molten Salt Reactor Neutronic Design Using MCNP6 and Serpent-2

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ABSTRACT

Passive Compact Molten Salt Reactor (PCMSR) is a thermal breeder molten salt reactor (MSR) developed in Universitas Gadjah Mada, Indonesia, run in thorium fuel cycle. Its design was initially developed using deterministic code SRAC2006 but has never been compared with other codes. This paper attempts to compare PCMSR neutronic design using Monte Carlo codes MCNP6 and Serpent-2 with ENDF B/VII.0 continuous neutron cross-section library. The reactor was run in a pure thorium fuel cycle with lithium fluoride as its carrier salt. The analyzed parameters were effective multiplication factor (k_{eff}), temperature coefficient of reactivity (TCR), void coefficient of reactivity (VCR), and conversion ratio (CR). The result shows that there are several important discrepancies between the original calculation and this research. The Monte Carlo calculations implied that PCMSR core was able to be critical using lower fissile concentration than previously designed, but failed to reach CR above unity. While the TCR value was found to be negative, the VCR value was positive up until the 10 % void fraction. The PCMSR core suffered from ineffective neutron moderation and high neutron leakage. These findings imply that the previous PCMSR neutronic design is inaccurate. For PCMSR to be able to operate as a thermal breeder MSR, geometrical modifications must be performed to improve neutron moderation and reduce neutron leakage.

INTRODUCTION

Molten salt reactor (MSR) is one of the six Generation IV nuclear reactor designs proposed in Generation IV Forum (GIF). It offers many advantages compared to conventional light water reactors (LWR), such as passive safety systems, atmospheric operating pressure, high operating temperature, and no fuel fabrication requirement. Its online reprocessing capability enables MSR to achieve breeding in thermal spectrum using thorium fuel cycle while maintaining high fuel burnup [1-3].

The idea of thermal breeder MSR was conceived in Oak Ridge National Laboratory (ORNL) during the 1960s. As a part of MSR development, the prototype of Molten Salt Reactor Experiment (MSRE) was built and tested successfully for 4.5 years. However, before the ORNL-designed thermal breeder MSR, the Molten Salt Breeder Reactor (MSBR), was realized, the development was stopped abruptly by the United States government in favor of fast breeder reactor [2,4]. Interests on thermal breeder MSR were then resurfaced after MSR was selected by GIF.

Recent researches on thermal breeder MSR have been performed in several designs, such as ORNL-designed MSBR [5-9], Japanese MSR-FUJI [10-12], and the more recent Chinese Thorium Molten Salt Reactor (TMSR) [13-16], to name a few. Many of the aforementioned researches were focused on the fuel cycle and transition into the thorium fuel cycle. Another thermal breeder MSR design is the Passive Compact Molten Salt Reactor (PCMSR). It is currently being developed in Universitas Gadjah Mada, Indonesia [17-19], and designed to possess a passive safety system with a

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compact modular design. it differs from other thermal breeder MSR designs in terms of integral module concept, higher operating temperature, and thermal efficiency, among others [17]. PCMSR refers more to a whole reactor module rather than the core design; thus, PCMSR can use one fluid or two fluid-core.

A design study has previously been performed for one fluid PCMSR using deterministic code SRAC2006 [17]. The result implied that the core design can achieve thermal breeding with a negative temperature coefficient of reactivity. However, the calculation has never been compared with other codes, such as Monte Carlo-based codes. The calculation also ignored the void coefficient of reactivity. Other publications on PCMSR [18-20] were performed similarly using SRAC2006, ignoring characterization of its inherent safety and none using Monte Carlo-based codes.

This paper attempts to compare PCMSR neutronic design using Monte Carlo codes, MCNP6 and Serpent-2. The objective was to make a model comparison of PCMSR neutronics using probabilistic codes to study whether the initial calculation using deterministic code has been modelled accurately or not. The neutronic parameters analyzed in this study were effective multiplication factor (k_{eff}), inherent safety parameters, i.e., temperature coefficient of reactivity (TCR) and void coefficient of reactivity (VCR), as well as conversion ratio (CR).

THEORY

PCMSR is a thermal breeder MSR run in thorium fuel cycle. It uses liquid fluoride salt mixture as fuel, graphite as moderator and structure, and eutectic Flinak salt (LiF-NaK-KF) as intermediate coolant. The latter has its lithium-7 isotope unenriched, as there is no necessity to do so. Instead, the unenriched lithium-7 will act as a protective layer to prevent criticality during an accident.

Its operational temperature is 1200 °C, much higher than the typical MSR (around 700 °C) [17]. To support such a high temperature, it employs lithium-7 fluoride (^{7}LiF) as its carrier salt. The omission of beryllium fluoride from the fuel salt increases salt melting point and boiling point, providing a sufficient safety margin. However, due to the limitation of the available cross-section library in MCNP6 and Serpent-2, this study employed PCMSR at a lower temperature of 930 °C. Consequently, its thermal power was increased from 460 MWt to 570 MWt to compensate for lower thermal efficiency as operating temperature decreased.

PCMSR core configuration is a virtual one-and-half fluid [2]. It means that PCMSR has a single fluid/fuel stream, but the core has two moderating zones meant for different purposes. The first is called the "core" zone, with a narrow fuel channel dedicated mainly to optimize fission reaction. The second is a "blanket zone" with a wider fuel channel and therefore less moderation, meant to optimize neutron capture by thorium. This configuration is similarly used in SD-TMSR [13] and has proven to be effective to optimize thorium conversion.

PCMSR reactor module is an integral module consisting of a reactor core, heat removal system, and post-shutdown cooling system. The module is designed in such a way so that the fuel is always sufficiently confined by secondary coolant salt which acts as the heat transfer medium as well as radiation shielding. The general schematic of a PCMSR system is shown in Fig. 1 [18].

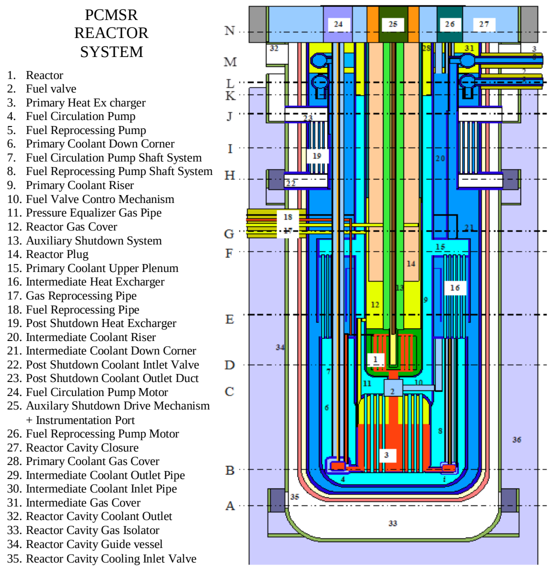


Fig. 1. PCMSR Reactor System [18].

PCMSR core parameters used in this study are provided in Table 1.

Table 1. PCMSR core parameters [17].

PCMSR core parameters	Values
Thermal Power	570 MWt
Core diameter	180 cm
Core height	179 cm
Active core diameter	260 cm
Active core height	220 cm
Graphite density	2.2 g/cm^3
Hastelloy thickness	5 cm
Core channel radius	4.5 cm
Blanket channel radius	6.5 cm
Operational temperature	930 °C
Fuel type	Molten salt
Composition	LiF- ThF_4-UF_4
Molar composition (%)	70-29.4-0.6

METHODOLOGY

The neutronic calculation was performed using two Monte Carlo-based codes. The first code was the MCNP6 neutron transport code, developed by Los Alamos National Laboratory (LANL). The code is well-known to be able to model a complex geometry for radiation transport cases and validated for many reactor types [21-23]. MCNP6 was employed to model the MSR-FUJI reactor, which was initially modelled using the SRAC95 code. The calculation result showed that the MCNP model was comparable and able to predict MSR-FUJI neutronic simulation [10]. It was also used to model MSBR [5]. Thus, MCNP6 can be considered suitable to model MSR. The second code was Serpent-2. It is a 3D continuous energy Monte Carlo neutron and transport code developed at VTT Technical Research Center of Finland, Ltd [24-26]. Serpent-2 has been employed previously to model SD-TMSR and MSBR, both showing good agreement with the previous results [7,27]. Both codes use ENDF/B-VII.0 continuous neutron cross-section library.

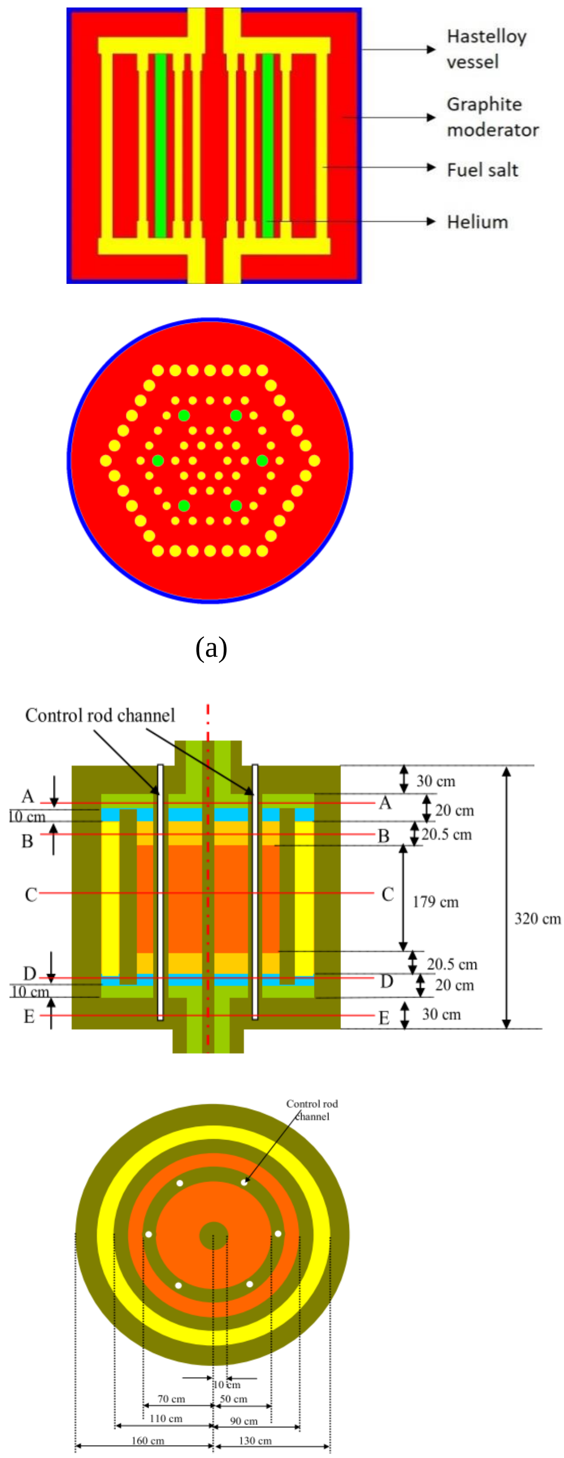
The previous calculation was performed using SRAC2006 [17], which uses geometrical homogenization. Thus, no actual detailed geometry was designed. However, a general model of PCMSR has been visualized. Here, we attempt to translate the visualized model into MCNP6 and Serpent-2. The comparison is shown in Fig. 2.

Although the visualization shows a cylindrical core, the actual model was hexagonal. Thus, the design approach in both Monte Carlo codes is considerably accurate. The exception is for the control rod channel, which is quite difficult to model in the current MCNP and Serpent-2 model. Since the calculation does not involve control rods, or in other words, the control rods are fully withdrawn, the incomplete control rod channels can be ignored for this calculation.

Criticality was calculated in the initial condition. Neutrons simulated at each cycle were set to be 10,000 neutrons, 250 cycles in total, and the 50 first cycles were discarded. The fuel composition was calculated so that the core is critical with k_{eff} below its effective delayed neutron fraction (β_{eff}), for the ease of reactivity control. From there, the TCR, VCR, and CR were then calculated.

TCR calculation was divided into fuel temperature coefficient (FTC) and moderator temperature coefficient (MTC). To calculate FTC, criticality calculations were performed with fuel temperature lowered to 30 °C, 330 °C, and 630 °C, while moderator and vessel temperatures were kept unaltered. Liquid fuel expands when temperature increases, lowering its density and pushing a fraction of fissile nuclides outside the core. Thus, FTC and TCR in MSR is also a factor of fuel density, and therefore the density was corrected accordingly.

MTC was calculated similarly with FTC, with the exception that temperature was altered for moderator only and graphite density change was ignored. Thermal scattering library S(α,β) for graphite was adjusted to the corresponding temperature.



(b)

Fig. 2. PCMSR model visualization in MCNP6 and Serpent-2 (a), and in the reference [17] (b).

Meanwhile, fuel density change due to gaseous fission product formation or helium bubbling in liquid fuel can be treated as VCR. Density reduction for VCR calculation was set from 0-50 %, with a 10 % change at each step.

CR was used to evaluate thorium conversion performance and calculated using reaction rate. Traditional CR definition was used and expressed in Eq. (1), modified from [28].

$$CR = \frac{R_c({}^{232}_{90}Th)}{R_A({}^{233}_{93}U)} \quad (1)$$

where R_c represents neutron capture reaction rate of fertile nuclide (${}^{232}_{90}Th$) and R_A represents neutron absorption reaction rate of fissile nuclide (${}^{233}_{93}U$). CR value was calculated at the beginning of cycle (BOC) only to obtain a maximum value. At BOC, the reaction rate is yet to be tampered by fission products and impurities buildups, such as neutron-absorbing Xe-135 and Sm-149. As such, no burnup calculation was actually performed, and reaction rates from other fertile and fissile nuclides that might be formed during burnup were ignored.

RESULTS AND DISCUSSION

Effective multiplication factor (k_{eff})

For k_{eff} calculation, the expected value is $1 < k_{eff} < 1+\beta_{eff}$. Using parameters mentioned in Table 1, the PCMSR core can achieve criticality. The k_{eff} value comparison is provided in Table 2.

Table 2. k_{eff} and β_{eff} values of PCMSR using different codes.

Code	k_{eff}	β_{eff}
SRAC2006 (from [17])	1.000082	-
MCNP6	1.08675 ± 0.00048	0.00236 ± 0.00038
Serpent-2	1.08800 ± 0.00041	0.00319 ± 0.00051

Both MCNP6 and Serpent-2 calculations resulted in far higher k_{eff} values compared to SRAC calculation. While the core is barely critical in SRAC calculation, MCNP6 and Serpent-2 calculations show excess reactivity of more than 8000 pcm. Such discrepancy is beyond any tolerated deviation. Thus, one of the calculations must be wrong.

Since MCNP6 and Serpent-2 generated relatively similar k_{eff} values, the modelling can be said to be consistent in both codes. The models were also modelled in a detailed way, considering geometrical heterogeneity. Both codes can also visualize the core geometry to help determine if the model is sufficiently accurate. Either way, both MCNP6 and Serpent-2 cannot run the input case if the geometry is wrong. Since the model was able to be run and provided k_{eff} values, it can be safely implied that there were no problems with geometrical modelling, i.e., the model was accurate for given geometrical parameters.

Even though the temperature simulated in this study was lower than the original one, as previously mentioned, the difference in reactivity is far too large to be considered as a calculation deviation. MSR is not known as possessing extremely negative TCR, especially when fuelled by ^{233}U-Th. Excess reactivity difference of 8000 pcm requires that the PCMSR possesses a TCR of around -26.7 pcm/K. This is virtually impossible, as thermal MSR can only achieve TCR around a tenth of said value [7,29]. TCR in PCMSR is even lower, as will be discussed later in this section. From these rationales, it can be argued that the initial SRAC model was incorrect, whereas MCNP6 and Serpent-2 models provided the accurate representation of the PCMSR core model.

The idea of PCMSR is to be operated with minimal excess reactivity, below its β_{eff} value. For the current fuel composition, the k_{eff} values are significantly larger than required, thus the fuel composition must be readjusted to fulfil the aforementioned criterion. It must be noted that MSR fuel is circulating through the primary loop, and consequently, a fraction of β_{eff} may be "lost" from the core. However, the lost β_{eff} fraction was ignored in this study, instead of calculated β_{eff} was used. The result is shown in Table 3.

Table 3. Fuel composition and k_{eff} value from new calculations.

Code	k_{eff}	β_{eff}
MCNP6	1.00205 ± 0.00043	0.00328 ± 0.00052
Serpent-2	1.00227 ± 0.00043	0.00305 ± 0.00050

The core can be critical using 0.495 % of UF_4, 0.105 % lower than the initial calculation. Calculation results from MCNP6 and Serpent -2 are in good agreement with each other. Excess reactivity values are both below their respective β_{eff}, therefore the values are acceptable and used for inherent safety calculations.

Neutron spectrum

PCMSR neutron flux per unit lethargy at BOC is shown in Fig. 3. Flux profile is in good agreement between MCNP6 and Serpent-2. Compared to other MSR designs [5,7,28,30], PCMSR has a harder spectrum, seen in high flux peaks in fast neutron spectra. Usually, MSR has a soft spectrum at BOC and becomes harder as the core enters the equilibrium state, as implied for instance in [5,7]. The harder spectrum shown in PCMSR implies that the neutron moderation is quite ineffective and neutron leakage is relatively high. Considering the small size of the PCMSR reactor core, the phenomenon is understandable. This spectrum profile can affect the inherent safety criteria, as will be discussed in the next subsections.

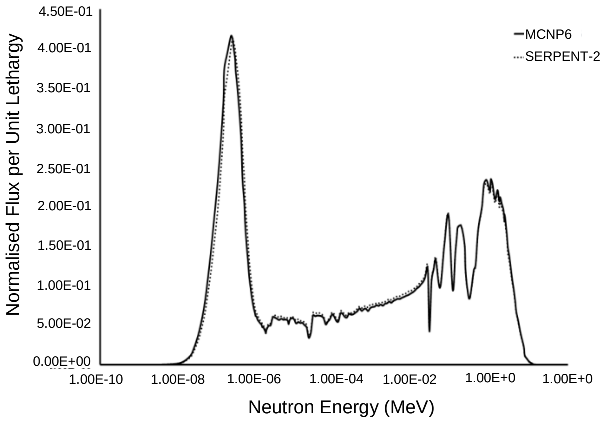


Fig. 3. PCMSR neutron spectrum profile.

Temperature coefficient of reactivity (TCR)

TCR value is broken down into FTC and MTC. Both values are shown in Figs. 4 and 5.

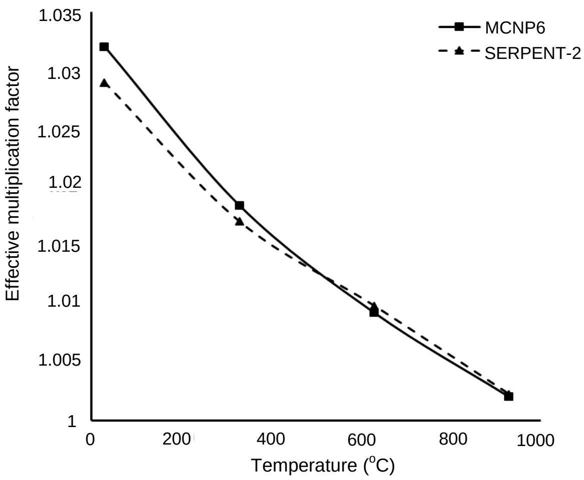


Fig. 4. FTC of PCMSR.

FTC is negative for all temperature range in both codes, and the values are similar for both codes. FTC consists of the Doppler feedback coefficient and fuel density coefficient. Doppler coefficient is relatively better in the harder spectrum, as it favors Th resonance over ^{233}U resonance. Since PCMSR has a relatively hard spectrum, the Doppler coefficient may be improved. The negative FTC is consistent with various calculations with different MSR core designs [5,7, 28-30].

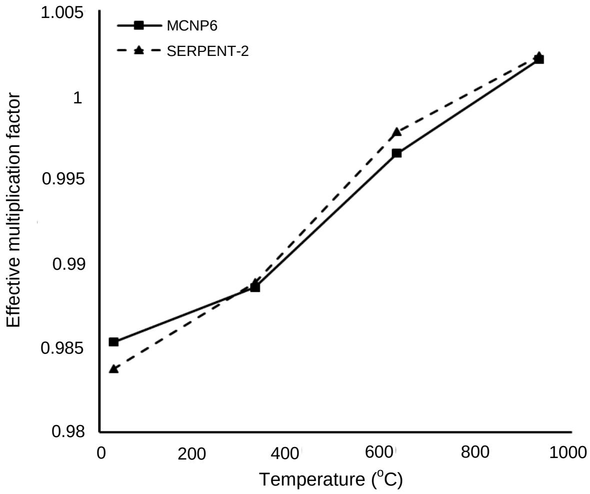


Fig. 5. MTC of PCMSR.

The reduction of fuel density due to temperature increase causes the fissile nuclide to be partially ejected from the core, reducing the macroscopic fission cross-section in the core. In an over-moderated core, an increased moderator-to-fuel ratio does not result in increasing fission, as the neutron spectrum softening is insufficient to compensate for the loss of fissile fuel from the core.

Conversely, MTC values are always positive for all cases. Graphite moderator heating causes a spectral shift to the thermal part so that fission reaction rates increase. The positive feedback is quite strong as the PCMSR core uses high-density graphite at 2.2 g/cm^3, whereas other MSRs generally use lower graphite density at around 1.84-1.86 g/cm^3 [10,28], exception for SD-TMSR that uses similarly high graphite density [30]. The effect will be less apparent in larger core radius as moderator volume decreases and spectrum hardens.

In total, despite a positive MTC value, the TCR of PCMSR is negative. It ensures that PCMSR fulfils the first inherent safety criteria. The Serpent calculation resulted in less negative TCR, caused by the fact that the calculated MTC is more positive than MCNP6 calculation, which is further exacerbated by less negative FTC. These total TCR values are lower than MSBR but comparable with SD-TMSR [7,30]. The obtained TCR value also invalidates the initial neutronic calculation of PCMSR, as previously discussed. The most negative TCR value calculated in MCNP6 is only 5.1 % of the required value to be able to prove that the SRAC calculation is valid.

The total TCR value is provided in Table 4.

Table 4. Total TCR value of PCMSR.

Temperature Coefficient	Codes	
	MCNP6	Serpent-2
FTC (pcm/K)	-3.22	-2.88
MTC (pcm/K)	+1.88	+2.09
TCR (pcm/K)	-1.34	-0.79

Void coefficient of reactivity (VCR)

VCR value is shown in Fig. 6. At the void range of 0-10 %, the VCR is positive. This applies to both MCNP6 and Serpent-2 results. Higher void ranges show negative value, i.e., higher void formation in the fuel salt resulted in lower reactivity. This is the indicator that the PCMSR core is not necessarily in over-moderated condition for all cases. Instead, the core is actually in slight under-moderated condition. When fuel density is reduced, the moderator-to-fuel ratio increases and softens the spectrum, increasing fission reaction. In void fraction more than 10 %, however, the lost fissile cannot be compensated by neutron spectrum, and reactivity is subsequently decreased even more drastically in higher fraction.

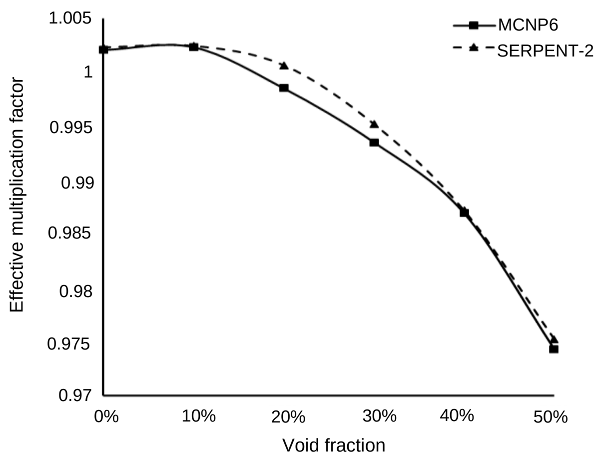


Fig. 6. VCR of PCMSR.

VCR value from 0-10 % void range is higher in MCNP6 calculation, around twice that of Serpent-2 result. Nevertheless, for both sets of calculations, a positive VCR value cannot be sufficiently compensated by a negative TCR value. Thus, it can be concluded that the PCMSR core does not necessarily fulfil inherent safety criteria at all conditions. To ensure that inherent safety is truly fulfilled, the core design needs reconsideration in terms of moderation conditions by adjusting the fuel channel radius. VCR is not discussed in publications about MSBR and SD-TMSR, but one analysis on FUJI-12 MSR [31] shows a positive VCR. There is no explanation on whether the VCR remains constant as void fraction increases, nevertheless, and therefore the complete comparison is impossible.

Detailed k_{eff} change against void fraction is provided in Table 5.

Table 5. VCR value of PCMSR.

Void fraction range	MCNP6	Serpent-2
0-10 %	+2.59	+1.39
10-20 %	-38.07	-17.85
20-30 %	-50.50	-54.73
30-40 %	-67.11	-81.64
40-50 %	-131.25	-123.82

Conversion ratio (CR)

The last parameter to be calculated was CR. The value was calculated using Eq. 1 at BOC and then compared with the initial SRAC calculation. The result is shown in Table 6.

Table 6. Comparison of CR value of PCMSR.

Calculated by	CR value of PCMSR
Initial calculation (from [17])	1.14
MCNP6	0.977
Serpent-2	0.992

While MCNP6 and Serpent-2 calculations are in good agreement, both values show another huge discrepancy between initial and new calculations. Initial calculation implied that PCMSR core can breed with a relatively large breeding ratio, even when compared to other MSR designs with larger core sizes [7,29,30]. However, new calculations reveal that the PCMSR core is unable to even merely break even. The CR value is below unity, despite the fact the calculation was assuming ideal conditions. Therefore, the studied PCMSR design can only be operated as a high conversion reactor instead of a breeder reactor.

This result is not unexpected in two ways. First, the initial CR value is remarkably large, as previously mentioned, for such a small core. The largest obtainable CR for large-core thermal MSR is around 1.1 [29,30]. Even MSBR can only achieve CR for about 1.062 [32]. Thereby, the notion that small size PCMSR core can obtain CR of 1.1 without special design adjustments is rightly questionable. Second, the small core size of PCMSR resulted in poor moderation and hard spectrum, as discussed previously. Neutron leakage is understandably high, and therefore neutron utilization for breeding is inefficient. In a poorly moderated, high leakage core, the fertile fuel cannot capture sufficient neutrons to breed more fuel than it consumes. Therefore, its CR value was understandably unable to surpass unity.

In short, the studied PCMSR design cannot be defined as a breeder reactor, as it failed to reach CR above unity. To be able to breed from thorium, major geometrical modifications must be applied.

CONCLUSION

Initial neutronic calculation of PCMSR was compared using probabilistic code MCNP6 and Serpent-2. From the findings, many discrepancies were found which resulted in the conclusion that the initial calculation was flawed and inaccurate. First, PCMSR was able to be critical in a lower fissile concentration (0.495 mole%) compared to the initial calculation (0.6 mole%). Second, although the TRC value was negative, the VCR value was positive up until the 10 % void fraction, implying that inherent safety criteria were not satisfied in all conditions. Third, the CR value was less than unity, due to high neutron leakage and inefficient neutron moderation shown by considerably hard neutron spectrum for a thermal reactor. In conclusion, the initial PCMSR core calculation using deterministic code SRAC2006 was inaccurate. For PCMSR to be able to be defined as a thermal breeder reactor, its core geometry must be modified to improve moderation and reduce neutron leakage. This issue must be resolved in future works.

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AUTHOR CONTRIBUTION

R. Andika Putra Dwijayanto and M. Rizki Oktavian are the main contributors of the article. All authors read and approved the final version of the paper.

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