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MCNP performance on neutronic calculation of VERA benchmark cases

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Original Research Abstract:

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1. Introduction

Indonesia is the largest archipelagic country in the world with most of its territory consisting of small islands. The need for electrical energy on these small islands was only a few hundred megawatts of electricity (MWe) and the power demand in these remote areas [1] can be fulfilled by Small Modular Reactors (SMR). SMR has the advantage that it can be built in remote areas that are difficult to reach and do not have the infrastructure to transport fuel. Another advantage of SMR technology is a simpler modular design, developed with passive safety systems, long life cycles, and resistance to proliferation [2].

SMRs become a trend in advanced nuclear reactor technology, especially to reduce the initial capital cost investment typically required by large-scale nuclear power plants [3]. Advanced SMRs can provide affordable nuclear power options while ensuring safe and clean energy. Furthermore, the advanced SMR technology offers not only a simpler modular design in nuclear power generation applications but also safer while being cheaper and easier to manufacture relative to a typical large-scale reactor by the economy of scale [4, 5]. Water-cooled SMR represents a mature technology considering that most of the nuclear power plants operating today are water-cooled reactors. Therefore, around twentyfive designs of water-cooled SMR use either light water or heavy water technologies for large to small remote grid applications, also for district heating [6].

The SMR design was proposed since its simpler and safer

safety concept relies on a passive system with safety characteristics inherent in the reactor [7]. In recent years, research to design SMRs was promoted through the Virtual Environment for Reactor Applications (VERA) benchmark cases [8]. VERA benchmark cases have been introduced by Oak Ridge National Laboratory (ORNL) and detailed guidelines have been provided including the burnup chain data for a depletion analysis. The VERA benchmark cases consist of 9 cases of single pin (SP) and 16 cases of fuel assembly (FA) with various fuel temperatures, ²³⁵U enrichments, control rods, and burnable poisons. These benchmark cases can be used to validate the neutron transport code's capability in calculating criticality and neutronic parameters.

Various studies on the modeling and simulation of VERA benchmark cases have been performed since the benchmark results were provided by Kim in 2018 [9]. Park consistently compared depletion calculations between four neutronic analysis codes with the VERA depletion problems [10]. Yu verified the OpenMC capability using the VERA depletion benchmark for all 26 cases including 10 pin-cell cases and 16 fuel assembly cases, and also carried out comparisons with published KENO results [11]. In Park's study, McCARD burnup analyses for the VERA depletion benchmarks were performed to examine its newly implemented depletion analysis modules [12]. Albugami presented results to VERA benchmark problems utilizing the OpenMC code and showed a code-to-code comparison with CASL VERA data [13]. Collins simulated the BEAVRS benchmark using VERA [14] while Nguyen presented a benchmark solution to the VERA problem using MCS codes with a study consisting of code-to-code comparisons with KENO-VI and Serpent 2 [15]. Mai analyzed several VERA benchmark problems with the deterministic transport code STREAM for 2D and 3D calculations [16]. All the codes performed their depletion capability to simulate the VERA benchmark with good results. In this study, it was expected that the MCNP6 wolud show its ability to accurately predict

the criticality and nuclide composition of VERA benchmark fuel.

The purpose of this paper was to develop fuel assembly from VERA benchmark cases using MCNP Monte Carlo code and providing the Doppler temperature coefficient (DTC) of reactivity, the moderator coefficient of reactivity (MTC) and effective delayed neutron fraction (β_{eff}) on each case. The VERA 2B and VERA 2P were selected as a representation for a typical fuel assembly of light water reactor (LWR) configurations. These benchmark cases were 2D fuel lattices without and with gadolinium. The MCNP code was chosen due to its flexible modeling capability and neutron transport solved using the Monte Carlo method with continuous energy nuclear data library [17]. MCNP tracks the neutron history started from the initiated source particle position and fission neutron while ENDF/B-VII.1 nuclear data library was used in this study, also the CINDER module was used to calculate fuel burnup for up to 60 MWd/kg [18, 19]. The neutronic parameters resulting from both benchmark cases can then be compared with VERA benchmark results and the various studies using other neutronic codes.

2. Materials and methods

2.1 VERA benchmark cases

VERA benchmark cases have been developed to test the performance of neutronic code, evaluate computational model, and validate their result by performing a code-to-code comparison. Table 1 presents the geometrical and material data for VERA 2B and 2P benchmark cases consisting of a fuel assembly on 17×17 fuel pins configuration, made up of 264 fuel rods, 24 guide tubes, and one instrumentation tube.

2.2 Calculation model

In this work, a series of calculations have been carried out from VERA benchmark cases using MCNP code with ENDF/B-VII.1 library to evaluate users' capability to develop those cases. MCNP was a well-established Monte

 Table 1. Geometry and material data for VERA 2B and 2P benchmark cases.

Core					
Pressure (bar)	155.13				
Power density (W/gU)	40.00				
Fuel assembly power (MW/cm)	0.050324728				
Assembly pitch (cm)	21.5000				
Pin pitch (cm)	1.2600				
Fu	lel				
Pellet radius (cm)	0.4096				
Material	UO ₂ (3.1% ²³⁵ U)				
Density (g/cm ³)	10.2570				
Gadolinium rod					
Pellet radius (cm)	0.4096				
Material	$UO_2 (1.8\%^{235}U) + 5\% Gd_2O_3$				
Density (g/cm ³)	10.1110				
Cladding					
Inner radius (cm)	0.4180				
Outer radius (cm)	0.4750				
Material	Zircaloy-4				
Density (g/cm ³)	6.5600				

Carlo transport code that can model 3-dimensional complex geometry including the reactor core and all its components to analyze interactions between radiation and matter using its continuous neutron energy spectra. MCNP has successfully demonstrated its capability in simulating the neutronic behavior of various reactors [20–37].

The VERA 2B fuel assembly consists of 264 UO₂ fuel pins with $3.1\%^{235}$ U enrichment while the VERA 2P fuel assembly uses 240 fuel pins of this type with additional 24 fuel pins of mixed UO₂+Gd₂O₃, with $1.8\%^{235}$ U enrichment and 5% wt. of Gd. Gadolinium (Gd₂O₃) was used as a burnable poison since it was a neutron absorber that burned (depleted) during reactor operation. From these models, it was known that the VERA 2P case would have lower fissile material content and lower heavy metal loading due to these 24 mixed fuel pins.

The VERA benchmark cases consist of a fuel pin which was a fuel rod surrounded by a helium gap inside a Zircaloy-4 clad with the dimensions mentioned in Table 1. Water as a coolant and moderator with a boron concentration of 1300 ppm surrounds the fuel pin, making up a fuel lattice with a pitch of 1.2600 cm. The moderator, cladding, and fuel temperatures were set to 600 K and 900 K for the VERA 2P fuel assembly while for the VERA 2B was set to 600 K. The guide tube and instrumentation tube as part of the structure were designed to guide the movement of the control rod and provide space for detectors, in-core instrumentation, and other measurement tools for monitoring the reactor core. Both tubes were modeled by modeling a tube with the size mentioned in Table 1 and the same lattice pitch as the fuel pin lattice pitch. The MCNP model for the fuel pin, guide tube, and instrumentation tube is shown in Figure 1 while the atomic number density for each material is presented in Table 2.

The VERA 2B and 2P benchmark cases were fuel assem-

blies arranged in a square lattice of 17×17 configuration with a fuel assembly size of 21.50 cm. These fuel assemblies were modeled by arranging 264 standard fuel pins for case 2B while for case 2P, the 240 standard fuel pins and 24 fuel with gadolinia pins were used, with both cases using 24 guide tubes and 1 instrumentation tube. The MCNP models for both cases are seen in Figure 2.

The total neutron histories employed for k_{inf} calculations was 125 million neutrons using 500,000 neutrons per cycle with 300 total cycles (50 inactive), giving a statistical uncertainty of around 6 pcm. The initial fission neutron source was located at the center of the fuel pin, making a 264-point source at the middle of each fuel pin. Thermal scattering data $S(\alpha, \beta)$ for light water was applied while reflective boundary conditions were used on all six surfaces of the fuel assembly. The burnup calculation was performed with a thermal power density of 40.0 W/gU, analog to 18.41 MW for the 365.76 cm height of the modeled fuel assembly. The burnup calculation starts from 0.0, 0.01, 0.25, 0.50, 0.75 to 1.0 MWd/kgU, followed by the interval of 1 MWd/kgU for 1 - 20 MWd/kgU and the interval of 2.5 MWd/kgU for 20-60 MWd/kgU. The Beginning of Cycle (BOC) was defined as 0 MWd/kgU while the Middle of Cycle (MOC) was 30 MWd/kgU and the End of Cycle (EOC) for 60 MWd/kgU. The MCNP simulation was carried out using a workstation with specification Intel(R) Core(TM) i7-X5960CPU, 3.0GHz-6core, RAM 32GB, with execution time of \sim 2460 minutes for each case.

The calculated multiplication factors will be compared to benchmark results (McCARD) [9] and previous studies that use OpenMC [11], MCS [15, 38], and STREAM [19, 39] codes. OpenMC was an open-source Monte Carlo transport code, while MCS was developed by the Ulsan National Institute of Science and Technology (UNIST) which both could solve 3-D continuous-energy neutron physics code



Figure 1. MCNP model for fuel cell, guide tube and instrumentation tube.

for particle transport based on the Monte Carlo method. STREAM was a deterministic neutron transport analysis code developed to use the method of characteristics to solve the multi-group neutron transport equation for 2D and 3D core analysis, also developed by UNIST.

The Doppler temperature coefficient (DTC) of reactivity, the moderator coefficient of reactivity (MTC), and the effective delayed neutron fraction (β_{eff}) were also calculated for each case. The DTC also known as fuel temperature reactivity coefficient came from the Doppler broadening in the resonance region of neutron interaction cross-sections of the fertile material (²³²Th, ²³⁸U, ²⁴⁰Pu). While MTC was correlated with changes in moderator temperature and density both MTC and DTC were considered dominant temperature reactivity coefficients which became part of the inherent safety parameters in nuclear reactors. The DTC and MTC were calculated by the following equation:

$$DTC = \frac{k_2 - k_1}{k_2 \times k_1} \frac{1}{\Delta T}$$
(1)

$$MTC = \frac{k_3 - k_1}{k_3 \times k_1} \frac{1}{\Delta T}$$
(2)

with k_1 was the multiplication factor with moderator and fuel temperature at 600 K for VERA 2B and 900 K for

VERA 2P, while k_2 was calculated with moderator temperature at 600 K while fuel was at 1200 K. k_3 was calculated with moderator temperature of 565 K for 600 K fuel temperature for VERA 2B and 900 K fuel temperature for VERA 2P. From this equation, negative values in both DTC and MTC correlate with a decrease in reactivity when its corresponding physical temperature increases.

On another hand, the effective delayed neutron fraction (β_{eff}) was calculated using the Iterated Fission Probability (IFP) that has been implemented on MCNP.

3. Results and discussion

The infinite multiplication factor (k_{inf}) or criticality result of VERA 2B and 2P benchmark cases is seen in Table 4 while Table 4 shows its comparison to other codes. In comparison to the MCS and STREAM code, MCNP shows a good agreement at the BOC with a difference of less than 100 pcm. The Monte Carlo method was implemented on MCNP and MCS gives a different response on depletion calculation so that the k_{inf} at MOC and EOC were differentiated on both codes within the range of 200 – 700 pcm. The difference between MCNP to STREAM shows a great discrepancy for case 2P of fuel assembly with burnable absorber during the BOC that can be rooted in the difference in multigroup cross sections generated for STREAM and its

Table 2. Atomic number density for each material.

Fuel UO ₂ (3.1% ²³⁵ U enrichment)						
²³⁴ U	6.11864E-06	²³⁶ U	3.29861E-06	¹⁶ O	4.57642E-02	
²³⁵ U	7.18132E-04	²³⁸ U	2.21546E-02			
Fue	$UO_2 + Gd_2O_3$	(1.8% 235	U enrichment, 5	% Gd coi	ncentration)	
234		152 ~ 1		157 ~ 1		
²³⁴ U	3.18096E-06	¹⁵² Gd	3.35960E-06	¹⁵⁷ Gd	2.62884E-04	
²³³ U	3.90500E-04	¹⁵⁴ Gd	3.66190E-05	¹⁵⁰ Gd	4.17255E-04	
²³⁰ U	1.79300E-06	¹⁵⁵ Gd	2.48606E-04	¹⁰⁰ Gd	3.67198E-04	
²³⁸ U	2.10299E-02	¹⁵⁰ Gd	3.43849E-04	100	4.53705E-02	
			Helium			
⁴ He	2.68714E-05					
		(Cladding			
⁹⁰ Zr	2.18865E-02	¹¹⁸ Sn	1.16872E-04	⁵² Cr	6.36606E-05	
⁹¹ Zr	4.77292E-03	¹¹⁹ Sn	4.14504E-05	⁵³ Cr	7.21860E-06	
⁹² Zr	7.29551E-03	¹²⁰ Sn	1.57212E-04	⁵⁴ Cr	1.79686E-06	
⁹⁴ Zr	7.39335E-03	¹²² Sn	2.23417E-05	¹⁷⁴ Hf	3.54138E-09	
⁹⁶ Zr	1.19110E-03	¹²⁴ Sn	2.79392E-05	¹⁷⁶ Hf	1.16423E-07	
¹¹² Sn	4.68066E-06	⁵⁴ Fe	8.68307E-06	¹⁷⁷ Hf	4.11686E-07	
¹¹⁴ Sn	3.18478E-06	⁵⁶ Fe	1.36306E-04	¹⁷⁸ Hf	6.03806E-07	
¹¹⁵ Sn	1.64064E-06	⁵⁷ Fe	3.14789E-06	¹⁷⁹ Hf	3.01460E-07	
¹¹⁶ Sn	7.01616E-05	⁵⁸ Fe	4.18926E-07	¹⁸⁰ Hf	7.76449E-07	
¹¹⁷ Sn	3.70592E-05	⁵⁰ Cr	3.30121E-06			
Moderator (1300 ppm boron, 600 K)						
¹⁶ O	2.33753E-02	^{10}B	1.00874E-05			
^{1}H	4 67505E-02	^{11}B	4 06030E-05			



Figure 2. MCNP model for VERA benchmark cases.

treatment for burnable absorber modeled within STREAM. By comparing the calculated results with benchmark data by McCARD, it was found that the results show a good agreement at the BOC, but at MOC-EOC the deviations from the McCARD values were observed to be within the range of 175 - 1500 pcm. This high deviation to benchmark data might come from the difference in nuclear data being used for burnup calculation (depletion chain and nuclear energy-branching ratio) which was ENDF/B-VII.0 for McCARD while our MCNP used ENDF/B-VII.1. Previous studies also showed that the differences between the ENDF/B-VII.0 and ENDF/B-VII.1 were around 30 pcm on fresh pin cell problem [15]. In comparison to other codes, k_{inf} value at BOC calculated using MCNP for VERA 2B case shows a good agreement compared to KENO, Serpent,

and OpenMC with a difference of less than 60 pcm while for VERA 2P case with a difference of less than 90 pcm. Figure 3 illustrates the changes in k_{inf} during fuel burnup for both VERA 2B and 2P benchmark cases that show the burnable poison acting on case 2P to reduce k_{inf} at the beginning of cycle. The sudden k_{inf} drop in both cases at the BOC correlates to the production of ¹³⁵Xe and ¹⁴⁹Sm fission products that absorb neutrons during reactor operation with their equilibrium concentration. The k_{inf} of VERA 2P assembly peaked at ~ 1.02 around 11 MWd/kg when gadolinium (¹⁵⁵Gd and ¹⁵⁷Gd) was fully depleted, and the decreasing of k_{inf} followed similar trends to the 2B case. Table 5 summarizes the Doppler temperature coefficient (DTC) of reactivity, the moderator coefficient of reactivity (MTC), and the effective delayed neutron fraction (β_{eff})

Table 3. Comparison of calculated kinf by MCNP with MCS [38]; STREAM [39], and McCARD [9].

						Difference* (pcm)		
VERA	Burnup	MCS	Stream	McCARD	MCNP			
cases	condition					with MCS	with Stream	with McCARD
VERA 2B	BOC	1.18291 ± 0.00004	1.18204	1.182710	1.18208 ± 0.00006	-83	+4.0	-6.3
	MOC	0.90010 ± 0.00003	0.90087	0.895640	0.89740 ± 0.00006	-270	-347	+176
	EOC	0.77322 ± 0.00003	0.77438	0.761262	0.77029 ± 0.00006	-293	-409	+902.8
VERA 2P	BOC	0.92677 ± 0.00003	0.92734	0.919643	0.92067 ± 0.00006	-610	-667	+102.7
	MOC	0.87890 ± 0.00003	0.87944	0.885197	0.88344 ± 0.00006	454	+400	-175.7
	EOC	0.74304 ± 0.00003	0.74447	0.760579	0.74568 ± 0.00006	264	+121	-1489.9

*Relative difference = (MCNP-MCS; Stream; McCard) ×100000 pcm.

Fable 4. Comparison of calculated k_i	f by MCNP (ENDF VII.1)	with KENO, Serpent and O	penMC (ENDF VII.0) [11].
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						Difference* (pcm)		m)
VERA cases	Burnup condition	KENO	Serpent	OpenMC	MCNP	with KENO	with Serpent	with OpenMC
VERA 2B	BOC	1.18240 ± 0.00012	1.18156 ± 0.00013	1.18217 ± 0.00016	1.18208 ± 0.00006	-32	+52	-9
VERA 2P	BOC	0.91993 ± 0.00016	0.92017 ± 0.00017	0.91983 ± 0.00012	0.92067 ± 0.00006	+74	+50	+84

*Relative difference = (MCNP-KENO; Serpent; OpenMC) ×100000 pcm.



Figure 3. *K*_{inf} of VERA benchmark cases

in each case. Table 5 shows that the DTC and MTC were all negative, which is below $-4 \times 10^{-5} \Delta k/k \text{ K}^{-1}$ for the VERA 2B case and below $-7 \times 10^{-6} \Delta k/k \text{ K}^{-1}$ for the 2P case. Both became more negative as the fuel burned, ensuring the safety of the reactor from the beginning of reactor operation through the end. Table 5 also confirms that the VERA 2B assembly without Gd₂O₃ content shows a more negative DTC and MTC compared to the VERA 2P assembly containing Gd₂O₃ fuel rods. Since these lower DTC and MCT of the 2P case happened during subcritical conditions at the BOC, the 2P fuel assembly was already reducing core overall reactivity during this burnup step. The effective delayed neutron fraction (β_{eff}) reflects the fraction of delayed neutrons relative to the total neutron population in the reactor, and it was related to the controllability of the reactor. Table 5 shows that the β_{eff} values of VERA 2B and VERA 2P were within the range of 670 - 685 pcm since both cases use ²³⁵U fissile nuclear material which has similar fractions of delayed neutrons and delayed neutron precursors. The decrease in β_{eff} value during fuel burnup comes from other fissile materials being produced from the transmutation of ²³⁸U, i.e. ²³⁹Pu and ²⁴¹Pu in combination with the remaining 235 U within the fuel assembly.

The depletion of heavy metals in the VERA benchmark cases was interesting to evaluate since the use of uranium could produce plutonium isotopes through a transmutation process that becomes the main contribution to fuel proliferation analysis. Since uranium and plutonium isotopes were essential for reactor operation by sustaining the nuclear chain reaction, Figure 4 and Figure 5 show both isotopic elements in each case. As previously mentioned in methodologies, the ²³⁵U concentration of VERA 2B fuel assembly at BOC was higher than VERA 2P assembly as could be seen in Figure 4, but towards the EOC their concentrations were almost the same, ~ 1000 gr, which came from the use of 24 mixed uranium (lower enrichment) and gadolinium fuel pins. The use of Gd₂O₃ absorbs neutrons but the depletion gradients of ²³⁵U and ²³⁸U were not fully affected since the number of fissions should be maintained to achieve the same amount of power, so the neutron flux will be increased to compensate for absorbed neutrons by gadolinia at the beginning of cycle, and these neutron flus not only induce fission but also transmutation on fuel material.

Figure 5 illustrates five plutonium isotopes, i.e. ²³⁸Pu, which comes from the beta decay of ²³⁸Np while ²³⁸Np comes from irradiated ²³⁷Np, and ²³⁷Np comes from irradiated ²³⁶U. ²³⁸Pu can be used for long-life nuclear batteries, as well as providing a long-lived heat source to power NASA space missions. The ²³⁸Pu and ²³⁹Pu concentration in VERA 2B assembly at EOC was around thousand times more than that of the VERA 2P assembly which comes from the higher ²³⁸U in VERA 2B at first. It can be seen

Table 5. Temperature coefficient of reactivity and effective delayed neutron fraction (β_{eff}).

VERA cases	Burnup condition	Doppler coefficient of reactivity (DTC, $\Delta k/k \text{ K}^{-1}$)	Moderator coefficient of reactivity (MTC, $\Delta k/k \ K^{-1}$)	Effective delayed of neutron fraction (β_{eff})
	DOC	4.02427E.05	4 00 4755 05	0.00005 + 0.00010
VERA 2B	BOC	-4.03437E-05	-4.094/5E-05	0.00685 ± 0.00010
	MOC	-6.01477E-05	-9.47981E-05	0.00478 ± 0.00008
	EOC	-6.98148E-05	-1.75884E-04	0.00426 ± 0.00008
VERA 2P	BOC	-2.36304E-05	-7.41383E-06	0.00670 ± 0.00009
	MOC	-2.78369E-05	-1.11634E-04	0.00479 ± 0.00008
	EOC	-3.22049E-05	-1.83914E-04	0.00426 ± 0.00008



Figure 4. Uranium concentration of benchmark cases.



Figure 5. Plutonium concentration of benchmark cases.

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in Figure 5(c-e) that the ²⁴⁰Pu, ²⁴¹Pu, and ²⁴²Pu VERA 2P were higher than VERA 2B with similar trends but delayed that might come from the hardened neutron spectrum shifting since thermal neutrons absorbed by gadolinia. ²⁴¹Pu was a formed when ²⁴⁰Pu captures a neutron while ²⁴²Pu was produced by successive neutron capture of ²³⁹Pu, ²⁴⁰Pu, and ²⁴¹Pu. Like some other plutonium isotopes, especially ²³⁹Pu, ²⁴¹Pu was fissile, with a neutron absorption cross section about one-third larger than ²³⁹Pu, and a fission probability around 73% similar to the neutron absorption.

4. Conclusion

The MCNP calculation of VERA benchmark cases has been conducted and was in good agreement with the MCS, STREAM, McCARD, and other neutron transport codes. In comparison to the MCS and STREAM, the infinite multiplication factor (k_{inf}) calculated by MCNP shows a good agreement at the BOC with a difference of less than 100 pcm while at MOC and EOC were within the range of 200 - 700 pcm. In comparison to the benchmark data by McCARD, it was found that the results show a good agreement at the BOC, but at MOC-EOC the deviations were within the range of 175 - 1500 pcm which might come from differences in nuclear data being used. The DTC of both cases were negative which was lower than $-4 \times 10^{-5} \Delta k/k \text{ K}^{-1}$ for VERA 2B case and lower than $-2 \times 10^{-5} \Delta k/k \text{ K}^{-1}$ for VERA 2P case. On another hand, the MTC was lower than $-4 \times 10^{-5} \Delta k/k \ \mathrm{K}^{-1}$ and $-7 \times 10^{-6} \Delta k/k \text{ K}^{-1}$ for VERA 2B and 2P cases respectively, while both became more negative as fuel burned. The β_{eff} values of VERA 2B and VERA 2P were 685 and 670 pcm respectively, since both use ²³⁵U fissile nuclear material, and slightly decrease caused by other fissile material being produced through fuel burnup. The ²³⁵U concentration of ²³⁵U concentration of VERA 2B fuel assembly at BOC was around ~ 600 gr higher than VERA 2P assembly, with almost the same amount on EOC, around \sim 1000 gr since VERA 2P case has lower fissile material content and lower heavy metal loading due to 24 mixed fuel pins. The discrepancy in plutonium concentration between VERA 2B and 2P cases comes from the hardened neutron flux on case 2P caused by mixed uranium-gadolinia fuel pin. It can be concluded that these findings can be used for further calculation on the whole core analysis.

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Authors Contributions

All the authors have participated equally in the intellectual content, conception and design of this work or the analysis and interpretation of the data, as well as the writing of the manuscript.

Availability of data and materials

Data presented in the manuscript are available via request.

Conflict of Interests

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

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