NEUTRONIC ASSESSMENT ON THE USE OF ADVANCED COATED PARTICLES IN A FLUIDIZED BED NUCLEAR REACTOR

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ABSTRACT
Neutronic calculations have been performed to a fluidized bed nuclear reactor that uses advanced coated particles to improve its endurance against irradiation and high temperature. The calculation is intended to determine whether reactor characteristics have been signiﬁcantly compromised. The characteristic of the reactor is assessed by investigating the change in criticality from packed bed condition to a full expansion of the particle bed. The particle used in this calculation was based on the standard TRISO fuel particle as being used in the HTR-10 reactor, and the use of advanced fuel particle was performed by replacing the SiC layer by a ZrC layer. A packed bed of 50 cm high was used in this research with an additional 20 ppm of boron in the side reﬂector. At packed condition, replacing SiC by ZrC in TRISO particles signiﬁcantly decreases the criticality with a range of -336 ± 138 pcm to -2809 ± 99 pcm. Calculation on expanded bed shows similar behaviors, in which case the decrease in reactivity spans from -269 ± 101 pcm to -1286 ± 121 pcm. The use of standard TRISO particles and advanced coated particles might create positive reactivity coefﬁcients for particular height of expanded beds.

Keywords: ﬂuidized bed Nuclear reactor, advanced coated particles, neutronics, ZrC, SiC, SERPENT.

INTRODUCTION
Small and modular reactors are desirable for developing countries whose electrical infrastructure is not adequate. The reasons for these are due to: (i) its ﬂexibility to develop, plan and construct the plant, (ii) increased safety level based on passive features, (iii) easy in operation and maintenance, (iv) economic competitiveness, (v) easier plant siting close to industrial and/or populated areas, and (vi) suitability for use in areas with or without grids [1], [2].

A ﬂuidized bed nuclear reactor (FLUBER) is one of high temperature reactors, which uses helium gas as coolant. The fuel is uranium dioxide in the form of coated particles, called TRISO. Those particles are suspended in graphite tube cavity. The ﬂuidized bed reactor is design in such a way that the reactor is subcritical when the helium gas does not ﬂow into the core. Criticality only occurs when the coolant ﬂows into the core and lifts up the TRISO particles. Recent researches have shown that the ﬂuidized bed nuclear reactor can be operated as should be and can be controlled by adjusting the coolant ﬂow rate [3-7]. This feature reduces a need of active control rod mechanism.

Some issues, however, need to be addressed, for example, regarding the strength and endurance of TRISO particles during ﬂuidization process. In a ﬂuidized bed where particle-particle and particle-wall collisions occur, integrity of the particles must be maintained and failure probability of the particles should be kept as low as possible. Furthermore, the ﬂuidized bed nuclear reactor is designed for long-term operation with high discharge fuel burnup. For such reasons, mechanical stability of the particles for long irradiation time becomes a very important factor.

Some options have been proposed to improve the performance of the TRISO particles, for example by using ZrC as coated materials to replace SiC. ZrC has higher melting point than SiC and it also has better performance against irradiation [8]. ZrC is also mechanically more stable than SiC [9]. Advanced coated particles have also been recommended for high temperature reactor, either by replacing the whole layers of SiC with ZrC (TRIZO particles), by adding a refractory buffer layer, or by adding ZrC layer between the fuel kernel and the graphite buffer [10-12].

The superior thermal and mechanical properties of ZrC are advantageous for its application in a ﬂuidized bed nuclear reactor. From a neutronic point of view, however, Zr has higher capture cross-section (n, γ) as compared to Si. This will inﬂuence the neutron economy. It is thus very important to investigate the performance of advanced coated particle in term of neutronics in a ﬂuidized bed nuclear reactor. Will an addition of Zr lead to signiﬁcant decrease in performance? Should the design be changed to accommodate such phenomena?

This article describes the neutronic assessment of a ﬂuidized bed nuclear reactor, fuelled with standard TRISO particles and its possible replacement with advanced coated particles. The structure of this article is as follows. Section 2 gives an overview of the reactor. The methods in modeling and calculation using the Monte Carlo code SERPENT are described in Section 3. The results of the simulations are explained in Section 4 and the ﬁnal section gives the conclusions and remarks for future research.

DESCRIPTION OF THE REACTOR
FLUBER is an innovative nuclear reactor employing gas-solid ﬂuidization concept. The reactor consists of TRISO fuel particles, ﬁlled into a cavity in a graphite cylindrical reﬂector. Helium is used as coolant as well as ﬂuidization medium. If the coolant does not ﬂow,
or the upward flow is too small, the fuel particles are suspended at the bottom of the core and the reactor is subcritical due to lack of neutron moderation. When the coolant flow increases, the fuel particles are fluidized, the core expands and the reactivity increases along with an increase in moderating process at the graphite reflector [3]. General specification of FLUBER is shown in Table-1 and the schematic of the reactor in both packed and expanded condition can be seen in Figure-1.

<table>
<thead>
<tr>
<th>Table-1. FLUBER specification [4].</th>
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<tbody>
<tr>
<td>Core radius [cm]</td>
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<td>Core height [cm]</td>
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<tr>
<td>Reactor total height [cm]</td>
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<tr>
<td>Axial and radial reflector width [cm]</td>
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<tr>
<td>Helium pressure [bar]</td>
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<tr>
<td>Maximum power (at full expansion) [MW]</td>
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<tr>
<td>Maximum fuel temperature [K]</td>
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<td>Maximum gas temperature [K]</td>
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<table>
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<tr>
<th>Table-2. Characteristic of standard TRISO fuel particles [13].</th>
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<tr>
<td>Material</td>
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<tr>
<td>--------------------</td>
</tr>
<tr>
<td>UO₂ kernel</td>
</tr>
<tr>
<td>Porous carbon layer</td>
</tr>
<tr>
<td>Inner pyrolytic carbon layer</td>
</tr>
<tr>
<td>SiC layer</td>
</tr>
<tr>
<td>Outer pyrolytic carbon layer</td>
</tr>
<tr>
<td>Fuel enrichment [wt %]</td>
</tr>
<tr>
<td>Natural boron impurity in kernel [ppm]</td>
</tr>
<tr>
<td>Natural boron impurity in graphite [ppm]</td>
</tr>
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The use of ZrC as structural and coated materials in TRISO particle is intended to replace or as an additional substance to the SiC layer. ZrC has attractive properties for nuclear fuel as its melting point above 3,500 K, large thermal conductivity at high temperature and good resistance against chemical corrosion by fission products. With such desirable properties, it is expected that ZrC may withstand temperature higher than 1873 K at operational and fuel burnup larger than 200 GWd/MTU [14]. Investigations to compare the strength of SiC and ZrC against irradiation showed also that ZrC could maintain its crystalline structure at high fluence as compared to SiC [15].

There are several types of proposed advanced coated particles [16]. The first type is replacing the whole layer of SiC by ZrC. Such fuel particles are also called ZrC TRISO or sometimes it is called TRIZO. Another type is by replacing the fuel kernel with UO₂*, which is similar to a common TRISO particle but the UO₂ kernel is coated with carbon and thin layer of ZrC of 10 μm in width [17]. Another type of UO₂* is by dispersing ZrC (with equal amount of 10 μm layer) in the graphite buffer layer.

**METHODOLOGY**

The particles and the core were modeled and simulated using a Monte Carlo code, SERPENT [18]. Figure-2 shows the scheme of FLUBER plotted by SERPENT.
the packed bed height for reactor with SiC lies around 40 cm (without boron at side absorber) and around 63 cm (with 50 ppm boron). Those values were found by considering the shutdown margin being set at 0.95. For a reactor with ZrC fuel, the range of packed bed height is between 42 cm (without boron) and 72 cm (with 50 ppm boron).

The graphical data can be interpreted as follows. From safety point of view, the level of sub-criticality of the reactor should be larger than the shutdown margin (or more negative in terms of reactivity). Therefore, the bed height of 40 cm is the maximum height of packed bed to be fulfilled in case no boron absorber presents in the side reflector. Increasing the packed bed height (by adding more particles to the reactor) will cause the multiplication factor become higher than the shutdown margin. Should the side reflector contain absorber boron, the multiplication factor at 40 cm height will be below the shutdown margin. Hence, the fuel inventory in the reactor can be increased if one requires a close-to-shutdown-margin criticality. If SiC were replaced by ZrC, the limitation of maximum packed bed height is still valid, considering that the packed bed of advanced coated particles is higher than the standard TRISO with the same parameter. Filling the cavity with less amount of advanced coated fuel particles will cause the reactivity become lower than the shutdown margin. Therefore, the height of packed bed was determined based on the use of standard TRISO fuel particles.

Figure-3(c) shows the difference in multiplication factor between standard TRISO particles and advanced coated particles. It can be seen clearly that advanced coated particles has lower reactivity than standard TRISO due to a higher integral resonance in Zr. Significant reactivity reduction can be seen also in Figure-3(c), with the range between $-336 \pm 138$ pcm and $-2809 \pm 99$ pcm. A consistent trend can be found also, that is the lower the packed bed height, the lower the difference multiplication factor. Along with an increase in packed bed height, the particle inventory also increases, meaning that the volume of Si or Zr also become larger. Therefore, the total neutron absorption on Zr increases, causing a significant decrease in reactivity at higher packed bed.

**RESULTS AND DISCUSSIONS**

**Determination of packed bed height**

This step was performed to determine the bed height at packed condition. Figure-3 shows the multiplication factor of the packed bed for reactor fuelled with standard TRISO particles as well as ZrC advanced coated particles. Calculations were performed at various boron concentration at side reflector absorber, from 0 ppm up to 50 ppm. By interpolating the results, it is found that

$$m_f = \frac{e \times M_{U235} + (1 - e)M_{U238}}{e \times M_{U235} + (1 - e)M_{U238} + M_{O2}} \times \rho_f \times \frac{V_f}{V_p} \times PF \times H_b \times A \approx 547.32 \text{ kg}$$

where $e$ is the uranium enrichment, $M_{U235}$, $M_{U238}$ and $M_{O2}$ are the molecular mass of U-235, U-238 and O$_2$, respectively, $\rho_f$ is the density of the fuel kernel, $V_f$ and $V_p$ are the volume of fuel kernel and of TRISO particles, respectively, PF and $H_b$ are the packing factor and the height of the bed at collapsed condition, and $A$ is the area of the bed. Total number of TRISO particles in the bed is thus $N_p \approx 9.12423 \cdot 10^8$. 

![Figure-2. A schematic view of FLUBER plotted by the SERPENT code.](image-url)
The bed is expanded by keeping the inventory constant, but varying the packing factor (or the bed height) according to the following relation

\[(PF \times H_b)_{\text{packed}} = (PF \times H_b)_{\text{expanded}}\]

Figure-4 shows the multiplication factor of the reactor from packed condition up to a full expansion to the maximum height of the reactor cavity, i.e. 600 cm. Both figures represent the reactor at cold zero power for reactor using standard TRISO particles and advanced coated particles. Reactivity increases along with the bed height, although not linearly. At maximum height, the differences in reactivity at some values of boron concentration are not as large as those at packed condition. These show that neutron absorption by boron is more effective when the bed height is low, while at larger expansion, the effectiveness of boron is not too significant.

At power operation condition, i.e. at high temperature (temperatures of the fuel and helium are 1200 K and reflector temperature is 750 K. The fuel and the helium temperature are set at the same due to excellent heat transfer properties of the TRISO particle and good mixing of fluidization process) the behavior of multiplication factor as a function of expanded bed also show a similar trend (Figures-5(a) and 5(b)). Variation of \(k\) to the boron concentration at packed bed is much larger than that at full expansion. Considering the shutdown margin at cold zero power and variation of multiplication factor at full expansion at power operation, it can be inferred that the minimum concentration of boron in the side absorber should be 20 ppm for packed bed of 50 cm.

Figures-6(a) and 6(b) show the multiplication factor as a function of bed expansion for both reactor with standard TRISO and with advanced coated particles. Those figures clearly show that the excess reactivity of the reactor at higher operational temperature is larger than that at room temperature. This poses a serious concern as it indicates a positive temperature reactivity coefficient. Further analysis is presented in the next section.

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**Figure-3.** Multiplication factors of FLUBER with standard TRISO fuel particles coated with SiC layer and with advanced ZrC-coated fuel particles and their differences as a function of packed bed height for various boron concentration in the side absorber. The errors of each calculation results for SiC and ZrC are not shown due to small values compared with the scale of the graph. The maximum error value is 99 pcm.
Figure-4. Multiplication factors of FLUBER with standard TRISO fuel particles coated with SiC layer and with advanced ZrC-coated fuel particles as a function of expanded bed height for various boron concentration in the side absorber. Temperatures of the fuel, helium coolant and reflectors are 300 K.

Figure-5. Multiplication factors of FLUBER with standard TRISO fuel particles coated with SiC layer and with advanced ZrC-coated fuel particles as a function of expanded bed height for various boron concentration in the side absorber. Temperatures of the fuel and helium coolant are 1200 K and temperature of the reflector is 750 K.
Figure-6. Multiplication factors of FLUBER with standard TRISO fuel particles coated with SiC layer and with advanced ZrC-coated fuel particles and their differences as a function of expanded bed height with 20 ppm concentration in the side absorber. The fuel temperature is 300 K and 1200 K.

Figure-7. Doppler coefficient for reactor with standard TRISO fuel particles and with advanced ZrC-coated fuel particles as a function of expanded bed with 20 ppm of side boron absorber.
The difference in multiplication factor between advanced coated particle and standard TRISO is shown in Figure-6(c). The minimum value of $-269 \pm 101$ pcm is achieved at 400 cm of bed expansion and 1200 K while the maximum of $-1286 \pm 121$ pcm is obtained at 50 cm height and 300 K. However, the data do not show clear and consistent trends. At room temperature, the difference in reactivity is roughly around -1250 pcm at lower bed expansion (less than 100 cm) while at larger expansions the difference is about -700 pcm. At 1200 K, the variations in the differences are larger. Therefore, no systematical information on errors can be inferred from the bed expansion.

Temperature reactivity coefficient

The Doppler coefficients for reactor with standard TRISO and with advanced coated particles at 1200 K are shown in Figure-6. For both types of particles, the Doppler coefficient could be positive or negative, depends on the height of expanded bed. For standard TRISO, the positive coefficient can be found at 150 cm of expanded bed (with a maximum positive of around 17 pcm/K), 250 cm and 350 cm. The negative coefficients, however, are not so large, even at expansion higher than 300 cm; the Doppler coefficient is very close to 0 pcm/K within one standard deviation. Some positive Doppler coefficients for advanced coated particles can be found at 150 cm, 200 cm, 250 cm and 450 cm of expanded bed. However, compared with the standard TRISO particles, in general advanced coated particles have more negative Doppler coefficients. This is influenced by a higher resonance integral of Zr.

The moderator temperature coefficient, MTC, (in the context of FLBER, the moderator is the reflector, as helium is practically transparent to neutrons) is shown in Figure-8. In a reactor with standard TRISO fuel, all MTCs...
are positive as a function of expanded bed. This is quite predictable due to spectral hardening caused by a shift in thermal neutron flux as temperature increases. However, some of the MTCs of advanced coated particles are negative. At lower bed expansion (for example at 50 cm and 100 cm), the influence of boron side absorber is dominant, thus an increase in boron resonance integral due to higher temperature causes a decrease in reactivity. Similar behavior can also be observed for standard TRISO particles at 50 cm of bed height, in which the MTC is minimum but not negative. On the other hand, at larger expansion where the side absorber is less influential, the MTCs are expected to be positive due to spectral shift. However, at expanded bed height of 400 cm, the MTC is negative. This phenomenon needs further investigation.

The sum of the two reactivity coefficients is presented in Figure-9. It can be clearly seen that the total reactivity coefficient could be positive at different bed height of reactor with standard TRISO and with advanced coated particles. No consistent relation can be found between the total reactivity coefficient and the expanded bed height, so that it is not so easy to explain the phenomena. These results are different from the preceding researches, for example as reported in [3], where the total temperature reactivity coefficient was always negative, although spectral hardening occurred also at the reflector.

Considering that a positive total reactivity coefficient is undesirable, further investigations are required. These might include a benchmark study with other Monte Carlo codes, such as SCALE/KECO-VI or MCNP. In addition, it is necessary to redesign the FLUBER, in terms of fuel design and core design. This is to be performed to ensure that the reactivity coefficient to be negative.

CONCLUSION AND REMARKS

Based on the calculation using Monte Carlo code SERPENT, it is found that the use of ZrC to replace SiC as coated layer in a standard TRISO particles gives the following:

a) A significant decrease in reactivity was observed with range of -336 ± 138 pcm to -2809 ± 99 pcm at packed bed condition and -269 ± 101 pcm to -1286 ± 121 pcm at expanded condition. Consequently, to achieve the same value of excess reactivity as in the standard TRISO, the use of advanced coated particles requires larger fuel inventory, or less boron concentration in the side absorber.

b) The use of standard TRISO and advanced coated particles in a fluidized bed nuclear reactor might cause a positive reactivity coefficient at particular bed expansion. The maximum positive coefficient of 25.96 ± 12.36 pcm/K was found at 150 cm of bed expansion, and a maximum negative coefficient of -33.31 ± 8.53 pcm/K was found at 400 cm of bed expansion, both in a reactor with advanced coated particles. The positive values were not only caused by spectral hardening of the graphite reflector, but also could be found at the change in fuel temperature. Nevertheless, no systematic relation can be found between the temperature reactivity coefficient and the height of expanded bed.

Further investigation or research should be performed considering the possible positive reactivity coefficient. Such future research may include:

a) Performing a code-to-code comparison/benchmark against other Monte Carlo code, to ensure the consistency of the computational results. If consistent results be found, the positive reactivity coefficient is thus not caused by user’s error in modeling the reactor using SERPENT code. The physical phenomena are thus the dominant factor in the reactor system.

b) Redesigning the fluidized bed nuclear reactor, in terms of fuel design and core design. Regarding the design of fuel particles, the geometry of the kernel, the coating layers in the TRISO as well as the material compositions of the TRISO particles could be varied. The calculation is then performed to fuel particles by assuming an infinitely large three-dimensional reactor to ensure the Doppler coefficient of the isolated fuel particles is negative. In terms of reactor design, the geometry of the core can also be modified. Instead of using a simple graphite cylinder with a helium cavity inside, the core might be in conical shape or by using small parallel channels embedded in the graphite reflectors. Modifications to the composition of the reflector material could also be performed, for example by varying the impurities in the graphite.

c) Performing calculations related to the dynamics factor of the reactor as well as fluidization aspects. In this case, a simplified approach is to use the point dynamics model with neutronic parameters obtained from static calculations. In addition, it is also necessary to perform calculation or simulations using computational fluid dynamics (CFD) without neutronic coupling to observe the behavior of fluidized particles in the geometrically redesigned reactor.

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