Evaluation of the neutronic performance of $^{11}B_4C$ as an alternative coating layer in TRISO fuel

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Evaluation of the neutronic performance of ^{11}B$_4$C as an alternative coating layer in TRISO fuel

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Abstract   This work explores the viability of using boron carbide (B$_4$C), substantially enriched in ^{11}B at about 99%, conveniently named ^{11}B$_4$C, as a coating material for Tri-structural Isotropic (TRISO) particle fuel. Utilizing the open source OpenMC VHTR fuel benchmark file as a reference, the SiC coating layer is replaced with ^{11}B$_4$C at varying enrichment levels to generate three TRISO fuel compact models. Using the models, multiple eigenvalue simulations are conducted with an appropriate number of batches of enough thousands of neutrons, calculating the infinite multiplication factor, with tallies for the neutron flux spectrum, and neutron absorption by the ^{11}B$_4$C layer against the reference TRISO with SiC coating. Results show that for highly enriched ^{11}B$_4$C the fuel element remains critical. For lower ^{11}B enrichment, the expected neutron absorbing properties of ^{10}B render the fuel element subcritical. Flux spectra and neutron absorption rates are tallied and plotted to further understand the neutronic performance of this coating.

Keywords   TRISO, Boron Carbide, Fuel Performance, Neutron Spectrum, Advanced Coating Materials, Ceramics, Monte Carlo

INTRODUCTION

The neutronic performance of ^{11}B$_4$C as a coating material for TRISO fuel, acting as a primary containment barrier against fission product release, a function typically met by a SiC coating layer [1] is assessed. TRISO fuel is characterized as Accident Tolerant Fuel (ATF), enhancing safety performance in beyond design accident scenarios [2]. Boron Carbide (B$_4$C) is renowned for its exceptional mechanical and thermal properties. It possesses high hardness and Young's modulus, contributing to significant resistance to ballistic impact, which makes it broadly used as a protective material. The thermal conductivity of B$_4$C is comparable to usual TRISO coating materials; additionally, B$_4$C exhibits high thermal stability, maintaining its structural integrity at elevated temperatures [3]. These attributes of B$_4$C, combined with its established use in nuclear systems as a neutron absorber, make ^{11}B$_4$C a candidate worth considering for enhancing the performance and safety of TRISO fuel particles. Neutron irradiation experiments with ^{11}B$_4$C have already been performed, characterizing the material as highly applicable for use in reactors [4]. In addition, synthesis capabilities and a supply chain for ^{11}B-enriched B$_4$C (with greater than 99% enrichment) already exist, primarily developed for neutron optics applications [5].
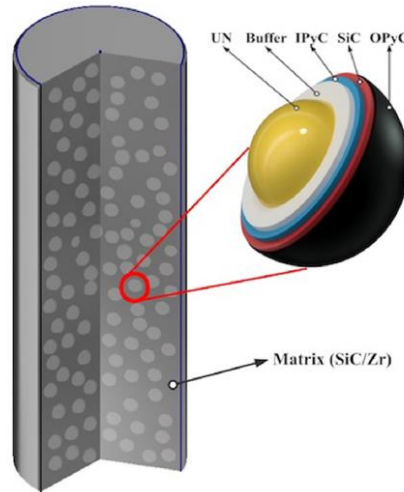
TRISO AND FUEL GEOMETRY

A common form of TRISO particle fuel involves packing the particles into cylindrical fuel compacts, as illustrated in Fig. 1. These fuel elements can be inserted into prismatic graphite blocks or Zircalloy clad, to create fuel assemblies suitable for High Temperature Gas Reactors (HTGRs) or Light Water Reactors (LWRs). The most common materials used for these cylindrical compacts are graphite or silicon carbide (SiC) [2].
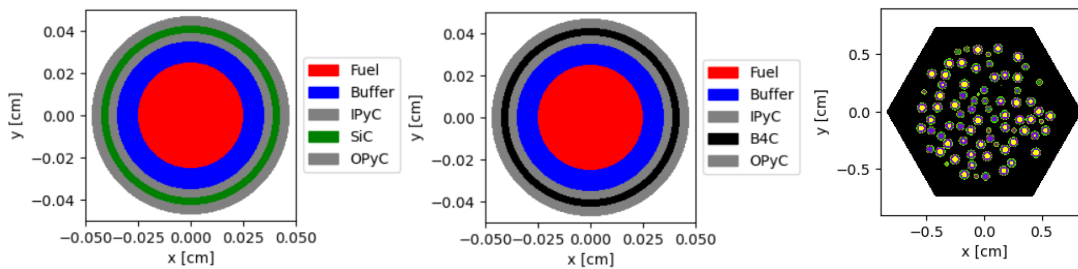
In the present study, a fuel element is replicated following the OpenMC [6] library Very High Temperature Gas Reactor (VHTR) benchmark file generated by the MIT Computational Reactor Physics Group [7]. First, the reference TRISO particle is generated using standard layer thicknesses. For the ^{11}B$_4$C-coated particle, the geometry of the reference particle is duplicated, with the SiC layer replaced by a ^{11}B$_4$C layer of the same thickness, as shown in Fig. 2. The fuel used is 4% enriched UO$_2$.

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The cylindrical fuel compact element is then generated by randomly packing the TRISO particles into a graphite cylindrical matrix, with a selected packing fraction of 0.28. The fuel compact is inserted in a hexagonal graphite prismatic block to form the fuel element, as per the benchmark file. The outer graphite block boundary and the top and bottom compact boundaries are considered as neutron reflective, generating a critical element for the reference geometry. The key elements of the model geometry are illustrated in Fig. 2.

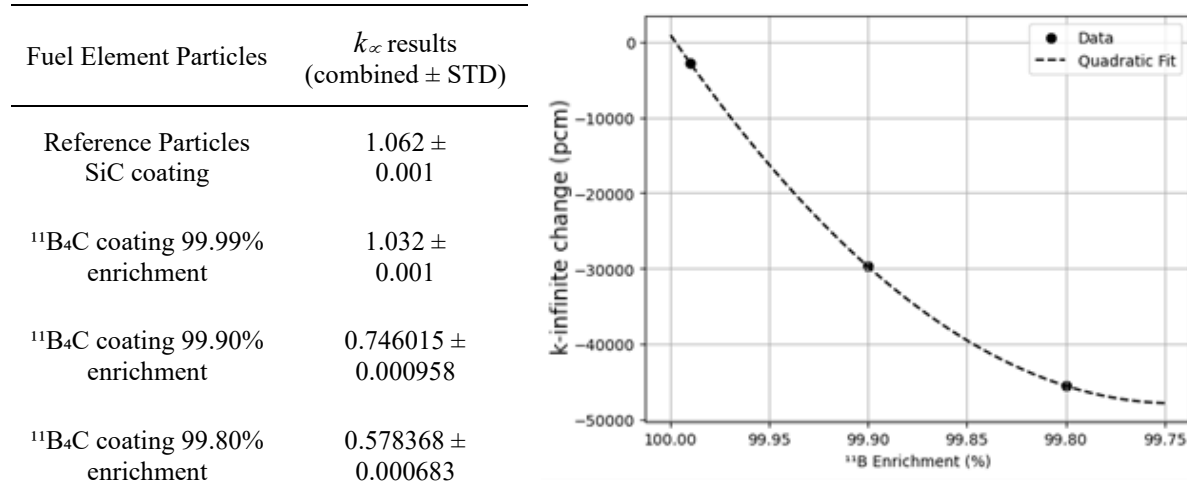**Figure 1.** *Visual Representation of a fuel compact element as in [2]*

Figure 2. *Cross-Sections of the model geometries.* **LEFT:** *Reference TRISO particle,* **CENTER:** *$^{11}B_4C$ coated particle,* **RIGHT:** *Hexagonal Fuel Element packed with TRISO,* **IPyC:** *Inner Pyrolytic Carbon,* **OPyC:** *Outer Pyrolytic carbon*
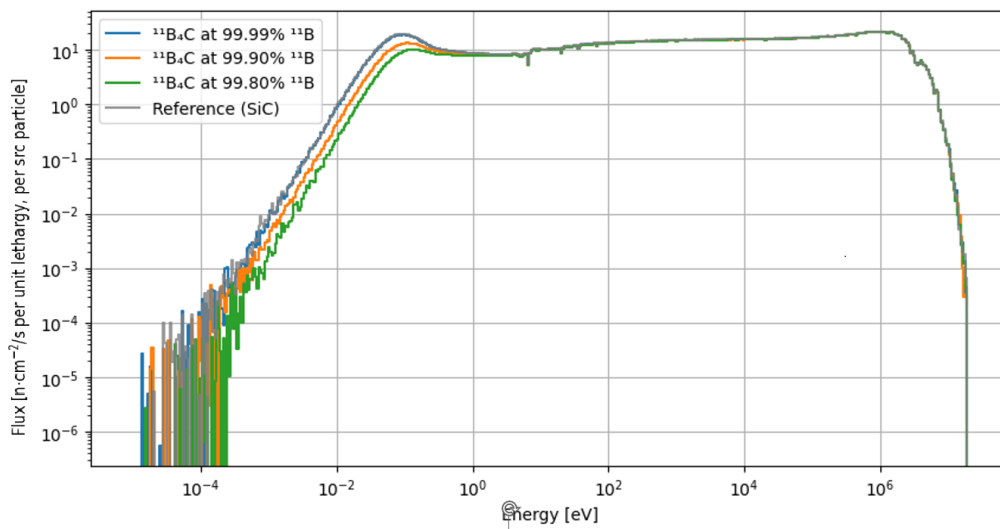
NEUTRONIC PERFORMANCE EVALUATION

To evaluate the performance of $^{11}B_4C$, k-eigenvalue k_∞ simulations were conducted for the reference fuel element and three $^{11}B_4C$ fuel elements at 99.80%, 99.90% and 99.99% isotopic enrichment in ^{11}B. The ENDF/B-VIII.0 library was used for the nuclear reaction cross sections. In addition to the calculated k_∞, two tallies were used to evaluate the $^{11}B_4C$ performance, namely a neutron flux spectrum tally and an absorption tally. The former records the neutron flux as a function of energy, allowing direct comparison of spectral differences between the reference fuel element and the $^{11}B_4C$-enhanced variants. As per standard practice, a logarithmically spaced energy filter with 500 bins is applied to the tally, spanning from 10^{-5} eV to 20 MeV, ensuring comprehensive spectral resolution across the entire neutron energy range. The flux $\Phi(E)$ is normalized as $\Phi_r(E)$ per unit lethargy, ensuring that each energy bin contributes equally in logarithmic energy space. This transformation is necessary since the logarithmic binning inherently causes a variable energy width. The lethargy-normalized flux is expressed as:

$$\Phi_r(E) = \frac{\Phi(E)}{\Delta \ln E} \left[\frac{\text{ns}^{-1}\text{cm}^{-2} \text{ per source neutron}}{\text{unit lethargy}} \right]$$

The later (absorption) tally records the neutron absorption rate as a function of energy, allowing direct comparison of absorption behaviour between the $^{11}B_4C$-enhanced fuel elements and the reference SiC-coated TRISO. A material filter is applied restricting the tally to $^{11}B_4C$ and SiC. The absorption reaction is tallied via an "absorption" score, accounting for all reactions that do not produce secondary neutrons as well as fission. Multiple eigenvalue simulations were conducted with 100 batches of 100.000 neutrons, calculating the infinite multiplication factor, and tallies for the flux spectrum and neutron absorption by the $^{11}B_4C$ layer against the reference TRISO with SiC coating. Results are shown in Figs. 3, 4 and 5.

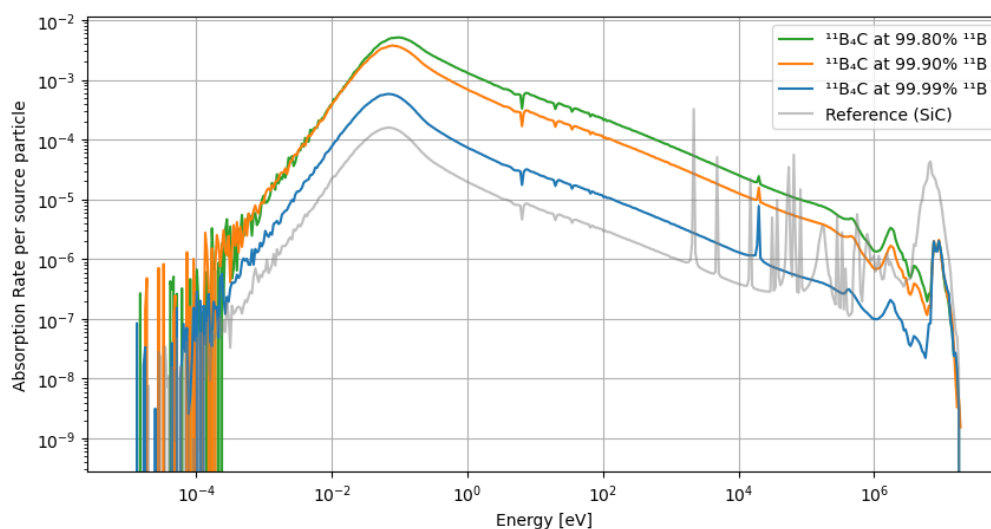| Fuel Element Particles	k_∞ results (combined ± STD)
Reference Particles SiC coating	1.062 ± 0.001
$^{11}B_4C$ coating 99.99% enrichment	1.032 ± 0.001
$^{11}B_4C$ coating 99.90% enrichment	0.746015 ± 0.000958
$^{11}B_4C$ coating 99.80% enrichment	0.578368 ± 0.000683

Figure 3. LEFT: *Simulation results for k_∞ of three $^{11}B_4C$ fuel elements of different ^{11}B enrichments and the reference fuel element.* **RIGHT:** *Results plotted in a quadratic fit, showing k_∞ change in pcm (i.e. %Δk/k).*

Figure 4. *Neutron flux spectrum per source particle in fuel element, normalised per unit lethargy, for reference and $^{11}B_4C$ coated particles.*

For a very high level (99.99%) of ^{11}B enrichment in the $^{11}B_4C$ coating, the fuel element remains critical with a ~3000 pcm drop in reactivity and a similar neutron spectrum (Figs. 3 and 4). However, as expected, for lower ^{11}B enrichment, the ^{10}B neutron absorption properties dominate (Fig. 5), leading to a subcritical element.

Figure 5. *Absorption rate per source particle in the* [11]B$_4$C *coating layers and the* SiC *reference.*

DISCUSSION

The present preliminary results suggest that [11]B$_4$C exhibits neutronic performance comparable to SiC, making it a viable candidate for TRISO fuel coatings – provided that high levels of [11]B enrichment can be achieved. In addition, the [10]B present in B$_4$C will act as a burnable absorber, gradually depleting over the reactor's lifetime. This characteristic could be leveraged in reactor design to manage excess reactivity at the beginning of life, control burnup, and regulate power distribution in [11]B$_4$C-coated TRISO fuel. However, further investigation is required to assess these potential advantages, to validate the neutronic findings and to evaluate the thermal and chemical stability of [11]B$_4$C for TRISO applications when needed.

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