### **Neutronics Study on LEU Nuclear Thermal Rocket Fuel Options**

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## **1. Introduction**

The development of the LEU (Low-Enriched Uranium) nuclear thermal rocket (LEU-NTR) has been heavily based on the legacy work of the NERVA [1][2][3] program in the 1960s and 1970s in the United States [4][5]. This has resulted in a non-trivial simplification of the tasks needed to develop such an engine and the quick initial development of the concept. There are, however, a series of key core-design choices that are currently under scrutiny in the field that have to be resolved in order for the LEU-NTR to be fully developed. The most important of these is the choice of fuel: carbide composite or tungsten cermet. This study presents a first comparison of the two fuel types specifically in the neutronic application to the LEU-NTR, keeping in mind the unique neutronic environment and the system requirements of the system. The scope of the study itself is limited to a neutronics study of the two fuels and only a cursory overview of the material properties of the fuels themselves.

# 2. Fuel Summary

The two major fuel types under consideration for future NTR development are the carbide composite and tungsten cermet. Both are similar in that they are able to operate at extremely high temperatures in the range of 2400 - 3000 K or higher. The similarities, however, stop there.

The carbide composite fuel was the one of the last iterations of the fuel developed during the US NERVA program. The evolution began with NbC coated  $UC_2$ particles dispersed in a graphite matrix and PyC coated UC<sub>2</sub> sphere (the precursor to the modern TRISO particle) dispersed in a graphite matrix [6]. These initial fuel forms, however, had the large issue of having extensive hydrogen corrosion of the graphite matrix due to a mismatch of coefficients of thermal expansion (CTE) between the fuel and the hydrogen barrier between the fuel and hydrogen coolant [7]. This resulted in the significant loss of fuel and structural integrity of the fuel elements during reactor operation. In order to mitigate this, the NERVA program developed the carbide composite fuel which had similar operating parameters as the previous fuels developed and had a significantly better match of CTE with the hydrogen barriers implemented [7]. The fuel itself is a continuous carbide matrix consisting of UC and ZrC inside of a larger graphite matrix, resulting in a (U,Zr)C di-carbide material.

The Tungsten Cermet fuel was a fuel option which was originally developed in parallel to the NERVA graphite-based fuel by researchers at General Electric and Argonne National Laboratory. The fuel consisted of  $UO_2$  spheres evenly dispersed inside of a W-Re matrix. The benefits behind this form stemmed from the high operating temperatures of tungsten and its ability to survive in a hot environment without interacting with the hydrogen. The result was a strong, durable fuel form that could ensure fission product retention throughout the operating life time of the reactor core [6]. When applied to the LEU-NTR, however, it has been shown that the tungsten matrix must be enriched in <sup>184</sup>W in order to mitigate the large neutron absorption cross-section of natural W [5].

It is important to note that almost all of the physical data pertaining to these two fuel types were determined in the 1960s and 70s, and have been largely untouched since then. Recently, however, there has been an effort in the US to recapture not only the manufacturing techniques, but also improve the fuel types by researchers at the Center for Space Nuclear Research (CSNR) for the Tungsten Cermet and Oakridge National Laboratory (ORNL) for the graphite fuels.

The summary of the legacy operating parameters for the two fuel is given in Table 1.

Table 1. Summary of legacy fuel operating parameters from the NERVA and ANL research programs [6].

Parameter	Carbide Comp.	W-Cermet
Max. Operating Temperature (K)	2800-3100	2900-3270
Thermal Conductivity (W/m*K)	8.2-10.0	~ 60
Coefficient of Thermal Expansion ( (µm/m*K) <sup>2</sup> )	7.8	Matrix : 5.0 UO <sub>2</sub> : 10.1
Failure Stress (MPa)	75-140	100-600

### **3. LEU-NTR Core Concepts**

A single factor dominates the neutronics of the LEU-NTR reactor core: the scarcity of fissile material in the active core. This follows from the need to have minimum size core and the desire to implement LEU fuel. Consequently, not only is the density of the fissile material low relative to HEU legacy designs, the absolute amount of fissile fuel is also similarly low. In order to compensate, the fission cross-section of the fissile material has to be maximized while simultaneously keeping the parasitic absorption in the fuel and the structural material to a minimum along with the core leakage. The result is that the typical LEU-NTR requires a thermalized neutron spectrum and an effective reflector, minimizing the effect of external factors on the neutronics of the inner core [8].

Another factor that must be taken into account is the fact that the core itself has heterogeneous core configuration with fuel elements interspersed among moderator elements. A typical LEU-NTR core configuration is shown in Fig. 1.



Fig 1. Typical NTR core configuration.

### 4. Fuel Neutronic Parameters

As a consequence of the neutronic environment in an LEU-NTR, the fuel has a series of characteristics that are particularly relevant in determining their neutronic suitability for the system: fuel loading, moderating ability, and neutron absorption. The first parameter determines the density and ultimately how much fissile material can be physically present in the core, countering the reduction of fissile material due to the reduced enrichment of the fuel. The second influences the spectrum by increasing or decreasing the thermalization of the spectrum, and therefore having a significant effect on both the minimum amount of fissile material needed in the core as well as the reflector size and average neutron path length in the moderator elements and the reflector region. Finally, the parasitic absorption by the fuel itself noticeably affects not only how much fissile material is needed in the core, but will also affect the average neutron path length in the fuel and determine the degree to which fuel self-shielding will occur.

#### 4.1 Fuel Loading

The fuel loading is a critical parameter because not only is the macroscopic homogenized fission crosssection of the fuel linearly dependent on it, it also has a direct effect on the physical properties of the fuel. This ensures that both fuel types have a clearly defined range within which the fuel loading can vary, but cannot go beyond.

The carbide composite fuel is severely limited in the range of fuel loading it can have, going from a mere .05  $g/cm^3$  up to .65  $g/cm^3$ . This is because of the need for carbide composite to maintain the careful balance of having a continuous graphite matrix while also having a continuous carbide matrix throughout the fuel element. By having both as continuous structures the fuel is able to have both desirable thermal properties (reduced thermal expansion and enhanced thermal conductivity) as well has good structural properties (strength and hydrogen corrosion resistance). Consequently, the carbide volume fraction is limited to being between 30 and 35 volume percent of the fuel matric. Furthermore, the actual loading of Uranium in the carbide has to be further limited in order to prevent the formation of UC2 in the fuel as well as increasing the melting temperature of the fuel. This careful balance in the (U,Zr)C system can be seen in the phase diagram reproduced in Fig. 2.



Fig 2. Portion of pseudobinary phase diagram for U-Zr-C system for composite elements containing 35 vol% carbide [9].

In contrast, the tungsten cermet is able to have a large variability in terms of the fuel loading. This is because unlike the carbide composite, the tungsten cermet does not need to maintain two distinct solid matrices in the fuel element, and relies on the tungsten matrix to ensure both structural stability and good thermal properties. Consequently, the fuel component (present as UO2 spheres evenly dispersed in a tungsten matrix) are able to occupy a much larger volume fraction of the fuel without adverse effects. In fact, the fuel volume fraction in the fuel elements can vary from 0 up to 70 vol %, resulting in a significantly larger fuel loading than the carbide composite. At 55 vol % (demonstrated volume fraction using modern techniques), the fuel loading is equivalent to 4.83 g/cm<sup>3</sup>, close to an order of magnitude greater than the carbide composite [9].

The effect of the fuel loading on the reactivity is shown in Fig. 3. The data presented in the graph were created using MCNP5 with the same infinite lattice for both fuel types. Each data point differs only in the fuel composition where the fuel loading was changed in order to find the k-infinite for each configuration. Two things become obvious. First of all, that the carbide fuel is highly sensitive to changes in the fuel loading. This has the unfortunate consequence in severely limiting how large the coolant channels can be made in order to maximize the heat transfer area for the coolant channels. The tungsten cermet, on the other hand, is not similarly limited, and can have large changes in fuel loading without a significant effect on the reactivity. The second factor is that the carbide composite is able to achieve similar, if not higher reactivity than the tungsten cermet with significantly less fuel. This could translate in a minimum reactor mass using carbide composite fuel being significantly small than a minimum mass tungsten cermet core.



Fig. 3. Effect of fuel loading on the k-infinite for an infinite lattice (2:1 moderator-to-fuel ratio).

#### 4.2 Fuel Moderation and Absorption

The difference in the effect the fuel loading has on the reactivity of the core is largely due to a difference in the moderating ability and the absorption of the fuel. If the fuel is a relatively good moderator as well as having a low absorption cross-section, it is able to have a heavily thermalized spectrum with significantly increases the fission cross-section of the fissile material. If, on the other hand, it is neither a good moderator and has a noticeable absorption cross-section, the neutron keeps a relatively fast spectrum and makes rather inefficient use of the fissile material in the fuel. These are the two cases in fact where the carbide composite is the good moderator with low absorption while the tungsten cermet is the bad moderator with the noticeable absorption. The effect each has on the neutron spectrum in the fuel can be seen in Fig. 4. Here the carbide composite fuel clearly demonstrates a thermalized spectrum with a fast and thermal peak while the tungsten cermet spectrum only has a fast peak with a thermal tail.

This can be further seen in how well each fuel is able to successfully thermalize neutrons. As expected, using two-group homogenized cross-sections for the fuel, the moderating power and moderating ratio for the carbide composite is significantly higher than that of the tungsten cermet. At the same time, the average neutron path length is shorter in the tungsten cermet. This is due to the noticeable neutron absorption cross-section of the tungsten matrix. This is summarized in Table 2.



Fig. 4. Neutron spectrum for the carbide composite (red) and tungsten cermet (blue) fuels in an infinite lattice with a 2:1 moderator to fuel element ratio.

Table 2. Two-group moderating characteristics for carbide composite and tungsten cermet fuels.

Parameter	Carbide Composite	CERMET
Slowing Down		
Decrement: Fast/Thermal	0.1191 / 0.1264	0.0341 / 0.0409
(ξ)		
Moderating Power: Fast/Thermal ( $\xi \Sigma_s$ )	0.0404 / 0.0524	0.0145 / 0.0146
Moderating Ratio (w/o fission): Fast/Thermal ( $\delta \Sigma_{c} / \Sigma_{c}$ )	9.95 / 1.5358	0.0767 / 0.5469
Average Neutron Path Length in Fuel $(1/\Sigma_{tot})$	2.6424	1.9093

The effective thermalization of the neutron spectrum is further evidenced by how the infinite lattice using the carbide composite fuel is actually slightly over moderated resulting in slight decrease in reactivity with the addition of additional moderator. This is not true, however, for the tungsten cermet fuel. This can be seen Fig. 5, where the outer radius of the moderator sleeve in the moderator element is varied from .3 cm up to .65 cm. The over moderation of the infinite carbide composite lattice is clearly apparent as is the under moderated state of the infinite tungsten cermet lattice. This over- and under-moderated state has interesting implications especially when taking into account events where the moderator fraction in the core changes including moderator loss in the event of an accident or a full water submersion accident scenario. Either case is a believable accident scenario which will have to take into account the individual characteristics of the selected fuel.



Fig. 5. Over- and under-moderation of the infinite lattice with a 2:1 moderator to fuel element ratio for carbide composite and tungsten cermet fuels.

#### 4.3 Fuel Self-Shielding

In the current standard fuel element design, fuel selfshielding is an issue specifically for the tungsten cermet fuel. Fuel self-shielding occurs when the average neutron path length is less than the size of the fuel element through a combination of having high macroscopic fission and absorption cross-sections. Due to the epithermal neutron spectrum, high fuel loading, and the noticeable tungsten absorption cross-section, both of these are true for the tungsten cermet fuel, creating a situation where after 60 hours of full power operation, the fuel shows a noticeable radial burn up profile where more fuel is utilized on the exterior of the fuel element than the center. In comparison, the carbide composite fuel does not display a similar trend, having an almost flat power profile across the fuel element. This is because, while the neutron spectrum is more thermalized, it does not have the additional neutron absorption by the tungsten.

The self-shielding for both fuels is shown in Fig 6. For this calculation the hexagonal fuel element was simplified into a cylindrical fuel element and then divided into 15 equal volume radial zones. This was done in order to take advantage of the powerful burnup calculation capabilities of Serpent 1.



Fig. 6. Burnup calculation of fuel element in an infinite lattice using 15 radial zones for 12, 36, and 60 hours (burnup period).

# 5. Conclusions

The results of this study have led to two major conclusions. First of all is that the carbide composite fuel is, from a neutronics standpoint, a much better fuel. It has a low absorption cross-section, is inherently a strong moderator, is able to achieve a higher reactivity using smaller amounts of fissile material, and can potentially enable a smaller reactor. Second is that despite its neutronic difficulties (high absorption, inferior moderating abilities, and lower k-infinity values) the tungsten cermet fuel is still able to perform satisfactorily in an LEU-NTR, largely due to its ability to have an extremely high fuel loading. This then enables the tungsten cermet fuel to have larger coolant channel radii due to its relative insensitivity to the fuel loading.

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