INL/CON-10-20346
PREPRINT

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## Nuclear and Emerging Technologies for Space 2011

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February 2011

Proceedings of Nuclear and Emerging Technologies for Space 2011
Albuquerque, NM, February 7-10, 2011
Paper 3276

# A Combined Neutronic-Thermal Hydraulic Model of a CERMET NTR Reactor

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**Abstract.** Two different CERMET fueled Nuclear Thermal Propulsion reactors were modeled to determine the optimum coolant channel surface area to volume ratio required to cool a 25,000 $lb_f$ rocket engine operating at a specific impulse of 940 seconds. Both reactor concepts were computationally fueled with hexagonal cross section fuel elements having a flat-to-flat distance of 3.51 cm and containing 60 vol.% $UO_2$ enriched to 93wt.%$U^{235}$ and 40 vol.% tungsten. Coolant channel configuration consisted of a 37 coolant channel fuel element and a 61 coolant channel model representing 0.3 and 0.6 surface area to volume ratios, respectively. The energy deposition from decelerating fission products and scattered neutrons and photons was determined using the MCNP monte carlo code and then imported into the STAR-CCM+ computational fluid dynamics code. The 37 coolant channel case was shown to be insufficient in cooling the core to a peak temperature of 3000 K; however, the 61 coolant channel model shows promise for maintaining a peak core temperature of 3000 K, with no more refinements to the surface area to volume ratio. The core was modeled to have a power density of 9.34 GW/m3 with a thrust to weight ratio of 5.7.

**Keywords:** nuclear thermal propulsion, space reactor, tungsten alloys, nuclear fuels.

## I. INTRODUCTION

Nuclear Thermal Rocket (NTR) propulsion may represent the best near term advanced propulsion system, which can enable aggressive manned exploration of our solar system. In concept a nuclear rocket engine is fairly simple. A fission reactor is heated to a maximum temperature without melting, a low molecular mass fluid, such as hydrogen, cools the reactor and absorbs enthalpy, and finally, the hydrogen is expanded out a converging-diverging nozzle to produce thrust at a very high specific impulse.[1]

The most robust NTR program pursued to date was the combined ROVER/NERVA program, which involved the United States Air Force (USAF), the National Aeronautics and Space Administration (NASA) and the U.S. Atomic Energy Commission (AEC). A total of 22 epithermal graphite moderated reactors were built and tested under the ROVER/NERVA program which operated at temperatures as high as 2650 K and successfully achieved power densities as high as 2.34 GW/$m^3$.[2] Unfortunately, NERVA testing demonstrated significant fuel mass loss rates due to cracking of the graphite matrix and cladding material, which both had a low creep strength and a significant chemical affinity for high temperature hydrogen.[3]

The General Electric (GE) Corporation and the Argonne National Laboratories (ANL) led two separate programs from 1965 until 1972 to investigate the fabrication of tungsten based fuel elements; which encapsulated highly enriched uranium dioxide ($UO^2$).[3] Tungsten has a far higher creep strength and resistance to hydrogen corrosion than the graphite materials used during the NERVA program and offered the potential for longer duration reactor operation at refractory temperatures. General Electric was successful in fabricating fuel elements, which consisted of 54 vol.% $UO_2$ and 46 vol.% tungsten. Approximately 10 mol.% $ThO_{1.5}$ was added to the fuel kernels which acted as a stabilizer to prevent fuel migration during peak temperature operations and fuel cycling.[4] General Electric also experimented with a uranium mononitride (UN) fuel within a W-3wt.%Re matrix for power reactors which would operate with a peak temperature of 2000 K[5]. However, the melting temperature of UN prohibited the use of the W-UN fuel type towards a NTR reactor which might see a peak temperature exceeding 2700 K.

In a separate program the Argonne National Laboratory fabricated W-$UO_2$ fuel elements to slightly higher fuel to tungsten volumetric ratios of 60/40 and used $GdO_{1.5}$ as a stabilizer, which decreased fuel loss over that of $ThO_{1.5}$, which was used by the General Electric Corporation. Fuel elements fabricated by both organizations were subjected to hot hydrogen testing at temperatures as high as 3100 K and neutronic ramp rates which produced temperature gradients of 16,000 K per second.[3-6] Fuel elements fabricated by both organizations showed it was possible to fabricate fuel elements which could operate for thousands of hours and hundreds of restarts at temperatures in excess of 2500 K. The specific heats and thermal conductivity of W-$UO_2$ fuels also show the promise for power densities in excess of 10 GW/$m^3$, which translates to increased thrust-to-weight ratios and a decrease in gravity losses when the rocket engine exits a gravity well.

In order to help support the resurgence of W-$UO_2$ Ceramic-Metallic (CERMET) based fuel elements for nuclear propulsion applications, the Center for Space Nuclear Research is developing an in house NTR reactor design, appropriately titled the Phoenix reactor. The modeling suite is still being developed, but will eventually be used to help guide fuel element geometry requirements as well as all-up reactor design. The current generation modeling tool includes a coupling between MCNP5, which determines the volumetric energy deposition, and STAR-CCM, which determines the temperature distribution within various reactor components.

## II. REACTOR DESIGN

The reactor design investigated in this study was developed to produce 512 MW of power to support a 25,000 $lb_f$ rocket operating at a specific impulse of 940 seconds for a total of 10 hours. Previous studies conducted by the General Electric Corporation determined that a 30,000 $lb_f$ reactor operating at a specific impulse of 900 seconds would require a cold clean excess reactivity of \$2.55 in order to account for 100 hours of burnup as well as the hydrogen moderation and fuel thermal expansion.[7] Without having conducted a robust burnup analysis for a 10 hour lifetime, the GE results were used for criticality design and a minimum excess reactivity of \$2.55 was set as the design target.

### II.A Fuel Design

The fuel elements were modeled to consist of 60 vol.% percent $UO_2$ and 40 vol.% tungsten, where the uranium is enriched to 93 wt.% $U^{235}$. Each fuel element is modeled to have a hexagonal cross section with a flat-to-flat distance of 3.51 cm; however, two coolant channel configurations were modeled. A configuration based on the P&W XNR-2000 reactor was modeled where each fuel hex contained 37 coolant channels lined with a 0.025 cm thick W-25%Re cladding layer and another was modeled to have 61 coolant channels each lined with a 0.009 cm W-25%Re cladding layer.[10] The surface-area to-volume-ratio of the 37 coolant channel hex was 0.31 compared to the 0.6 ratio with the 61 coolant channel hex. The first 20 cm of the fuel element is filled with a beryllium oxide neutron reflector and the latter 70 cm is filled with the CERMET fuel mixture. Figure 1 demonstrates an isometric view of the 37 coolant channel hex to include the BeO neutron reflector shown in gold, the W-$UO_2$ CERMET fuel drawn in silver and the W-25wt.%Re cladding tubes drawn in blue.

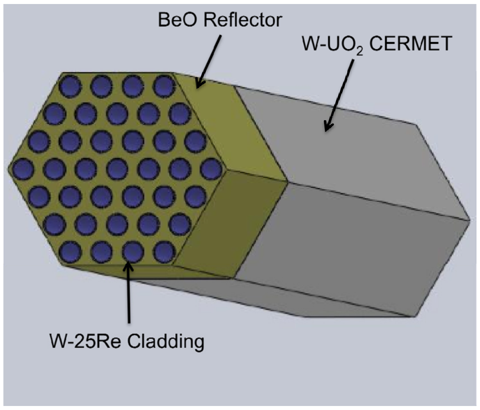

**FIGURE 1.** Diagram of a Tungsten CERMET Fuel Element.

### II.B. Core Design

The fission core consists of 151 fuel elements arranged in a lattice configuration. The fuel elements are surrounded by a 0.3 cm thick cylindrical pressure vessel; fabricated from a Ti-8Al-Mo-V alloy. The peripheral fuel elements are locked into place by the use of titanium alloy pinning rods inserted between the pressure vessel and the fuel elements. The inner pressure vessel is surrounded by a 16.45 cm thick beryllium neutron reflector, which is embedded with twelve control drums. Each control drum is fabricated with a core of beryllium oxide and a 0.5 cm sheath of $B_4C$ enriched to 90% $B^{10}$ which wraps around a $120^0$ segment of the control drum. The radial neutron reflector and the twelve control drums are encapsulated by an outer titanium alloy pressure vessel with a thickness of 0.4 cm. Figure 2 shows a top down view of the tungsten CERMET fission core to include the fuel elements, pinning rods, pressure vessels, neutron reflector and twelve control drums to include coolant channels within the radial reflector.

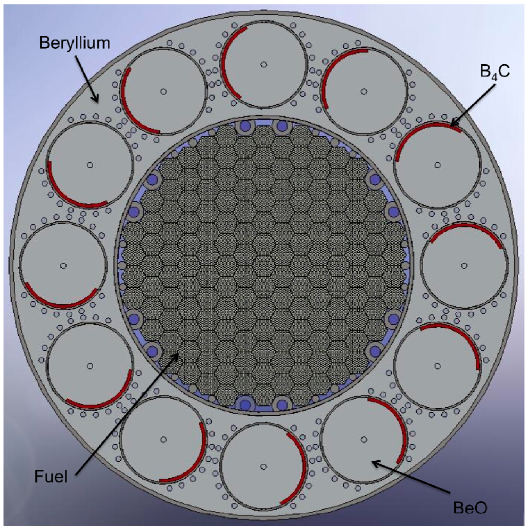

**FIGURE 2.** Drawing of a Phoenix CERMET Fission Core with 12 Control Drums and 151 Fuel Elements.

## III. CORE NEUTRONICS ANALYSIS

### III.A. Steady State Conditions

The Fission Core was neutronically modeled in MCNP5 using the ENDF-VII cross-section data-base.[11] The code was executed in a k-code Eigen value mode using 20,000 neutrons per cycle for 1800 cycles, in order to determine an estimate of the reactor systems neutron multiplication number (*k*). The first 100 neutron generations calculated by MCNP5 are skipped in order to achieve an acceptable fission source distribution. The configuration containing 61 coolant channels per fuel hex was found to provide the largest shutdown margin of both reactors and the most cold clean excess reactivity. With the control drums rotated to their most reactive position, the reactor was found to have a neutron multiplication number of 1.03012, with a delayed neutron fraction of $6.51935x10^{-3}$, yielding a cold clean excess reactivity ($\rho$) of \$4.48. In a dry shutdown state the reactor was found to have a neutron multiplication number of 0.97928, giving the drums an insertion worth of -\$7.73.

The W-Re alloy cladding tubes have a unique property in the fact that the rhenium has an absorption cross section spike in the thermal region. A scenario of concern for all space reactors is that of accidental water submersion, which might occur if a reactor were to fall back to earth. In such a scenario, the reflection and thermalization due to neutrons scattering in the water could very well force a reactor into a supercritical state, thus causing a mechanical explosion. The rhenium in the cladding tubes for the reactor modeled in this study can prevent excursions caused by water submersion by absorbing the thermalized neutrons before they can induce fissions. The MCNP model was manipulated to model a fully submerged reactor to include a neutronically infinite medium of fresh water around the reactor and flooded coolant tubes. In a completely wet environment with the control drums rotated to the least reactive position the reactor was found to have a deeply subcritical neutron multiplication number of 0.88781. The model was repeated with the drums rotated to the most reactive position to yield a neutron multiplication number of 0.9027, which is still deeply subcritical. Table 1 demonstrates all of the critical properties for the Phoenix reactor; however, other critical scenarios such as impact compaction and submersion in sand have not yet been modeled.

**TABLE 1.** Critical Properties of the Phoenix NTP Reactor with 37 and 61 coolant channels per fuel hex

| **Configuration** | ***k (37)*** | ***k (61)*** |
|---|---|---|
| Open | 1.02099 | 1.03012 |
| Closed | 0.97914 | 0.97928 |
| Bare | 0.85138 | 0.85043 |
| Wet (open) | 0.90213 | 0.9027 |
| Wet (closed) | 0.87436 | 0.88781 |
| β | 0.00664081 | 0.00651935 |
| ν | 2.496 | 2.500 |

## III.B. Volumetric Energy Deposition

The volumetric heating rates within the core and reflectors were determined using a track length flux estimator modified to account for the interaction cross sections of fission as well as neutron and gamma scattering events. The heating rates were imported from the MCNP5 code to STAR-CCM for thermal hydraulic analysis of the core. Figure 3 demonstrates the volumetric heating profile in units of W/m$^3$ as a function of axial and radial position within the core.

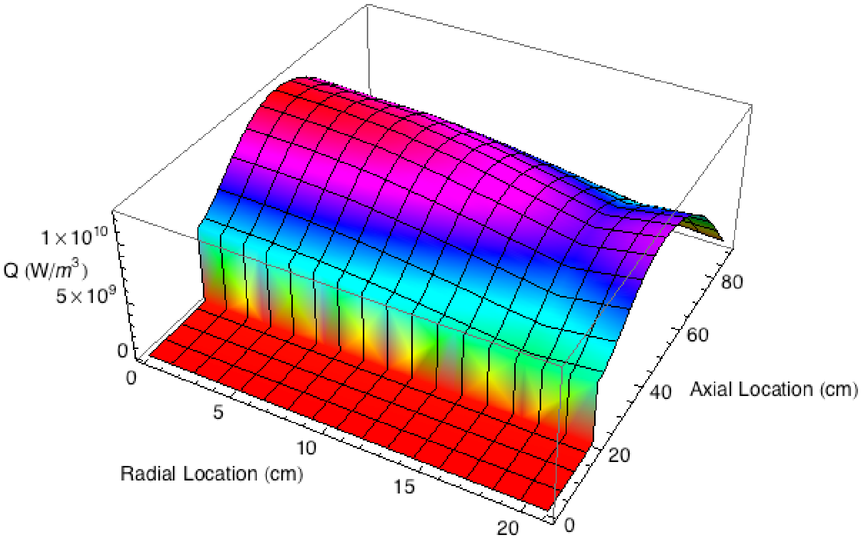

**FIGURE 3**. Volumetric heating rate in the Phoenix core as a function of radius and axial position.

Figure 3 demonstrates how highly reflected the reactor is as the flux and heating profiles decrease in a cosine fashion until the radial location of approximately 2/3$^{rd}$ the total core radius, where they begin to increase towards the radial reflector. The heating profile is very low over the first 20 cm in the axial dimension as expected. The first 20 cm of the fuel element are comprised of a BeO reflector, which is only heated through gamma and neutron scattering events. Each BeO section produces approximately 2 kW per fuel hex and each fueled portion generates an average of 3 MW. The power profile demonstrates that reactors of this power level do not need enrichment zoning in order to achieve a fairly uniform power distribution.

## IV. THERMAL HYDRAULICS

The phoenix NTP reactor is cooled with hydrogen at a mass flow rate of 12.06 kg/s. The hydrogen enters the core at a temperature of 300 K and a pressure of 5.5 MPa. The thermal-hydraulics calculation was performed using the STAR-CCM+ finite volume solver. The semi-structured mesh was generated using the GAMBIT software. Based on non-linear temperature dependent material properties,[12-20] core thermal-hydraulic optimization was performed. Due to the symmetry of the model, a 1/6 sector (60 degrees symmetry) was used to simplify the calculation and to speed up CPU calculation time.

### IV.A. CFD Methodology

The complete steady-state Navier-Stoke's equation, shown in Equations 1-3, was solved using the k-ε model to determine the turbulence in our system.

$$\nabla \cdot \left(\rho \vec{u}\right) = 0 \tag{1}$$

$$\nabla \cdot \left(\rho \vec{u} \otimes \vec{u}\right) + \nabla P = \nabla \cdot \vec{\tau} \tag{2}$$

$$\nabla \cdot \left[\rho\left(e + \frac{u^2}{2}\right)\vec{u}\right] + \nabla\left(\vec{u}P\right) = \nabla \cdot \left(\vec{u} \cdot \vec{\tau}\right) + \nabla \cdot k\nabla T \tag{3}$$

The solid equation was solved using the Laplacian heat conduction model demonstrated in Equation 4, with the energy source term from the neutronics calculation. A black body radiation model with an emissivity of 0.8 is applied to the outer shell exposed to vacuum.

$$\dot{Q} = \nabla \cdot k\nabla T \tag{4}$$

Significant time was spent to optimize the mesh configurations for both the 37 and the 61 coolant channel models in order to allow full convergence in 12 hours or less. Figure 4 shows the cross sectional CFD meshes for both the 37 coolant channel configuration and the 61 coolant channel configuration.

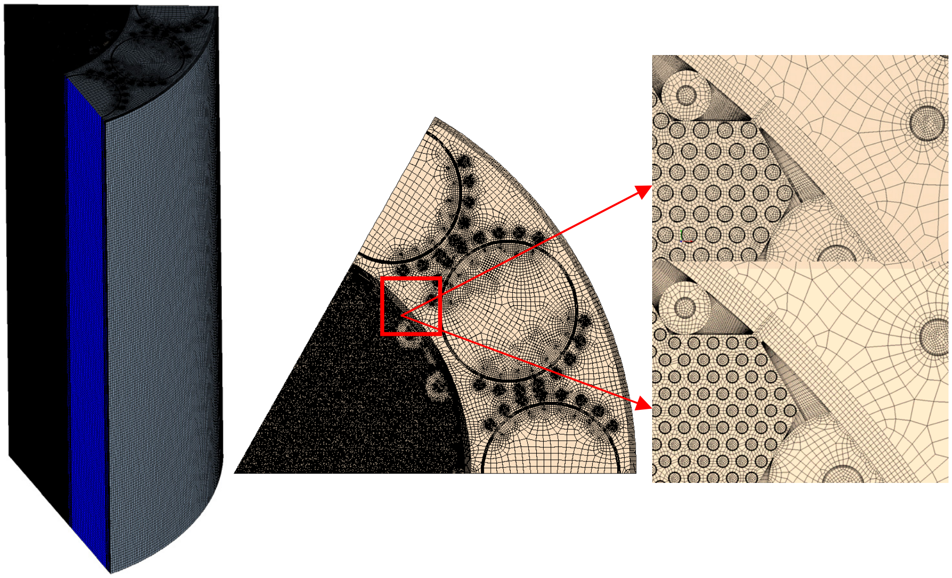

**FIGURE 4.** Cross Sectional Mesh of the full core (left) and a zoomed-in view of the 37 coolant channel model (top right) and of the 61 coolant channel model (bottom right) .

## IV.B. CFD Computational Results

The two models respectively consist of approximately 33.7 million and 40.1 million finite volume cells, allowing the thermal power profile to be calculated with an axial mesh spacing of 0.5 cm. A non-uniform mass flow rate was employed to take into account the non-uniform power profile in the radial dimension, thus allowing a more homogeneous temperature profile within the radial dimension. Basic calculations show that to achieve a specific impulse of 940 seconds with a thrust of 25,000 $lb_f$, a total mass flow rate of 1206 kg/s is required. Since this model was reduced to a 1/6 core model, the mass flow rate through the modeled section was held at 2.01 kg/s. Figure 5 demonstrates the average axial temperature profiles for both the CERMET fuel meat and the hydrogen coolant in the reactor, calculated using the STAR-CCM+ model.

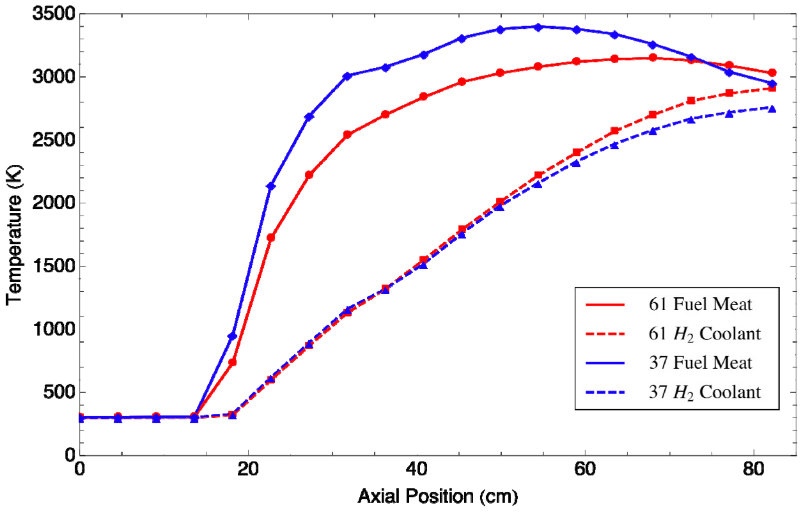

**FIGURE 5.** Axial Average Fuel Matrix Temperature Profile for the Fuel Meat and Hydrogen Coolant for the 37 Coolant Channel case (blue) and the 61 Coolant Channel Case (red).

The average hydrogen outlet temperature for the 37 and 61 coolant channel cases was approximately 2757 K and 2880 K respectively while the peak fuel temperature is at around 3600 K and 3470 K respectively. The 37 coolant channel model demonstrates a slight decrease in the temperature at an axial position of 40 cm; this short lived temperature decline is most likely due to a less than fully converged simulation. A cross-sectional temperature plot of the Z = 0.7 m plane are shown for the two cases in Figure 7 where the approximate peak temperature is observed.

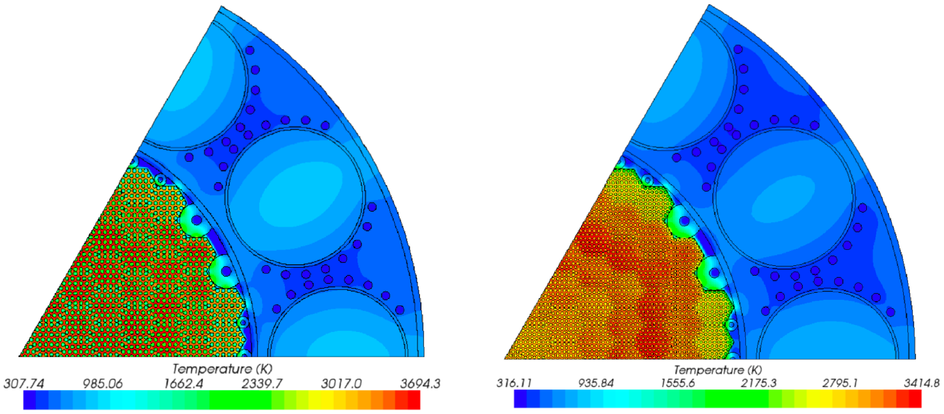

**FIGURE 7.** Temperature Profile of the Axial Location where Peak Temperature is observed for, 37 Channel (left) and 61 Channel (right).

As expected, due to the higher surface area to volume ratio, the peak temperature is lower for the 61 channel case than for the 37 coolant channel case. The radial temperature profile seen for the 61 coolant channel case in Figure 7 has its peak near a radial position of 17 cm, which is primarily due to the non-optimum mass flow rate distribution that is applied for this calculation. A non-uniform mass-flow distribution was calculated based on the power profile and mass flow rate per coolant channel in each block rings. In further studies, an optimization on the mass flow rate distribution must be performed to make the temperature profile as flat as possible in the radial direction. Figure 8 shows the radial dependence for mass flow rate modeled in the STAR-CCM+ code.

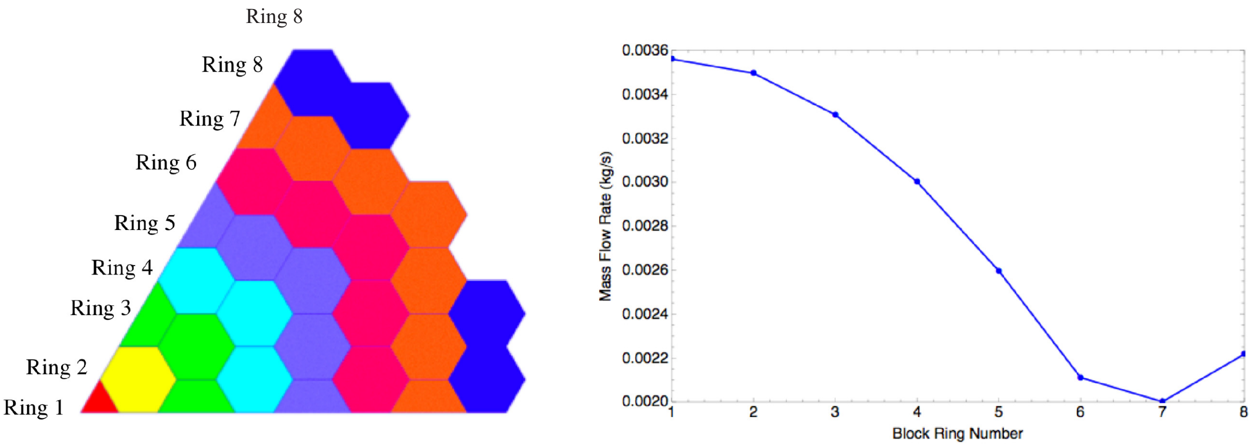

**FIGURE 8.** Mass Flow Rate Determination Diagram.

At the moment no hydrogen is pumped through the bypass flow area of the 61 coolant channel model. The bypass flow will substantially cool the outer blocks of the core, requiring less mass flow rate through these blocks, which can be diverted to cool the hotter spots to bring down the peak temperature. This optimization process is of interest to further design studies. At the end of the optimization phase, a grid convergence will be performed to assure convergence of the solutions in grid space.

## CONCLUSIONS

A computational model has been developed that combines the results of Monte Carlo neutronics and CFD thermal hydraulics calculations to determine spatial steady-state temperature profiles within a Nuclear Thermal Rocket engine. This model will be developed to include finer resolution in the hex power deposition profile as well as combine other programs such as MOCUP and DAGMC in order to account for time dependent burnup and a smoother power deposition profile transfer from MCNP to STAR-CCM+.

In order to prevent the melting and migration of the $UO_2$ fuel within the tungsten matrix, a CERMET NTR reactor should operate at a peak fuel temperature of 3000 K. Thus far the current suite of modeling tools seem to indicate that a fuel element containing a surface area to volume ratio of 0.3 (37 coolant channels) is insufficient to cool a 25,000 lbf NTR engine operating with a specific impulse of 940 seconds. The model consisting of 61 coolant channels (0.6 surface area to volume ratio) is more effective in cooling the core; however, the peak core temperature is still approximately 3400 K at the axial location of 0.7 m and the radial location of 17 cm. While the NTR modeled with the 61 coolant channels is still running to hot, it is believed that manipulation of the mass flow rate in the radial direction will keep all sections of the fission core at or below a temperature of 3000 K, with a power density of 9.34 $GW/m^3$. Future work will focus on reducing the core temperature to a maximum of 3000 K with the 61 coolant channel design. The core without any turbomachinery or attached nozzle was found to have a mass of 1984 kg, yielding a thrust to weight ratio of 5.7, which would most likely decrease to 5.0 when turbomachinery and the nozzle apparatus is attached.

# NOMENCLATURE

$\rho$ = density ($kg/m^3$) or reactivity ($)
$\tau$ = shear stress ($N/m^2$)
$e$ = internal energy (J)
$u$ = velocity (m/s)
$k$ = thermal conductivity (W/m-K) or neutron multiplication number
P = Pressure (MPa)
T = temperature (K)
Q = energy addition rate (J/s)

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