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Preliminary Benchmark Uncertainties for Deimos, a HALEU-Fueled and Graphite-Moderated Advanced Reactor Testbed

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INTRODUCTION

Many advanced reactor concepts will make use of various uranium fuels with levels of enrichment higher than previously seen in current light water reactors. In particular, High-Assay Low Enriched Uranium (HALEU), that is uranium enriched to $^{235}U \approx 20$ w/o% , is planned to be used in over ten new reactor concepts [1]. HALEU is attractive for advanced reactors as it enables longer intervals between refueling. Unfortunately, little to no experience with HALEU is available in experimental literature raising concerns for not only licensing advanced reactors but also fabrication and transportation of HALEU fuels [2]. This is where Deimos, a Los Alamos National Laboratory internal project, comes in. Deimos is a new critical experiment scheduled for FY24 at the National Criticality Experiments Research Center (NCERC). Deimos is a graphite moderated, graphite and beryllium reflected critical experiment making use of HALEU TRi-structural ISOtropic (TRISO) fuel from the Compact Nuclear Power System (CNPS) [3]. This transaction entails a brief description of efforts to benchmark Deimos for inclusion into the International Criticality Safety Benchmark Experiment Project (ICSBEP) Handbook [4].

DEIMOS CONFIGURATION

Deimos's primary purpose is to serve as the technical validation basis for many upcoming advanced reactor designs, the majority of which deviate from the typical light water reactor. For this reason, Deimos is comprised of a graphite moderated core with a beryllium reflector. The fueled core region is broken into five main components, a central cylindrical inner core and four outer core corner monoliths. In addition to these fueled graphite areas, there are graphite pieces that form both lower and upper reflectors to the core. Outside of the fueled region there is a beryllium reflector used to limit the size of the system by providing additional reactivity. This beryllium reflector, though solid in Figure 1, is actually hundreds of individual beryllium pieces from the Honeycomb critical assembly [5]. The end result is a critical assembly that is roughly a 5' x 5' x 4' rectangular prism.

The inner and outer core pieces have channels to accommodate over 300 fueled graphite rods between them, though this is much more reactivity than is needed to go critical. Therefore in the actual experiment the most outer perimeter is not fueled. Each graphite rod, referred to as "graphite cups", are one meter long graphite tubes in which 19 fuel compacts are held. The fuel compacts are from Compact Nuclear Power Source (CNPS) experiments back performed in the late 1980s at TA-18 at LANL [3]. The compacts, shown in Figure 2, were manufactured by General Atomics by converting 19.91% enriched UO_3 powder into UCO kernels. These kernels, were then coated with concentric layers of SiC and pyrolytic carbon to form TRISO particles 0.87 mm in diameter. Hundreds of individual particles are then pressed into a graphite substrate and baked to form the fuel compact. The dried compacts are roughly two inches long and one-half inch in diameter. The volumetric packing fraction of the CNPS TRISO is 60.1% whereas contemporary compacts have packing fractions near 40%. The outcome of the higher packing fraction is a higher fuel density, but it comes at the cost of a rather crumbly compact.

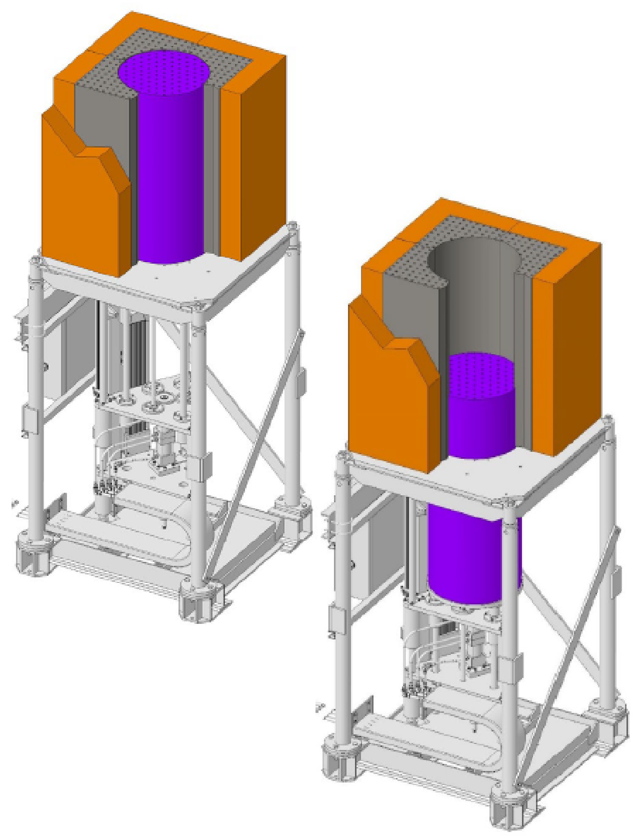

Fig. 1: Engineering assembly of the Deimos experiment on top of Comet. The inner core (purple and outer core (grey) are made of graphite and the axial reflector is beryllium (orange).

Neutronic models of Deimos were developed to inform the engineering design of the system as well as predict the reactivity of the system during loading sequences. These models were initially created in MCNP 6.2 ®[6][1] and later revised in 6.3 and developer versions. The latter enables the use of delta-tracking to speed up the computation time of the fully modelled TRISO particles [7]. Simplifications such as removing the Comet vertical lift machine and homogenizing the beryllium reflector into a single piece were done to aid in lowering model complexity and speeding up simulation time. Other than those changes, the core was simulated as is for the following uncertainty analysis.

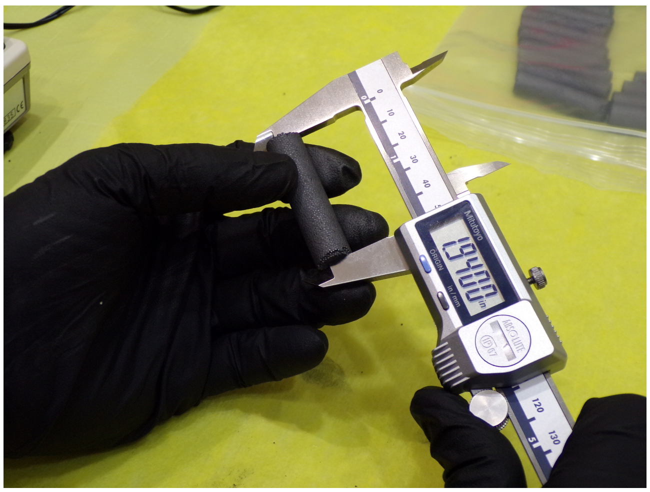

Fig. 2: Photo of a HALEU TRISO compact from the CNPS taken during the 2021 unpacking at NCERC.

UNCERTAINTY ANALYSIS

As Deimos is an advanced reactor testbed, desired outcome from the experiment is to create a benchmark from which reactor engineers can validate their designs on.Benchmarking is a rigorous peer-review of an experiment to go over any and all areas of uncertainty and how this affects the reported multiplication factor k_{eff}[4]. Uncertainties are most often cited in terms of per cent mille (pcm) or 0.001% of k_{eff}. Variations in key system factors such as enrichment, component dimensions, densities, material impurities, and temperature are all studied to see their impact on the final uncertainty. Critical experiments with total uncertainties $\leq$ 150 pcm are considered exceptional. Whereas uncertainties between 150 and 250 pcm are common and generally acceptable in modern experiments. Experiments that are older, missing key uncertainties, and/or have poor recording of experimental conditions can have uncertainties ranging well into the 400s - 1000+ pcm.

As the Deimos experiment has not been fully executed yet, a preliminary benchmarking effort was undertaken to identify key areas which the experimental team can focus on to reduce uncertainties during execution. Hence, for the sensitivity and uncertainty methods below some of these values had to be estimated for the evaluation. Uncertainty analysis involves perturbing the model in order to obtain sensitivities of $k_{\text{eff}}$with respect to a certain parameter, p.

$$S_{k,p_i} \equiv \frac{p_{i,0}}{k_{eff,0}} \frac{\delta k_{eff}}{\delta p_i}\bigg|_{p_i=p_{i,0}} \tag{1}$$

Here δp_i is the perturbation to initial parameter $p_{i,0}$. The sensitivity is then multiplied by the relative uncertainty ($\frac{\delta p_i}{p_{i,0}}$) in the experimental parameter to get the propagated uncertainty in terms of k_{eff}, Equation 2 [8].

$$u_{k,i} = \frac{\delta p_i}{p_{i,0}} k_{eff,0} |S_{k,p_i}| \tag{2}$$

Two methods for calculating sensitivity were utilized for this work, adjoint-based sensitivity and finite central difference. The former utilizes an adjoint neutron flux during the transport solver to calculate sensitivities to isotopes (densities). The latter, shown in Equation 3 is a direct perturbation to the model geometry with a positive and negative perturbation to then calculate the slope (sensitivity).

$$S_{k,i} = \frac{1}{2\delta p_i} |k_{eff}(p_{i,0} + \delta p_i) - k_{eff}(p_{i,0} - \delta p_i)|, \tag{3}$$

Of course using the central difference method, one already obtains the actual change in $k_{\text{eff}}$from the perturbation calculations so the uncertainty can be calculated as Equation 4.

$$u_{k,i} = \frac{p}{2\delta p_i} |k_{eff}(p_{i,0} + \delta p_i) - k_{eff}(p_{i,0} - \delta p_i)|, \tag{4}$$

MCNP6.3 and ENDF/B-VIII.0 [9] data library were used for all the adjoint and central difference sensitivities calculations.

RESULTS

To begin the sensitivity studies, an adjoint-based calculation was performed to see which isotopes were contributing to reactivity the most. As Table I reports, ^{12}C and ^{9}Be contribute the most to k_{eff}, moreso than even ^{235}U, the fissile fuel. The third and fourth top contributors are thermal scattering laws for the beryllium and graphite pieces. Finally, ^{238}U and ^{10}B round out the list with both acting as poisons, ^{238}U in the TRISO and ^{10}B in the graphite.

TABLE I: Major Isotopes of Interest

Isotope	Sensitivity
^{12}C	0.4288
^{9}Be	0.1582
^{235}U	0.1135
^{9}Be - TSL	0.1086
^{12}C - TSL	0.0847
^{238}U	-0.0481
^{10}B	-0.0173

The results shown in Table I were used to guide decisions on which isotope to focus on and studies into the dimensions and densities of the moderators and reflector were undertaken as were studies into the fuel enrichment and packing fraction of the compacts.

[1]MCNP® and Monte Carlo N-Particle® are registered trademarks owned by Triad National Security, LLC, manager and operator of Los Alamos National Laboratory. Any third party use of such registered marks should be properly attributed to Triad National Security, LLC, including the use of the designation as appropriate. For the purposes of visual clarity, the registered trademark symbol is assumed for all references to MCNP within the remainder of this paper.

Core Component Dimensions and Densities

The uncertainty analysis started with the volume and densities of the graphite and core components, as they appeared to be the most sensitive for system reactivity. Adjoint weighting methods via the KSEN card in MCNP were used to analyze the impact of changing various carbon and beryllium pieces' densities by 0.1% [10]. The impact of this study is shown in Table II with only the beryllium having a noticeable impact on k_{eff}. However, it's important to note that this is for a 0.1% uncertainty on the density which is unlikely for the beryllium reflector let alone the graphite pieces. If the uncertainty on the graphite density is 1% then the uncertainty is roughly 20 pcm which is more reasonable from both manufacturing tolerances as well as previous experiments. Beryllium being a metal can have an uncertainty on density around 0.2% but this may be impacted from the homogenization done by combining individual beryllium pieces into a single reflector component in the model. When these more realistic uncertainties are added, the densities are contributing nearly 100 pcm worth of uncertainty.

TABLE II: Impact of Densities on Reactivity

Component	$\Delta k_{\text{eff}} \pm 0.1\%\rho$ **(pcm)**
Inner Graphite Core	1.921
Outer Graphite Core	1.927
Be Reflector	22.61
Inner Core Bottom	1.652
Top Reflector	2.191

Besides adjusting the densities of the major components, the dimensions were also studied. In particular the major dimensions of the largest components were varied to see what the impact would be on k_{eff}. From Table III, it's seen that only the air gap between the inner and outer core seems to give significant contributions. Uncertainties relating to the individual fuel channels and the air gaps present in those were considered but measurements using a coordinate measurement machine (CMM) showed that they were minimal (≤ 3/1000").

TABLE III: Impact of Dimensions on k_{eff}

Core Piece	**Parameter Change**	$\pm\Delta k_{eff}$ **(pcm)**
Inner Core OD	±0.01"	± 55
Outer Core ID	±0.01"	± 42
IC Bottom Height	±0.2"	± 15
Core Height	±0.2"	± 6

CNPS Compacts and Constituent TRISO Uncertainties

Parameters relating to TRISO particles such as the packing fraction (PF) and the enrichment of the fuel were analyzed as these parameters are some of the hardest to quantify from the older CNPS fuel. Packing fraction was adjusted by performing a finite central difference method by manual perturbation of the cell volume used in the MCNP lattice geometry. The mean packing fraction of 60.1 volume% was perturbed ±2%, which is assumed to be a bounding value for purposes of this preliminary evaluation. The effect of this perturbation, IV, is quite significant resulting in k_{eff} uncertainty of 361 pcm.

TABLE IV: Packing Fraction Sensitivity on Reactivity

Packing Fraction	$\mathbf{K}_{eff}$
58.1%	1.00734
60.1%	1.01025
62.1%	1.01358
Sensitivity	90.25×10^{-2}

As this is the dominating uncertainty discussed, serious efforts were undertaken to determine ways to better characterize the TRISO fuel compacts, including destructive analysis of two compacts. Enrichment is another fuel characteristic expected to have a high sensitivity. For this calculation the ratio of $^{235}U/^{238}U$ was perturbed so the resulting enrichment was ±0.1 wt.% from its nominal value of 19.9 wt.%. The effects of changing the enrichment by 0.05 wt.% is unclear due to the nonlinear effects of changing the $^{235}U/^{238}U$ ratio. The range of enrichment for the UCO kernels has a large sensitivity and is again an area of interest to be reduced in the final benchmark evaluation. Studies have shown that this can be reduced by a combination of SIMS and inductively coupled plasma mass spectroscopy (ICP-MS) analysis.

TABLE V: Enrichment Sensitivity on Reactivity

Enrichment	$\mathbf{k}_{eff}$
19.85%	1.01057
19.90%	1.01025
19.95%	1.01122
Sensitivity	7.51×10^{-4}

Combined Uncertainty

An approximated uncertainty for k_{eff} can be obtained by summing all the uncertainties in quadrature. The results for the total uncertainty from applied uncertainties is presented in Table VI. According to the analysis here, an uncertainty of at least 222 pcm is expected for the Deimos experiment. This uncertainty is driven largely from the description of the fuel compacts which given their age and poorer quality information is understandable. As mentioned earlier, characterization of the HALEU compacts and constitute TRISO particles is necessary for a successful benchmark and the experiments are looking into a suite of analytical tests to be done on two sacrificial compacts. Careful mass and volume measurements using calibrated scales, calipers, and CMM are expected to be

TABLE VI: Combined k_{eff}Uncertainty

Uncertainty (Perturbation)	Δk_{eff}
Enrichment (0.5%)	0.00075
Packing Fraction (1%)	0.00180
Density (0.2% Be and 0.7% C)	0.00105
Volume Uncertainties (0.001 in.)	0.00015
Total Expected k_{eff} Uncertainty	0.00222

able to minimize the volume and density uncertainties.

FUTURE WORK AND CONCLUSION

The preliminary uncertainty analysis for Deimos was performed to gauge the expected uncertainties related to the experiment as well as highlight areas where extra effort should be expended to lower uncertainties. To this end, sensitivity analysis of MCNP models led to the conclusion that the density of the major assembly components as well as the characteristics of the HALEU TRISO compacts were the dominant factors. Further measurements for these two areas are planned as part of the benchmarking work and are expected to provide a tighter bounding on the uncertainty. Besides these measurement areas, expanding uncertainty analysis to temperature is a key next step. Temperature impacts not only the density but the Doppler broadening of resonance as well as thermal scattering corrections. The latter is also dependent on the type of graphite used which is another area of study as there are varying opinions relating the density to porosity and how this should be corrected with nuclear data models. With these areas addressed, Deimos should have uncertainties below 300 pcm and be the first graphite moderated, beryllium reflected HALEU TRISO reactor benchmark.

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