TREAT LEU Conversion Analyses Performed 2016-2018

Nuclear Science & Engineering Division

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Executive Summary

TREAT is an experimental nuclear reactor designed to produce high neutron flux transients for the testing of reactor fuels and other materials. After more than 20 years of non-operational standby, TREAT has been restarted under the U.S. Department of Energy's Resumption of Transient Testing Program. The conversion of TREAT from its current highly enriched uranium fuel to a low enriched uranium fuel is being pursued in keeping with the mission of the Department of Energy National Nuclear Security Administration's Material Management and Minimization Reactor Conversion Program. This report documents additional analyses performed over the timeframe of 2016 to early 2018 to evaluate the LEU Conceptual Design for the TREAT reactor, following the initial design studies documented in the 2016 Conceptual Design Report. The analyses documented in this report include neutronic and thermal hydraulic sensitivity studies to evaluate the effect of key design parameters on predicted core behaviors, as well as a simple investigation into the effect of fuel thermal expansion.

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1 Introduction

The Transient Reactor Test Facility (TREAT) is an experimental reactor designed for transient testing of reactor fuels and other materials. TREAT is located at the Idaho National Laboratory (INL) and was operated from 1959 until 1994, when it was placed on non-operational standby. TREAT has now been restarted under the U.S. Department of Energy's (DOE) Resumption of Transient Testing Program. In addition, work was performed for several years to support the conversion of TREAT from its current highly enriched uranium (HEU) fuel to low enriched uranium fuel (LEU, defined as uranium with $<20\%$ ^{235}U), in keeping with the mission of the DOE National Nuclear Security Administration (NNSA) Material Management and Minimization (M3) Reactor Conversion Program. At this time, the TREAT LEU convert program is now entering a cold standby.

Following pre-conceptual and conceptual phase LEU fuel design analyses [1-3], a baseline conceptual LEU fuel design was established in collaboration with INL and Los Alamos National Laboratory (LANL). Detailed analysis of the TREAT LEU conceptual design (LEU-CD) was presented in the March 2016 report ANL/RTR/TM-16/1 [4], with a subset of this information also included in the TREAT convert program's conceptual phase deliverable report.

This report documents additional studies of the TREAT LEU Conceptual Design, which were performed over the timeframe of 2016 to early 2018, following the publication of ANL/RTR/TM-16/1. Neutronic and thermal hydraulic simulations were performed to evaluate the effect of changes in key design parameters on the predicted behavior of the LEU-CD core. In addition, a simple study of fuel thermal expansion was performed, in order to confirm that thermal expansion has a negligible effect in the TREAT core.

It is anticipated that the performance requirements for an LEU conversion of TREAT could be further refined in the future. In particular, there could be further clarification of requirements for core transient behavior. Both the initial conceptual design study and the studies discussed in this report focused on the primary performance parameter of achievable energy deposition in the test samples being irradiated in the TREAT core.

2 Model and Methods

2.1 TREAT Description

TREAT is a homogenous, air-cooled, graphite-moderated and graphite-reflected reactor currently fueled with 93% enriched UO_2 dispersed in graphite, with a fuel carbon-to- ^{235}U ($\text{C}/^{235}\text{U}$) ratio of approximately 10000:1.

The reactor cavity can accommodate a maximum of 361 assemblies in a 19x19 array. The TREAT fuel elements are approximately four-inch x four-inch square, with an active ~four-foot long zircaloy-clad fuel region and ~two-foot long aluminum-clad graphite reflectors above and below the fuel region. The fuel assemblies feature chamfered corners, which form square passageways for forced flow of cooling air provided by two blowers. The air flow through the core travels downward axially from the top of the core. TREAT is controlled by a set of B_4C -bearing control rods, arranged in three banks: (1) four pairs of control/shutdown rods, used to set the reactor to a critical state, (2) four pairs of transient rods, used to introduce the reactivity changes which drive TREAT transients, and (3) four compensation/shutdown rods which are used for reactivity compensation when an experiment vehicle is removed.

During irradiation experiments, a small number of fuel assemblies (typically two to four) near the center of the core are replaced with an experiment vehicle containing the test sample(s). Graphite dummies are utilized in corner locations as needed to provide the core loading size required for appropriate excess reactivity. In addition, a central row (or half row) of fuel assemblies is frequently removed in order to provide an unimpeded path for neutron travel between the test sample and an ex-core neutron collimator and detector system called the hodoscope. The TREAT core is surrounded by a radial graphite reflector, which is in turn enclosed in a concrete bioshield. Both the reflector and bioshield feature a variety of holes to allow for instrumentation use. Detailed descriptions of the current HEU fuel assembly design and TREAT facility can be found in previous conversion team reports [1, 5] and in the facility's design summary report [6].

2.2 LEU Conceptual Design

The TREAT LEU Conceptual Design (LEU-CD) was established based on lessons learned in the analysis and fabrication development efforts of the pre-conceptual and conceptual phases of the project [1-3]. The baseline design parameters and key assumptions are outlined in the November 2015 revision of the program's analysis guide [7].

The LEU-CD fuel element is similar in geometry to the existing HEU fuel element, and is designed to fit into the existing core layout on the current grid plate. Like the HEU, the LEU-CD is fueled with UO_2 dispersed in graphite. Key differences between the LEU Conceptual Design and the existing HEU fuel are listed in Table 1. Additional detail on the design, as well as the calculated performance of the LEU-CD core, can be found in ANL/RTR/TM-16/1 [4]. It should be noted that for the LEU design, the carbon-to-uranium ratio is generally reported as carbon-to-total uranium, rather than just ^{235}U as was typically reported for the HEU fuel. The HEU C/U value is similarly reported relative to total uranium in this table, for comparison with the LEU value.

Table 1. Key Properties of the HEU and LEU Conceptual Design TREAT Fuel

	HEU	Conceptual Design LEU
Cladding Material	Zircaloy-3 (Fuel) / Aluminum (Reflectors)	Zircaloy-4 (Single Can)
Cladding Thickness	25 mil	25 mil
Fuel-to-Clad Gap	50 mil	15 mil
Fuel Graphite Content*	59%	85%
Fuel Boron Impurity	7.6 ppm	2 ppm
Fuel Density	1.73 g/cm ³	1.85 g/cm ³
C/U_{total}	9257	2370

* Ratio of graphite-to-total carbon in the fuel mixture

2.3 Analysis Tools and Methods

Steady-state neutronic modeling was performed using the MCNP5 v1.60 Monte Carlo software code [8], with ENDF/B-VII.0 cross-sections used as the reference set. Transient analyses are performed with TREKIN, a point kinetics code which was used during TREAT's original operation, and which has been updated for use in an Excel-based environment [9]. The historic M8CAL experiment [10] is used as the reference core loading. M8CAL was one of the latest, best-documented historic experiments. Its loading is consistent with the core loading utilized in the restart of TREAT. In addition, the M8CAL core's characteristics, such as a large loading and highly-absorbing experiment vehicle, are considered consistent with anticipated near-term future needs of TREAT. Thermal hydraulic modeling is performed using the

finite element software COMSOL® [11]. This thermal hydraulic modeling utilizes power distribution and power-time history information produced in the MCNP and TREKIN simulations.

Overall, analysis of the TREAT LEU design is intended to ensure that the design can meet core performance needs, while continuing to operate safely. The analyses presented in this report focus on evaluation of key core properties, including excess reactivity and peak fuel temperature, as well as the neutronic relationship between the TREAT core and experiment test samples. The most important test sample-related property is the achievable test-sample total energy deposition (TED). The TED is related to core operation through a parameter called the power coupling factor (PCF). The PCF represents the ratio of test sample power (or energy) per unit test sample mass to total reactor core power (or energy), and it is typically expressed in units of W/g/MW or J/g/MJ. The PCF is dependent upon a number of variables, including the neutron energy spectrum in the core and the composition and geometry of the test samples and experiment vehicle. A lower PCF means that more core energy is needed to achieve the same test sample TED. In the LEU design analysis, the calculated PCF for a given experiment is reported relative to the corresponding PCF calculated for the same experiment in the HEU core model, as a ratio (LEU Core PCF)/(HEU Core PCF) reported as a percentage.

3 Thermal Hydraulic Sensitivity Studies

A key limiting factor, which dictates allowable TREAT operation, is the peak temperature experienced by the TREAT fuel assembly cladding. Temperature limits of the cladding are in place to minimize oxidation and to prevent material phase change. In the HEU-fueled TREAT core, there is a temperature limit during normal operation (Limiting Safety System Setting, or LSSS) of 600°C, and an accident scenario temperature limit (Safety Limit, or SL) of 820°C. The converted LEU core therefore must be able to match HEU core performance for any transient which the HEU core can perform within these temperature limits.

The thermal-hydraulic analyses in this report examine the impact of thermal and geometrical properties of the fuel assembly on peak fuel temperatures, fuel cooling times, and corresponding cladding metal loss (by oxidation). Key thermal properties investigated are fuel heat capacity and density, fuel thermal conductivity, and contact resistance between adjacent fuel blocks. Cladding thickness was also investigated as a parameter. The purpose of this scoping analysis was to assist the discussions with the fuel manufacturers and the determination of the LEU fuel design requirements.

3.1.1 Cooling Time History and Cladding Oxidation

3.1.1.1 Model Description

Cooling time histories evaluated for a single fuel assembly have been analyzed with a 3D transient thermal-hydraulic (TH) model using the finite element software COMSOL®. The model and assumptions have been documented in previous reports [3, 4], and only key model assumptions and dimensions are summarized below.

The geometry for the LEU design concept fuel assembly is shown in Figure 1. Assuming negligible heat transfer between neighboring fuel assemblies, symmetry is utilized for the geometrical domain (a 1/8th section of the fuel assembly is modeled). The central section of the fuel assembly consists of twelve vertically stacked four-inch tall blocks to generate a four-foot fuel section. In direct contact, above and below the fuel section, are two ~24 in long blocks of graphite reflector. The cross-section of a fuel assembly (including cladding) is 3.96 in square with 0.625 in of chamfered corners. There is a nominal 0.040 in gap between adjacent assemblies on the flat region (sides) which, is assumed to be maintained across the reflector and fuel areas of the assemblies.

Figure 1. COMSOL® model of a single TREAT LEU fuel assembly, A) Cross-sectional view, B) Axial view showing reflector and fuel block region.

A single 25-mil thick can of Zircaloy-4 is used for the cladding material for the entire fuel assembly and is separated from the fuel and reflector by a 15 mil nominal gap around the entire fuel and reflector block circumference. The gap is not maintained around the full periphery of the fuel block in actual operation, however. The evacuation of the fuel-cladding gap during the manufacturing process will cause deflection of the cladding inward from the differential pressure between the evacuated inside and ambient air pressure. The deflection causes gap closure over portions of the can thus keeping the fuel and reflector blocks centered. Structural analyses performed by the INL team estimate 57% the cladding at the side region would be in contact with the fuel. Due to standardized dimensions of Zircaloy-4 sheets, it is possible that the cladding thickness may be increased to 26 mil in future updated LEU design iterations. The total cross-sectional areas of both the fuel and reflector blocks respectively is expected to remain the same, however, to a nominal area of 14.699 sq-in.

3.1.1.2 Cooling Assumptions

The reactor is cooled by an induced draft air system, and the cooling is controlled by two turbo-compressors, or blowers, operating in parallel. Under normal operation, TREAT may operate with one or two blowers. In the original TREAT core, each blower was rated at 3250 cfm [6]. For the reference TH model, the nominal flow-rate for each blower assumes 92% of rated capacity (3000 cfm). The blowers were replaced during the TREAT upgraded core modifications, and the current blowers have a capacity of 4000 cfm each.

The flow-rate entering the core was evaluated assuming normal temperature and pressure (NTP; i.e. $T=25^{\circ}\text{C}$ and $P=101.325\text{ kPa}$). It was identified following this work that given the elevation of TREAT, the pressure at the facility is lower than this value, estimated at 84.43 kPa at 25°C . Additionally, it is known that the *mass flow rate* is not constant, but is a function of inlet pressure and *temperature* to the blower, and that there may be pressure drop through the core. Due to a lack of measured data prior to TREAT restart, only limited validation of the thermal hydraulics models was feasible under the convert project. Additional benchmarking with new restart was not performed by the convert project, due to the project's standby. However, the reported work is still considered acceptable and conservative because it utilized the more conservative lower value 6000 cfm assumption (relative to the actual 8000 cfm capacity), and because the primary objective was HEU to LEU core comparisons and the same cooling assumptions were used for both cores. Additionally, it has been established in other analyses that the core cooling does not affect peak fuel and cladding temperature. Even with maximum air-flow, the fuel assembly remains near adiabatic conditions even minutes after the transient.

The flow through the system is distributed within three regions in the core denoted as R_i (see Figure 2), wherein four neighboring fuel assemblies form a cooling passage. 91.5% of the total air flow enters region

R_1 , which is assumed to be distributed uniformly across all assemblies in the core. The rest of the flow (8.5%) through the system is distributed equally in the flow passages between the radial reflector and core (Region R_2) and reflector/bio-shield (Region R_3). The areas and hydraulic diameters of the respective flow sections are based on nominal dimensions and clearances. In region R_1 , based on equal pressure drop along all of the channels, the majority (95.75%) of the air flows along the coolant passages formed at the chamfered corners of neighboring assemblies (CR) and 4.25% flows along the flat (side) regions of the assemblies (SR).

Figure 2. a) Schematic cross-section of TREAT, b) Four neighboring fuel assemblies form a cooling channel.

It should be noted that the flow distribution as calculated is based on an assumed uniform temperature (25 °C) across the core. However, in reality energy is not symmetrically deposited within the assemblies resulting in a non-uniform temperature distribution across the core (radially and axially). The non-uniform temperature will affect the flow distribution with more flow passing through the colder regions of the core. The flow distribution due to temperature non-uniformity could be further investigated using measured data from the restarted TREAT core. Traditionally in TREAT analysis (throughout TREAT's original operation) an assumption of uniform flow distribution was always used.

3.1.1.3 Fuel Geometry, Thermal Properties and Cladding Oxidation

The fabrication processes for fuel blocks and the final element are currently in development. The preferred design at this point are fuel blocks 4x4x4 inches using overcoat-compacting methods for fabrication. Desired thermal properties of the fuel are heat capacity within 3% of ASTM grade graphite, minimum density of 1.82 g/cm³, and thermal conductivity similar to or higher than the current HEU fuel. The LEU conversion program has considered the idea that if it were determined that acceptable fuel properties cannot be produced in the 4x4x4 inches configuration, blocks could be fabricated as 1 or 2 inch cubes which are then assembled to form a 4x4 inch cross-sectional area. Obtaining a high thermal mass, or heat absorbing capability of the fuel block, is important as this allows the LEU core to generate more core energy than the HEU core for the same peak fuel temperatures. Thermal conductivity of the fuel and contact resistance between individual fuel blocks, are inherently connected to the cooling behavior of the fuel assembly following a high power transient. The amount of oxidation of the cladding will depend on the cumulative temperature-time history that the cladding has experienced.

Thermal conductivities measured by LANL/INL [12] for a set of early LEU fuel development blocks are shown below in Figure 3. Characterization of LEU feasibility fuel compacts show a measured thermal conductivity between 12.7-19.1 W m⁻¹ K⁻¹. The difference in thermal conductivity (60-100% relative to the

HEU) is subject to uncertainty due to crack formation during compaction and outgassing. The fabrication development efforts have continued to produce more recent blocks which demonstrate improvements; the data from the early blocks was utilized for this study.

Figure 3. a) Axial thermal conductivity of LEU fabricated compacts

The reference TH model assumes an average thermal conductivity measured at INL based on four BWX Technologies (BWXT)-manufactured samples fabricated by overcoat-compacting methods [13]. Radial conductivity has been measured on some samples indicating (when compared to the axial conductivities) a high degree of anisotropy in thermal conductivity, as shown in Figure 4.

Figure 4 Reference thermal axial (circles) and radial (squares) conductivity values.

The sensitivity of fuel thermal conductivity (axially and radially) as well as fuel block geometry (1-4 inch cubes) on cladding oxidation has been evaluated for both normal operation and for an accident scenario. The axial and radial thermal conductivities as functions of temperature were varied between +/- 50%

relative to the LEU reference conductivities (Figure 4). For the investigation of contact resistance, data was used from preliminary measurements performed by LANL [14]. In these measurements, contact resistance was measured for two disks in contact, with no contact pressure, for both as-formed as well as machined surfaces.

In the cooling time history calculations, contact resistance between graphite blocks was varied from $4 \times 10^{-4} \text{ m}^2 \text{ K W}^{-1}$ (smooth surfaces) to $5 \times 10^{-3} \text{ m}^2 \text{ K W}^{-1}$ (conservative, upper-bound value). Cooling time histories assuming no contact resistance were analyzed as well for a comparison. Operational peak fuel temperatures ranging from 400°C to 600°C were considered in this study, to evaluate a range of high power transients. During normal operation, the reactor is always assumed to be convectively cooled by air at flow-rates up to 6000 cfm within 5 minutes after a transient. The accident scenario assumes no flow conditions (free convection ignored) and cooling occurs only due to thermal conduction. For the accident scenario all of the reactivity available at the beginning of the planned bounding shaped transient is inserted as a step. Peak fuel temperatures were investigated in the accident analyses, with 820°C as an upper bounding case. For each cooling time history, the cumulative metal loss of the cladding (Zircaloy 4) was evaluated based on post-transition corrosion kinetics¹. Details regarding corrosion kinetics have been reported in an earlier report [4]. Use of such kinetics may be viewed as conservative for periods where the cladding has not yet attained the post-transition region (i.e. the oxide layer remains dense and adherent to the metal).

3.1.2 Cladding Oxidation – Normal Operation

3.1.2.1 Base Case

Cooling time histories as a function of air flow-rates and peak fuel temperatures have been analyzed previously both during transients as well as at constant power operation [4]. An example case of cooling time history used for reference considers a peak fuel temperature of 600 °C, an air-flow of 3000 cfm through the core, with reference values of thermal conductivity and no contact resistance, Figure 5a. The temperature is shown at three different locations along the periphery of the cladding, denoted as T-S, T-SC, and T-C (side, side/corner, and corner points), respectively. The temperature of the cladding at the side location increases quickly until it approaches the fuel temperature. At that point, the time for that region of the cladding to cool down to near ambient temperature is nearly the same as for the peak fuel temperature. In contrast, the section of the cladding at the corner region (T-SC and T-C), which is where the majority of the cooling occurs, remains substantially cooler. Changing the cladding thickness from 25 to 26 mil did not change the temperature profiles of the cladding during cooldown (less than 0.1 °C difference).

The corresponding effect of cladding corrosion (metal loss) as function of peak fuel temperature (400-600°C) is shown in Figure 5b. Most of the corrosion of the cladding occurs in the fuel section of the assembly where the cladding is hottest. The metal loss peaks near the fuel mid-plane (highest axial power) and decreases rapidly to virtually zero near the reflector region. Most of the metal loss in the fuel region of the assembly will occur in the initial stages of cooling when temperatures remain high. Once temperatures are below 500 °C, corrosion rates are substantially reduced. Further, the metal loss at the corner section of the cladding will remain low, approximately 50 times lower than the side section due to the lower temperatures observed at the cooling channel.

¹ During the initial, pre-transition oxidation, the kinetic growth rate is usually controlled by cubic or parabolic kinetics and the reaction progresses by oxygen transport through a growing, protective, oxide layer. The post-transition regime reflects a break-down of the oxide scale with an increase in oxidation rates and transition to linear kinetics.

Figure 5a) Temperature of the Cladding at Three Different Locations as Function of Cooling Time (for 600°C Peak Fuel case). b) Axial Variation of Cladding (T-S) Metal Loss as Function of Peak Fuel Temperature

In evaluating lifetime oxidation of the TREAT fuel assembly cladding, the HEU core Safety Analysis Report utilizes a conservative assumption that each year the reactor performs 20 transients which reach 600°C, 60 transients which reach 500°C, and 120 which reach 400°C. In the lifetime calculation it is assumed that the same location experiences the peak temperatures for all 40 years.

The same set of assumptions are currently used for the LEU core. Assuming that cumulative oxidation does not impact cooling times considerably, the metal loss projected during 40 years of operation is shown in Figure 6. Here, the metal loss refers to the point of the cladding that experiences the highest temperature (fuel mid-height and side section of the cladding). As seen, temperatures reaching 600 °C contribute nearly 90% of the cladding loss, while corrosion at temperatures 400 °C or below is negligible. The amount of flow rate through the reactor has a significant impact on corrosion as decreasing the flow rate from 6000 to 3000 cfm increases the metal loss by ~40 %. While a metal loss of 5-7 mils is within the safety limit of a maximum metal loss of 10 mil, the analysis should be considered very conservative with respect to historical operations [12]. For perspective, during 15 years of operation with the HEU core (1968-1983) 150 transients produced peak core temperatures above 400 °C and only 20 of them reached higher temperatures than 500 °C, as documented in an internal 1983 study by N. A. Kramer.

Figure 6. LEU Fuel Assembly Metal loss during 40 years of operation according to HEU FSAR assumptions

3.1.2.2 Effect of Axial Conductivity and Fuel Block Size

The effect of axial conduction through the fuel block and its effect on cladding oxidation relative to the base case were investigated. Parameters of importance are thermal conductivity, fuel block geometry (1"x1", 2"x2", and 4"x4" inch blocks) and contact resistance (smooth vs rough surfaces). To reduce computational variations between all parameters, the effects of contact resistance and fuel block size were translated numerically into an effective conductivity (for convenience expressed as a quotient K/K_0 where K_0 is the thermal conductivity of the fuel). A high contact resistance and a larger number of fuel blocks decreases the heat transferred axially from the fuel to the reflector section and thus translated as a reduced heat conductivity of the fuel relative to the conductivity of a single fuel block. Figure 7a shows the effect of fuel block size and contact resistance translated to an equivalent effective axial conductivity of the fuel. For smooth surfaces, a change in fuel block length from 4" to 1" corresponds to an effective axial fuel conductivity in the range of 95%-82%. The effect is more severe, however, for rough surfaces where the effective conductivity drops to between 70%-40%.

Figure 7. a) Fuel Block Size and Contact Resistance Translated to an Equivalent Effective Axial Conductivity, (b) Effective Conductivity's Effect on Cladding Oxidation

The effect of the effective axial conductivity on cladding oxidation is shown in Figure 7b for the case of a 1" x 1" fuel blocks. Here, the change in cladding oxidation is relative to the base case condition (no contact resistance, K_0 =LEU base case thermal conductivity). For a base case thermal conductivity, the oxidation rate of 1x1 fuel blocks may be higher by 3-10% depending on contact resistance and air-flow rate through the core. If the thermal conductivity were to decrease by 50%, the effective axial conductivity for the smallest fuel block could be reduced to slightly below 20%. Still, even with no axial conduction, the change in cladding oxidation does not increase significantly, just 10-15% depending on the flow rate. The effect can be appreciated by comparing the cooling times for these two cases, as shown in Figure 8.

Figure 8. Effect of Axial Conductivity on Cooling Times

As a reduction in flow-rate increases the cooling time, there is negligible difference in cooling time behavior between the two extreme cases (nominal vs zero axial thermal conductivity) during the first couple of hours of cooling. Here, heat transfer by convection, rather by conduction, is the primary cooling mechanism. Once the temperature drops to below 400 °C, however, the effect of axial conduction starts to influence

cooling time. However, corrosion rates at that temperature and below are small and do not significantly affect the overall oxidation of the cladding. Since 90% of the total corrosion occurs at temperatures between 600-500 °C, the effect of axial conductivity as well as contact resistance do not affect overall corrosion behavior during *normal* operation with air flow.

3.1.2.3 Effect of Radial Conductivity and Fuel Block Size

The effect of radial conduction across the fuel block and its effect on cooling time and subsequently cladding oxidation relative to the base case was compared next. Neutronic analyses assume a uniform dispersion of UO₂ content within the graphite matrix. The reference modeling does not account for radial power distribution across a single fuel assembly (power peaking is evaluated radially element-to-element across the core, and axially within each element).

MCNP calculations were performed to confirm that the radial power distribution across each fuel assembly does not significantly affect core temperature distribution and core behavior. The analysis found that the radial power distribution across the core does lead to small temperature non-uniformities across individual fuel blocks. Given input from neutronic radial core power distribution profiles, the temperature non-uniformity across a fuel block after a power transient differs by approximately 10 °C relative to an average temperature, as shown in the left panel of Figure 9, below. At 30 seconds after the transient, the temperatures are somewhat equilibrated but not uniform across the fuel block. The temperature non-uniformities are too small, however, to necessitate switching to a full block model as opposed to a symmetric model (1/8th of a fuel cross-section, which is the current reference modeling approach).

Figure 9. Effect of Temperature Non-uniformity across the Fuel Plane as function of Radial Power Distribution; Temperature Difference is shown Relative to an Average Temperature

Depending on the fuel block sizes, conduction alone, versus a combination of conduction and contact resistance, can affect the radial heat transfer. For 2x2x2 inch fuel blocks, cooling time is affected only by conduction as each quadrant of the fuel block transfers its heat to its own neighboring cooling channel. The cooling time for the 1x1x1 inch fuel blocks will be affected by added contact resistance as well².

Given a peak fuel temperature of 600 °C, the cooling time was evaluated for an effective radial conductivity (K/K_0) in the range of 0.1-1.5 where K_0 refers (as previously) to the nominal LEU thermal conductivity. As shown in Figure 10, the change in cladding oxidation is not affected until the effective conductivity drops below 0.6. A further reduction in effective conductivity actually reduces cladding oxidation; this is observed

² It should be noted that 1X1 fuel blocks will need additional design configurations to align and holding them in place.

even if cooling times to below 500 °C are slightly increasing, as shown in the insert of peak fuel temperature vs time in Figure 11.

Figure 10. Change in cladding oxidation as function of radial effective conductivity

The lower cladding oxidation as the radial effective conductivity is reduced is due to the temperature gradients being formed within the fuel cross-sectional area. As shown in Figure 11, conductivities near the nominal values ($K/K_0=1$) produce a relatively flat temperature distribution, with exception near the corner region.

Figure 11. Temperature non-uniformity after 1000s of cooling. Cross section reflects peak fuel location.

The cladding section at the side which is in contact with the fuel will be at near thermal equilibrium with the fuel. A lower conductivity, on the other hand, produces larger thermal gradients with the center of the fuel being hotter. Lower radial conductivity reduces cladding corrosion due to cooler fuel temperatures near the cladding despite the slightly longer cooling time.

Even with a reduction of the fuel radial conductivity to 10% relative to the base case value, cooling still remains effective. The cooling rate of the cladding hottest location is not limited by fuel conductivity, but rather by peripheral heat transfer from the side section of the cladding to the corner region where the majority of convective cooling occurs. Thermal radiation, predominately at high temperatures, accounts for ~20% of heat transfer at the corner region.

3.1.3 Cladding Oxidation – Accident Scenario

Cooling times and consequently cladding corrosion values were shown above to be insensitive to conductivity during normal operation as convective cooling is the predominant mode of heat transfer. For an accident scenario, however, the analyses for the cooling time history of the fuel assembly assumes no flow conditions, i.e. both cooling blowers fail and natural convection is ignored. Thus the only mode of cooling in the accident scenario is by axial conduction through the fuel assembly.

An upper bounding accident case assuming 820°C peak fuel temperature for the hottest fuel assembly was analyzed. Even without flow and radial conduction throughout the core, the fuel assembly (including reflectors) is able to absorb the energy and reduce cladding temperatures such that corrosion rates remain low. However, the time until the axial temperature distribution within the fuel assembly (fuel and reflectors) is uniform is of importance. Assuming that the fuel assembly does not reject heat to the environment, a conservative cooling time history during the accident is shown in Figure 12a. The conductivity of the fuel was set at the nominal value (LEU reference), and a conservative value of contact resistance (CR) was used for the calculations. In case of no contact resistance, the fuel assembly reaches equilibrium (uniform temperature throughout the assembly) in a little less than 25 hours. Since the cladding is in thermal equilibrium with the fuel, peak fuel and peak cladding temperatures remain equal to each other.

Figure 12 . a) Cooling time history during an accident as function of fuel block size, b) Corresponding metal loss during an accident as function of contact resistance and fuel block size.

As a high contact resistance and increasing number of contact points along the fuel impedes heat transfer (from the fuel to the reflector blocks), cooling times to reach thermal equilibrium also increase. Within 25 hours of cooling, the peak cladding temperature of a 4X4 inch block will be slightly below 500 °C, while a 1X1 inch block still remains high at approximately 600 °C. It will require ~48 hours for a 1X1 inch block to reach thermal equilibrium across the entire fuel assembly.

The corresponding effect of cladding oxidation as function of fuel block size and contact resistance during an accident is shown in Figure 12b. Here, the cumulative cladding loss during the accident is evaluated during a cooling period of 48 h (i.e. thermal equilibrium). Once temperatures reach thermal equilibrium (temperature of 450 °C) cladding oxidation is slow and would equate to an additional metal loss of ~0.1 mils/week (assuming heat losses due to natural convection or conduction to the grid plate continue to be zero). As long as contact resistance remains low, the metal loss during the accident is insensitive to fuel block size with a total loss of ~2 mil of cladding during the cooldown. Metal loss increases exponentially with contact resistance, however, and further exacerbated with more fuel contact points. For a 1"x1" inch block and rough surfaces, the metal loss of the cladding increases to approximately 5 mil.

The minimum cladding thickness which must remain after a design basis accident in order to meet stress criteria was determined to be no less than 16 mils (based on stress-analysis by INL) [9]. Considering an initial cladding thickness of 26 mils, the maximum metal loss before a fuel assembly must be taken out of service is 10 mils. The amount of oxidation during normal operation may be substantially lower than estimated in Figure 9 depending on the amount of metal loss that can occur during a potential accident case. The metal loss during an accident with no air-flow is highly dependent on axial fuel conductivity, contact resistance, and fuel block size as shown below in Figure 13. Relative fuel conductivity, K/K_0 , is related to the LEU reference value (K_0) and contact resistance assumes rough surfaces in this scenario.

Figure 13. Cladding metal loss during an accident as function of fuel block size, contact resistance assuming rough surfaces and relative thermal conductivity.

The inserted horizontal lines consider the maximum allowable cladding that can be lost during an accident scenario following 40 years of normal operation with different operational core flow rates. For example, considering a case of no contact resistance, the thermal conductivity can be reduced to 40% relative to the base case value and the fuel element will still be within the lifetime maximum metal loss limit of 10 mils after normal operation for 40 years with two blowers and followed by the design basis accident. A conductivity below this value in combination with high contact resistance between fuel blocks would correspond to a lifetime oxidation which exceeds this limit following the accident scenario. Analysis of legacy data has indicated that the thermal conductivity of graphite may be reduced by fission fragment damage [4]; this behavior will be further investigated via irradiation testing of TREAT LEU fuel samples in the future. The key conclusions of this study were that a) the magnitude of axial contact resistance between fuel blocks should be as small as possible, b) 4 inch or 2 inch blocks should be considered only (as opposed to 1 inch blocks, which introduce more axial interfaces), and c) increases in the axial thermal conductivity, if possible, would improve the cooling of the fuel under the assumptions of the design basis accident scenario.

3.1.4 Effect of Fuel Thermal Mass

The thermal mass of the fabricated fuel assembly is the product of density and heat capacity. Obtaining a high thermal mass, or heat absorbing capability, of the fuel block is important as this allows the LEU core to generate more core energy for the same peak fuel temperatures. The thermal-hydraulic analysis focuses on examining the impact of fuel density and fuel heat-capacity on peak fuel temperatures for various core energies. For this analysis, the following perturbations and assumptions were made:

- Fuel Density Range = 1.80 – 1.90 g/cm³
- LEU/HEU PCF Range = 90 – 100%
- Range of Core Energy (CE) in Accident Scenario = 4018 – 4458 MJ
- Maximum Fuel Assembly Energy per Total Core Energy (E_{FA}) = 0.4454%
- Maximum Axial Relative Power Peaking (P_{AX}) = 1.18
- Heat capacity variation based on TREAT HEU and LEU fabricated samples

A preliminary analysis was first conducted to investigate the effect of fuel graphite content on the specific heat of the fuel. Assuming that the fuel is comprised of graphite, amorphous carbon and UO₂ only, the graphite content (i.e., ratio of graphite-to-total C in the fuel mixture) and presence of the UO₂ appear to have a small effect on the overall heat capacity of the fuel. Figure 14 below compares the heat capacity of the HEU fuel to pure graphite [15]. As shown in Figure 14a, the specific heat of the HEU fuel with an estimated graphite content of ~59% is nearly equivalent to that of pure graphite. The specific heat of amorphous carbon [16] is similar to, if not slightly higher than, graphite. Also, since the weight fraction of UO₂ in the fuel remains well below 1% (~0.24 wt. % for the original HEU fuel), the UO₂ content has a negligible contribution to the overall heat capacity of the fuel, Figure 14b. Thus graphite content should have a small effect on the specific heat of the fuel unless constituents other than graphite and amorphous carbon are present in significant quantities.

Figure 14. (a) Heat Capacity of HEU Fuel and Pure Graphite, and (b) Heat Capacity of Pure Graphite Compared to Heat Capacity of a Mixture of Graphite and UO_2 ($\text{UO}_2 = 1 \text{ wt}\%$)

Fuel heat-capacity has been re-examined based on historical data for HEU fuel and fabricated “LEU” compacts. Figure 15 shows the range in measured heat capacity and average value given four different fuel samples and pure graphite. The four fuel samples were the original TREAT HEU fuel, the fuel of the TREAT upgrade as well as two B&W test samples [13] (ID 13103 and 13104). The average heat capacity is close to the value used for the LEU conceptual design phase, differing by a constant deviation of $\pm 35 \text{ J kg}^{-1} \text{K}^{-1}$ regardless of temperature. This translates into a difference in heat capacity values of less than 3% for temperatures above 600 °C (873 K), in good agreement with the well-known experimental data for graphite [17].

Figure 15. Heat Capacity Measured for TREAT HEU Fuel, B&W Compacts, and Graphite

The effect of fuel density on peak fuel temperature during an accident scenario is shown in Figure 16. Data is plotted for two different PCF ratio (i.e., $\text{PCF}_{\text{LEU}}/\text{PCF}_{\text{HEU}}$) scenarios, where this ratio reflects the relative difference in core energy needed to achieve the same test sample energy deposition. The curve for PCF ratio = 100% represents the scenario where the LEU core requires the same energy as the HEU core. As

discussed in the previous conceptual design report, the PCF ratio range of 90-100% corresponds to total LEU core accident energies between 4018-4458 MJ. The peak fuel temperature as function of density and PCF ratio (evaluated for the hottest fuel assembly in reference M8CAL half-slotted LEU core) can be expressed by a simple formula as shown below:

$$T(^{\circ}\text{C}) \sim (1901 - 302.8 \times \rho - 6 \times \text{PCF}) \mp 15$$

Here, ρ denotes the fuel density and PCF the LEU-to-HEU PCF ratio. The uncertainty of 15 °C represents the deviation in fuel heat capacity of $\pm 35 \text{ J kg}^{-1} \text{ K}^{-1}$ as discussed previously and is reflected in the error-bars. As Figure 16 demonstrates, from a thermal perspective *only*, a high PCF ratio combined with a high fuel density is very important in maintaining temperatures well below the accident scenario temperature limit (Safety Limit, or SL), which is 820°C. For the current analysis assumptions, fuel densities as low as 1.80 g cm^{-3} are feasible, provided that the PCF ratio remains 95% or higher and the fuel heat capacity remains close to that of graphite. However as observed in the previous LEU-CD analysis, the PCF ratio may be below 95% for some high absorbing experiment vehicle scenarios.

Figure 16. Peak Fuel Temperature as a Function of Density and PCF Ratio

A good quality fuel should have a large heat capacity. Ideally, it is anticipated that heat capacity should be independent of graphite content and overall density. This was not the case in some preliminary results for the “feasibility” LEU UO₂ compacts [12]; however these samples represent early efforts at fuel fabrication. Figure 17a shows the measured heat capacity for some of those samples compared to the average (~ graphite heat capacity) previously discussed. The LEU LANL 13102 sample had a substantially lower measured heat capacity compared to that of graphite. (The measurements also indicate decreasing values at temperatures above about 1000 K, possibly reflecting a measurement error at the higher temperatures, or that the heat-treatment during resin carbonization was not complete.) The consequence of such low heat capacity during a reactivity accident scenario can be seen in Figure 17b (for the core energy corresponding to an LEU-to-HEU PCF ratio of 95 %). Even with a high fuel density of 1.90 g/cm^3 , a decrease in heat capacity by ~15% (LEU LANL 13102) relative to the average reference value translates to peak fuel temperature higher than the HEU core safety limit of 820 °C. The analysis did not consider the heat capacity for compact 13104, which was lower than that of 13102 (and consequently would produce even higher peak fuel temperature results). These LEU samples represent very early efforts to develop the LEU fuel fabrication process. More recent LEU samples demonstrate significantly improved heat capacity; the results of analyses with newer heat capacity data will be addressed in a future report. The objective of the study

presented here was to bound the anticipated core performance utilizing the lower heat capacity measurements.

Figure 17. (a) Heat Capacity for Sample LEU Feasibility Fabricated Compacts and (b) Effect of Heat Capacity on Accident Scenario Peak Fuel Temperature (for Energy Corresponding to PCF Ratio 95%)

In this analysis of the impact of heat capacity on peak fuel temperature, only the heat capacity was adjusted, assuming the same power pulse and total core energy as the reference accident scenario. However, in reality if the LEU heat capacity differs from the reference value, this will also have an impact on the neutronic behavior of the core, as it will influence the temperature rise during a transient and correspondingly will affect the reactivity feedback of the core as the core heats up. Therefore, the total LEU core energy corresponding to the maximum-allowed experiment in the HEU core, and the corresponding LEU core reactivity-accident energy, will both change as functions of fuel capacity. The effect of the heat capacity on core neutronics has not yet been investigated.

4 Neutronic Sensitivity Studies

In addition to the thermal hydraulic sensitivity studies discussed above, neutronic sensitivity studies were performed to further evaluate the effects of design parameters and modeling assumptions on the neutronic behavior of the LEU core.

4.1 Effect of Fuel Density and Carbon-to-Uranium Ratio

A detailed study was performed to investigate the relationship between the fuel properties of density and carbon-to-uranium ratio and the key core properties of neutron spectrum, excess reactivity, and test fuel PCF. The MCNP model of the LEU Conceptual Design (LEU-CD) core, using the historic M8CAL core loading and experiment vehicle as a reference configuration, was used in this study. The effective multiplication factor (k_{eff}) was calculated with an estimated statistical standard deviation of 0.00005 in all cases presented in this section.

For all of the simulations in Section 4.1, all three control rod banks were set at their fully withdrawn positions. The M8CAL experiment vehicle was modeled, with a single test “pin” located at the center of the vehicle. In general, for the same incident neutron flux and spectrum, the PCF changes with the size of the test pin (with a bigger pin diameter corresponding to higher self-shielding, which affects the radial power profile in the pin) and with the test sample’s material composition (high or low enriched ^{235}U fuel,

or plutonium-bearing fuel, etc.). For the purpose of this analysis, the pin was assumed to be filled with air, so self-shielding effects were not present, in order to provide more general results.

Simulations were first performed for the HEU and LEU-CD cores in order to obtain the LEU-to-HEU PCF ratio, core excess reactivity, and neutron spectrum inside the test “pin.” The HEU and the LEU-CD (referred to here as LEU-CD-Reference) fuel compositions used in the MCNP calculations are shown in Table 2 and Table 3, respectively.

Table 2: HEU Fuel Composition

HEU Fuel		
Isotope	Atom Fraction	Weight Fraction
U-235	1.0068E-04	1.9658E-03
U-238	7.2991E-06	1.4435E-04
C (graphite)	5.8973E-01	5.8845E-01
C (free gas)	4.0981E-01	4.0855E-01
Fe-54	7.5679E-06	3.3913E-05
Fe-56	1.1869E-04	5.5154E-04
Fe-57	2.7425E-06	1.2972E-05
Fe-58	3.6223E-07	1.7433E-06
O-16	2.1588E-04	2.8686E-04
B-10	1.6803E-06	1.3977E-06
B-11	6.7631E-06	6.1856E-06
Density	8.6267E-02 (at/b-cm)	1.72434 (g/cm ³)
Boron (ppm)	8.44 (by atom)	7.58 (by weight)
C/U_{total}	9257 (by atom)	472 (by weight)
C/U₂₃₅	9928 (by atom)	507 (by weight)

Table 3: LEU-CD-Reference Fuel Composition

LEU-CD Fuel-Reference		
Isotope	Atom Fraction	Weight Fraction
U-235	8.4073E-05	1.6321E-03
U-232	8.6241E-13	1.6527E-11
U-234	1.1115E-06	2.1486E-05
U-236	1.9499E-06	3.8013E-05
U-238	3.3427E-04	6.5721E-03
O	8.4281E-04	1.1134E-03
C (graphite)	8.4892E-01	8.4214E-01
C (free gas)	1.4981E-01	1.4848E-01
B-10	4.4579E-07	3.6866E-07
B-11	1.7943E-06	1.6316E-06
Density	9.2014E-02 (at/b-cm)	1.85 (g/cm ³)
Boron (ppm)	2.24 (by atom)	2.00 (by weight)
C/U_{total}	2370 (by atom)	120 (by weight)
C/U₂₃₅	11879 (by atom)	607 (by weight)

The LEU core MCNP calculations were repeated using the isotopic composition of LEU-CD-Reference for perturbed fuel density values of 1.80 and 1.90 g/cm³, which are now referred to as cases LEU-CD-var-1

and LEU-CD-var-2, respectively. Table 4 summarizes the results of the MCNP calculations for the HEU core and the three LEU-CD cases with different densities. (STD FA and CNTL FA represent the number of standard fuel assemblies and control-rod fuel assemblies, respectively.)

Table 4: Neutronic Calculations for the HEU Core and the LEU-CD Core with Fuel Densities 1.80, 1.85 and 1.90 g/cm³ (the LEU Cases had the same Isotopic Fractions). STD FA: Standard Fuel Assembly, CNTL FA: Control-rod Fuel Assembly.

	HEU	LEU-CD-var-1	LEU-CD-Reference	LEU-CD-var-2
C/U (atom ratio)	9257	2370	2370	2370
d (g/cm³)	1.72434	1.80	1.85	1.90
STD FA U235 (g)	37.4	33.9	34.9	35.8
CNTL FA U235 (g)	26.1	22.6	23.3	23.9
Excess Reactivity	7.72%	6.38%	7.73%	9.00%
LEU/HEU-PCF	100%	103.3%	100.5%	98.5%
LEU/HEU-Flux at Pin	100%	94%	91%	88%
Thermal/Total Flux	19.09%	21.25%	21.38%	21.71%

For the same isotopic composition, when the density of the LEU fuel changes the excess reactivity in the core also changes (the perturbation in density increases or decreases the amount of uranium in the core for constant C/U). Traditionally in the TREAT LEU core analysis it has been assumed that the LEU core needs to provide roughly the same excess reactivity as the current HEU core (in order to be able to accommodate the same in-core experiment hardware set). Therefore in order to match the excess reactivity of the HEU core, the C/U_{total} values of the LEU-CD-var-1 and LEU-CD-var-2 compositions were adjusted. The fuel compositions with the adjusted C/U_{total} ratios are shown in Table 5 and Table 6 for 1.80 and 1.90 g/cm³ fuel densities, respectively. These cases, which are now referred to as LEU-CD-var-3 and LEU-CD-var-4, represent more realistically what the recommended fuel composition might be for the LEU fuel density set at 1.80 or 1.90 g/cm³.

Table 5: LEU-CD-var-3 Fuel Composition

LEU-CD-var-3		
Isotope	Atom Fraction	Weight Fraction
U-235	9.0730E-05	1.7602E-03
U-232	9.3069E-13	1.7825E-11
U-234	1.1995E-06	2.3172E-05
U-236	2.1042E-06	4.0997E-05
U-238	3.6074E-04	7.0879E-03
O	9.0954E-04	1.2008E-03
C (graphite)	8.4884E-01	8.4152E-01
C (free gas)	1.4980E-01	1.4837E-01
B-10	4.4579E-07	3.6842E-07
B-11	1.7943E-06	1.6305E-06
Density	8.9469E-02 (at/b-cm)	1.80 (g/cm ³)
Boron (ppm)	2.24 (by atom)	2.00 (by weight)
C/U_{total}	2196 (by atom)	111 (by weight)
C/U₂₃₅	11007 (by atom)	562 (by weight)

Table 6: LEU-CD-var-4 Fuel Composition

LEU-CD-var-4		
Isotope	Atom Fraction	Weight Fraction
U-235	7.7780E-05	1.5108E-03
U-232	7.9785E-13	1.5300E-11
U-234	1.0283E-06	1.9890E-05
U-236	1.8039E-06	3.5189E-05
U-238	3.0925E-04	6.0839E-03
O	7.7973E-04	1.0307E-03
C (graphite)	8.4900E-01	8.4274E-01
C (free gas)	1.4982E-01	1.4858E-01
B-10	4.4579E-07	3.6888E-07
B-11	1.7943E-06	1.6326E-06
Density	9.4558E-02 (at/b-cm)	1.90 (g/cm ³)
Boron (ppm)	2.24 (by atom)	2.00 (by weight)
C/U_{total}	2562 (by atom)	130 (by weight)
C/U₂₃₅	12842 (by atom)	656 (by weight)

Table 7 summarizes the key results of the neutronic calculations for the two LEU-CD variant fuel composition variations, as compared to the reference LEU-CD core. These results demonstrate that with the isotopic compositions needed for the LEU core to provide roughly the same excess reactivity as the HEU fuel (for the M8CAL half-slotted core with vehicle), the LEU cores with fuel densities 1.80, 1.85, and 1.90 g/cm³ provide LEU-to-HEU PCF ratios of 98.2%, 100.5%, and 104.2%, respectively. These results represent a more realistic comparison of the three density cases than the comparison previously presented in Table 4 (which documents the cases with perturbations in density only, with the LEU-CD-Reference composition maintained).

Table 7: Neutronic Calculations for the LEU-CD-var3, LEU-CD-Reference and for the LEU-CD-var-4 with Adjusted C/U ratio to match the HEU Excess Reactivity

	LEU-CD-var-3	LEU-CD-Reference	LEU-CD-var-4
C/U_{total} (by atom)	2196	2370	2562
C/U₂₃₅ (by atom)	11007	11879	12842
d (g/cm³)	1.80	1.85	1.90
STD FA U235 (g)	36.6	34.9	33.2
CNTL FA U235 (g)	24.4	23.3	22.1
Excess Reactivity	7.70%	7.73%	7.64%
LEU/HEU-PCF	98.2%	100.5%	104.2%
LEU/HEU-Flux at Pin	91%	91%	90%
Thermal/Total Flux	20.80%	21.38%	22.28%

For a more complete set of results, the neutronic calculations were expanded to consider all three density values for the each of the isotopic compositions of LEU-CD-var-3 and LEU-CD-var-4. Table 8 and Table 9 show the results for these additional variants. For the LEU-CD-var-3 composition (with C/U=2196 that was selected to provide appropriate excess reactivity for the density of 1.80 g/cm³, the core excess reactivity with a higher density of 1.85 or 1.90 g/cm³ is too high. On the other hand, for the LEU-CD-var-4 composition (with C/U=2562), there is not sufficient reactivity with densities less than 1.90 g/cm³. It should be noted that while the lower densities of 1.80 and 1.85 g/cm³ (cases LEU-CD-var-7 and LEU-CD-Var-8) appear to give a “better” PCF than the case with 1.90 g/cm³ (LEU-CD-var-4) for the LEU-CD-var-4 composition, these results do not represent realistic LEU options because of low excess reactivity values.

Table 8: Neutronic Calculations for Fuel Densities 1.85 and 1.90 g/cm³ with the Isotopic Composition of LEU-CD-var-3

	LEU-CD-var-3	LEU-CD-var-5	LEU-CD-var-6
C/U (atom)	2196	2196	2196
d (g/cm³)	1.80	1.85	1.90
STD FA U235 (g)	36.6	37.6	38.6
CNTL FA U235 (g)	24.4	25.1	25.8
Excess Reactivity	7.70%	8.99%	10.19%
LEU/HEU-PCF	98.2%	94.9%	92.2%
LEU/HEU-Flux at Pin	91%	88%	86%
Thermal/Total Flux	20.80%	20.73%	20.79%

Table 9: Neutronic Calculations for Fuel Densities 1.80 and 1.85 g/cm³ with Isotopic Composition of LEU-CD-var-4

	LEU-CD-var-7	LEU-CD-var-8	LEU-CD-var-4
C/U (atom)	2562	2562	2562
d (g/cm³)	1.80	1.85	1.90
STD FA U235 (g)	31.4	32.3	33.2
CNTL FA U235 (g)	20.9	21.5	22.1
Excess Reactivity	4.89%	6.31%	7.64%
LEU/HEU-PCF	110.5%	107.5%	104.2%
LEU/HEU-Flux at Pin	96%	93%	90%
Thermal/Total Flux	22.08%	22.23%	22.28%

To support additional comparisons between the currently-evaluated variants, the U-235 mass in the standard fuel assembly, the core excess reactivity, the thermal-to-total neutron flux and the LEU/HEU-PCF presented as a function of C/U_{total} , C/U_{235} and total fuel density are documented in Table 10 through Table 14.

Table 10: U-235 Mass per Standard Fuel Assembly

U235 Mass (g) per Standard Fuel Assembly				
d (g/cm³)	1.80	1.85	1.90	C/U₂₃₅
C/U_{total}				
2196	36.3	37.6	38.6	11007
2370	33.9	34.9	35.8	11879
2562	31.4	32.3	33.2	12842
HEU values for comparison				
C/U_{total}	9257			
C/U₂₃₅	9928			
d (g/cm³)	1.72434			
Mass (g)	37.4			

Table 11: Excess Reactivity (Shaded Values are Close to the HEU Excess Reactivity)

Excess Reactivity (1-1/k_{eff})
--

$\frac{C}{U_{\text{total}}}$ \ d (g/cm ³)	1.80	1.85	1.90	C/U_{235}
2196	7.70%	8.99%	10.19%	11007
2370	6.38%	7.73%	9.00%	11879
2562	4.89%	6.31%	7.64%	12842
HEU values for comparison				
C/U_{total}	9257			
C/U_{235}	9928			
d (g/cm ³)	1.72434			
Excess Reactivity	7.72%			

Table 12: Thermal-to-Total Neutron Flux inside Test Pin (pin filled with air)

Thermal/Total Neutron Flux inside Test Pin				
$\frac{C}{U_{\text{total}}}$ \ d (g/cm ³)	1.80	1.85	1.90	C/U_{235}
2196	20.8%	20.7%	20.8%	11007
2370	21.3%	21.4%	21.7%	11879
2562	22.1%	22.2%	22.3%	12842
HEU values for comparison				
C/U_{total}	9257			
C/U_{235}	9928			
d (g/cm ³)	1.72434			
Thermal/Total Flux	19.09%			

Table 13: LEU/HEU-Total Neutron Flux at the Test Pin

LEU/HEU-Total Neutron Flux at Pin				
$\frac{C}{U_{\text{total}}}$ \ d (g/cm ³)	1.80	1.85	1.90	C/U_{235}
2196	91.4%	88.4%	85.6%	11007
2370	93.7%	90.8%	87.6%	11879
2562	96.3%	93.0%	89.8%	12842

Table 14: LEU/HEU-PCF Ratio

LEU/HEU-PCF Ratio				
$\frac{C}{U_{\text{total}}}$ \ d (g/cm ³)	1.80	1.85	1.90	C/U_{235}
2196	98.2%	94.9%	92.2%	11007
2370	103.3%	100.5%	98.5%	11879
2562	110.5%	107.5%	104.2%	12842

For the same fuel isotopic composition (including the same C/U_{total} ratio), the excess reactivity increases for higher fuel density values, which is consistent with the increase in ^{235}U mass in the fuel (see Table 10 and

Table 11). As the excess reactivity varies with fuel density, the fuel C/U_{total} ratio needs to be adjusted to achieve the equal excess reactivity with the HEU core. For example, for $C/U_{\text{total}}=2196$ and $d = 1.85$ g/cm³,

the excess reactivity changes from 8.99% to 7.73% and 6.31% for C/U_{total} values of 2370 and 2562, respectively (Table 11).

In addition to changing the excess reactivity, the fuel C/U ratio and ^{235}U loading also affect the neutron spectrum reaching the test pin and consequently affect the PCF. A higher Uranium content in the fuel (lower C/U_{total}) decreases the number of thermal neutrons reaching the test pin at the center of the core (harder neutron spectrum), and decreases the total neutron flux at the test pin, both of which correspondingly result in lower PCF. This is shown in Table 12 and in Table 13 where the thermal-to-total neutron flux and the LEU-to-HEU PCF ratios decrease for lower C/U_{total} values.

Table 15 summarizes the LEU fuel density and C/U_{total} combinations that produce LEU core excess reactivity approximately equal to the HEU core. For the experiment scenario considered in this analysis, a higher thermal/total neutron flux would be preferable as this allows the LEU core to better match the HEU core PCF and satisfy the core temperature limits (higher LEU/HEU-PCF demand lower total core energy to achieve equal to the HEU energy deposition in the test sample). However, a more thermal spectrum reaching the test region may also increase self-shielding in the sample (especially for thicker and/or multiple targets) resulting in most of the fissions occurring at the outer layers of the pin (which may not be desirable in some experiments). Therefore, to match the more detailed profile of the sample(s) in the HEU core, the thermal-to-total neutron flux at the experiment region in the LEU core should be close to the HEU core value. Additional calculations should be performed in the future to analyze the effect of thicker pins (with high or low enriched fuel) and multiple-pin-bearing test vehicles, which reflect the potential future experiment programmatic needs of the LEU core.

Table 15: LEU Fuel Density and C/U_{total} for Excess Reactivity close to the HEU Value (7.72%)

Excess Reactivity	d (g/cm ³)	C/U_{total}	U235 (g) per FA	LEU/HEU-PCF
7.70%	1.80	2196	36.3	98.2%
7.73%	1.85	2370	34.9	100.5%
7.64%	1.90	2562	33.2	104.2%

In earlier analyses of the LEU-CD core [4], it was observed that with the slightly more thermal spectrum in the current reference LEU core (as compared to the HEU core), the LEU-to-HEU PCF ratio decreased for higher density values of the M8CAL vehicle structural materials due to the higher neutron absorption of the more thermal incident flux. Therefore, the current analysis was expanded to also consider the neutronic performance for a subset of the LEU composition scenarios for the same M8CAL experiment configuration with the density of the experiment vehicle stainless steel components increased by a factor of 2 as compared to the reference vehicle (i.e. the vehicle utilized in all analyses discussed above).

The LEU composition and density combinations selected for this analysis were the cases yielding core excess reactivity similar to that of the HEU core. With the higher density vehicle, the general trend was the same, but the PCF ratio values were all slightly lower. This reduction can be expected to be larger if the absorption of the experiment vehicle is further increased (i.e. a thicker or more dense vehicle). Table 16 shows the effect of doubling the density of the experiment vehicle materials on the PCF and the excess reactivity.

Table 16. Excess Reactivity and LEU/HEU PCF Ratio Values for Reference and Higher Density M8CAL Experiment Vehicle Scenarios

Core		Reference Vehicle		Increase Density of Vehicle x2	
		Excess Reactivity	LEU/HEU PCF Ratio	Excess Reactivity	LEU/HEU PCF Ratio
HEU		7.72%	-	7.66%	-
LEU-CD-Reference	d = 1.85 g/cm ³ , C/U = 2370	7.73%	100.5%	7.67%	97.6%
LEU-CD-var-3	d = 1.80 g/cm ³ , C/U = 2196	7.70%	98.2%	7.63%	95.9%
LEU-CD-var-4	d = 1.90 g/cm ³ , C/U = 2562	7.64%	104.2%	7.56%	99.6%

4.2 Effect of Cross-section Library

Simulations were performed to evaluate the effect of the cross-section library dataset used on the core excess reactivity, temperature reactivity feedback, PCF values, and control rod worths. These values were calculated using the current reference cross-section library, ENDF/B-VII.0 and the cross-section library ENDF/B-VII.1 to identify the differences.

Both the HEU and LEU cores were found to display only a small change (1-2% increase) in PCF for a change from ENDF/B-VII.0 to ENDF/B-VII.1, for a cold core with M8CAL vehicle. Excess reactivity, on the other hand, shifts more significantly. Table 17 presents the effect of cross-section library on excess reactivity and temperature reactivity feedback (TRF) for the LEU core. The corresponding results for the HEU core are documented in Table 18.

The cold core excess reactivity changes from 7.71% with ENDF/B-VII.0 to 6.80% with ENDF/B-VII.1. Although the PCF showed minimal change, if the fuel C/U were adjusted to compensate for the reactivity change (to produce the same excess reactivity as the HEU core), there could be a change in PCF. However, this was not investigated at this time.

Table 19 and Table 20 present the calculated control rod bank worths and shutdown margins, respectively, for the LEU core using the two cross section libraries. The rod worths show minimal change with cross-section set. Therefore, a larger shutdown margin is calculated when using the ENDF/B-VII.1 library.

Table 17. Effect of ENDF Cross-section Library on k-eff and Temp. Fdbk 7.1/7.0 Ratio in the LEU Core

Cross Section T (K)	ENDF 7.0		ENDF 7.1		Excess Reactivity Diff 7.0 – 7.1	Temp. Fdbk Ratio 7.1/7.0
	Excess Reactivity	Temp. Fdbk	Excess Reactivity	Temp. Fdbk		
293	7.71%	0.00%	6.80%	0.00%	0.91%	n/a
400	5.71%	2.00%	4.77%	2.03%	0.94%	101.4%
500	3.83%	3.88%	2.95%	3.85%	0.88%	99.2%
600	2.04%	5.67%	1.13%	5.67%	0.90%	99.9%
700	0.36%	7.35%	-0.56%	7.36%	0.92%	100.1%
800	-1.20%	8.91%	-2.15%	8.95%	0.95%	100.4%
1000	-3.99%	11.70%	-5.00%	11.80%	1.00%	100.8%
1200	-6.68%	14.39%	-7.63%	14.43%	0.96%	100.3%

Table 18. Effect of ENDF Cross-section Library on k-eff and Temp. Fdbk 7.1/7.0 Ratio in the HEU Core

Cross Section T (K)	ENDF 7.0		ENDF 7.1		Excess Reactivity Diff 7.0 – 7.1	Temp. Fdbk Ratio 7.1/7.0
	Excess Reactivity	Temp. Fdbk	Excess Reactivity	Temp. Fdbk		
293	7.76%	0.00%	7.11%	0.00%	0.65%	
400	5.78%	1.98%	5.14%	1.97%	0.64%	99.4%
500	3.98%	3.78%	3.32%	3.79%	0.66%	100.2%
600	2.32%	5.44%	1.68%	5.43%	0.64%	99.7%
700	0.78%	6.98%	0.11%	7.00%	0.67%	100.3%
800	-0.65%	8.41%	-1.34%	8.45%	0.69%	100.4%
1000	-3.32%	11.08%	-3.97%	11.08%	0.66%	100.0%
1200	-5.75%	13.52%	-6.40%	13.51%	0.64%	99.9%

Table 19. Effect of ENDF Cross-section Library on Control Rod Bank Worth in LEU Core

Cross Section Library	Excess Reactivity	Rod Bank Worth		
		Transient	Shutdown	Compensation
7.0	7.77%	8.70%	9.21%	8.44%
7.1	6.85%	8.71%	9.25%	8.56%

Table 20. Effect of ENDF Cross-section Library on Rod Bank Shutdown Margin in LEU Core

Cross Section Library	Shutdown Margin (Excess Reactivity – Control Rod Worth)		
	Transient	Shutdown	Compensation
7.0	-0.93%	-1.45%	-0.68%
7.1	-1.86%	-2.40%	-1.70%

4.3 Effect of Fuel Boron Impurity

The effect of fuel boron impurity content on the excess reactivity and the PCF was investigated by evaluating changes from the reference impurity content of 2 ppm to 1 ppm and 3 ppm. The changes produced minimal differences in PCF, but approximate 1% change in excess reactivity per ppm of Boron. Although the PCF showed minimal change with changes in boron, changes in the boron content could necessitate an adjustment of the C/U to compensate for the reactivity change. A change in C/U would in turn, affect the neutron spectrum and PCF. This was not investigated further in this study.

Table 21. Effect of Fuel Boron Impurity on Excess Reactivity and PCF in LEU core

		ARO Reactivity	LEU/HEU PCF
HEU		7.74%	n/a
LEU	1 ppm	8.75%	100.2%
	2 ppm	7.72%	99.9%
	3 ppm	6.70%	100.6%

4.4 Effect of Fuel Graphite Content

The effect of fuel graphite content (i.e., fraction of total carbon in the fuel which is in the form of graphite) was investigated for a series of values, ranging from 0% to 100% graphite content. In the neutronic modeling, the graphite content has an impact on the scattering behavior of the neutrons in the reactor. The different scattering properties of two forms of carbon was simulated in MCNP by using the $S(\alpha, \beta)$ tables on the graphitized carbon and assuming the “free-gas” treatment for carbon. It is recognized that the $S(\alpha, \beta)$ may not be appropriate for the type the LEU fuel matrix manufactured for TREAT but in the context of the feasibility analyses for the TREAT conversion using the available inelastic scattering treatment provides valuable insight on the performance change due to carbon’s different crystalline structures.

This study evaluated the effect on excess reactivity and PCF for all the cross sections at 293.6K temperature. Results are presented in Table 22. The results for the PCF also plotted in Figure 18. This analysis found that there is an increase in PCF and decrease in excess reactivity with increasing graphite content. The relationship between the PCF and graphite inelastic scattering ($S(\alpha, \beta)$) will be further investigated in future analyses.

In the future, irradiation tests will be performed on LEU fuel samples, which will provide information on how the graphite content of the fuel may change over the fuel lifetime. Until further experimental data is gathered, the analyses will continue to assume the reference graphite content.

Table 22. Effect of Fuel Graphite Content on Excess Reactivity and PCF in LEU core

Core	Graphite Content (%)	ARO Reactivity	LEU/HEU PCF
HEU	59%	7.74%	-
LEU	0%	8.99%	95.1%
	42.5%	8.53%	97.1%
	80%	7.88%	100.2%
	85%	7.72%	99.9%
	90%	7.57%	100.1%
	100%	7.18%	102.7%

Figure 18. Effect of LEU Fuel Graphite Content on PCF

4.5 Effect of Axial Reflector Density

The effect of axial reflector density on the excess reactivity and PCF was investigated by evaluating changes from the reference density of 1.85 g/cm³ to 1.80 g/cm³ and 1.90 g/cm³. Results are presented in Table 23. The changes produced negligible differences in PCF, and only roughly 0.1% differences in excess reactivity.

Table 23. Effect of Axial Reflector Density on k-eff and Temperature Reactivity Feedback

Core	Axial Reflector Density (g/cm ³)	ARO Reactivity	LEU/HEU PCF
HEU	1.67	7.74%	n/a
LEU	1.80	7.63%	99.7%
	1.85	7.72%	99.9%
	1.90	7.84%	99.9%

4.6 Effect of Fuel Element Cladding Properties

Simulations were performed to evaluate the effect of cladding impurity content and cladding thickness on the excess reactivity and PCF. Results are presented in Table 24 through Table 26.

The study of cladding impurity content considered three cases:

1. The reference maximum anticipated impurity content, with all alloying and impurity elements explicitly modeled.
2. The reference maximum anticipated impurity content, with the alloying materials explicitly modeling and the impurity elements represented as boron equivalent.
3. A previous design cladding material specification, which included only the elements of Sn, Fe, Cr, and O, with no other impurities specified.

For the three cases, there was minimal variation in PCF. The case with lower impurity content (case 3) displayed a higher excess reactivity relative to the other two cases.

Table 24. Effect of Cladding Impurity Assumptions on Excess Reactivity and PCF

	ARO Reactivity	LEU/HEU PCF
Reference: All Impurities Modeled	7.72%	99.9%
Perturbation: Alloys + B _{equiv}	7.88%	100.6%
Perturbation: Previous spec - Sn, Fe, Cr, and O only	8.25%	100.7%

Changes in the cladding thickness were evaluated for a change from the LEU-CD reference thickness of 25 mils to an increased thickness of 26 mils. Table 25 presents the calculated PCF and excess reactivity assuming the reference fuel area, compared to the reference design. Table 26 presents the effect of assuming a change in the fuel area to compensate for change in cladding thickness (i.e., assuming the reference (25 mil thickness case) fuel-to-clad gap is maintained for the 26 mil cladding).

Based on the results of these studies, it was concluded that it would be acceptable to change the design from 25 mil to 26 mil thick cladding in future design iterations, if needed.

Table 25. Effect of Cladding Thickness on Excess Reactivity and PCF, Assuming Fuel Area is Unchanged

	ARO Reactivity	LEU/HEU PCF
Reference: 25 mil, All Impurities Modeled	7.72%	99.9%
Perturbation: 26 mil, All Impurities Modeled	7.58%	101.4%
Perturbation: 26 mil, Alloys + B _{equiv}	7.73%	101.1%

Table 26. Effect of Cladding Thickness on Excess Reactivity and PCF, Assuming Fuel Area is Adjusted

	ARO Reactivity	LEU/HEU PCF
Reference: 25 mil	7.72%	99.9%
Perturbation: 26 mil clad, 14 mil Gap, Reference Fuel Area	7.58%	101.4%
Perturbation: 26 mil clad, Reference 15 mil Gap, Smaller Fuel Area	7.52%	100.8%

5 Fuel Thermal Expansion

5.1 Fuel Thermal Expansion – Thermal Analysis

Fuel thermal expansion was evaluated during normal operating conditions with operating fuel peak temperatures in the range of 100 to 600 °C. The purpose of this study was to investigate if fuel thermal expansion has a notable effect in the TREAT core *for neutronic analyses only*, and the study excludes evaluation of thermal stress on the fuel assembly and cladding. For simplicity, the current analysis considered only the fuel (a stack of twelve 4x4x4 inch blocks) and reflector sections. Based on a specified thermal load, the fuel and reflector are free to expand longitudinally and laterally relative to a fixed position at the bottom of the lower reflector. An isotropic value of 6×10^{-6} /K was used for the coefficient of linear thermal expansion (CTE) [7, 18]. The same CTE values is used for both the fuel and axial reflector, and deemed conservative in the temperature range between room temperature and 600 °C.

The analysis of thermal expansion of the fuel assembly (cladding excluded) was performed using hot core temperature distributions evaluated based on the MCNP-calculated power distribution in the M8CAL half-slotted core. All calculations were done using the structural mechanics module in COMSOL 5.1a. The (MCNP-calculated) axial power profile (normalized to an axial-average of unity) is shown for the LEU fuel in Figure 19a. Assuming the LEU axial power profile is invariant as a function of temperature, the corresponding temperature profiles as a function of axial distance is shown in Figure 19b for various initial peak core temperatures after a transient pulse (evaluated after 10s cooling time – assuming conduction only). As shown in Figure 19c-d, essentially all of the thermal expansion occurs in the fuel section, as little heat has yet been transferred by axial conduction to the reflector regions. As the peak-to-average axial power ratio in a fuel assembly is highly non-uniform, there are significant temperature gradients along the fuel section.

Figure 19 a) Ratio of Fuel Element Power Density to the Core Average Power Density, b) Temperature Profiles of Fuel Assembly as Function of Axial Distance, c) Total displacement in mm given a peak fuel temperature of 600 °C, d) Cumulative axial displacement in mm given a peak fuel temperature of 600 °C.

The largest local volumetric expansion occurs near the center of the fuel section, where the temperature is highest. For a peak temperature of 600 °C, the expansion of a 4x4x4 inch fuel block is ~ 10 cm³; in contrast, the fuel block in the vicinity of the upper axial reflector has an average temperature of 420 °C and expands by ~ 6 cm³. The density of each fuel block will vary due to axially temperature differences, however, the average change in density variation is small (e.g., increasing from 1.831 to 1.838 g cm⁻³). To simplify neutronic calculations, the volumetric expansion (ΔV) of the entire fuel section is correlated as a function of peak fuel temperature (°C) according to the expression below,

$$\Delta V(\text{cm}^3) = 0.18017 \times T(^{\circ}\text{C}) - 4.5212$$

This relationship was provided for the neutronic evaluation of the effect of thermal expansion.

5.2 Fuel Thermal Expansion – Neutronic Analysis

To evaluate the neutronic effects of fuel thermal expansion, simulations were performed for a bounding case of uniform core heating to 600°C. The corresponding volume change for a standard fuel assembly is provided in Table 27.

Table 27. Standard Fuel Assembly Volume after Thermal Expansion at 600°C

Volume, no expansion	11562.20 cm ³
Volume, 600°C thermal expansion	11663.20 cm ³

Table 28 documents the thermal expansion-induced change in excess reactivity, calculated with all-rods-out. Table 29 documents the effective multiplication factor (k_{eff}) and LEU-to-HEU PCF ratio, calculated with the control rods inserted (to a reported critical configuration, which yields close to criticality in the current model). PCF values are presented for three different test sample compositions: the M8CAL test pins 433 and 462 and the low enriched fissile wire used in the M8CAL tests. The PCF for the wire and the 443 pin were calculated as isotopic reaction rates, meaning that these materials were not physically present in the MCNP model. In the actual model, the pin had the 462 material (this is what the asterisk is showing).

As anticipated, there is a small increase in neutron leakage with the thermal expansion, resulting in a small decrease in k_{eff} . There is minimal change in PCF. As noted above, these results are bounding as they are based on an assumed uniform core temperature of 600°C, the maximum allowed operating temperature. In reality, if a location in the core is at the peak allowable temperature of 600°C, the majority of the core is at a lower temperature than this.

Table 28. Effect of Uniform Thermal Expansion Corresponding to 600°C on Core Excess Reactivity

C/U	d (g/cm ³)	k_{eff}		ARO Reactivity
2370	1.85	1.08454	0.00018	7.795%
	1.83398*	1.08402	0.00021	7.751%

Table 29. Effect of Uniform Thermal Expansion Corresponding to 600°C on Power Coupling Factor

C/U	d (g/cm ³)	k_{eff} (std)	LEU-to-HEU Core PCF (%)		
			PCF-wire	PCF-433	PCF-462*
2370	1.85	1.01538 (0.00006)	97.4%	97.4%	97.5%
	1.83398*	1.01480 (0.00007)	97.6%	97.7%	97.7%

* Based on the MCNP model

6 Conclusions

This report documents the additional studies of the TREAT LEU Conceptual Design that were performed following the publication of report ANL/RTR/TM-16/1. Neutronic and thermal hydraulic simulations were performed to evaluate the effect of changes in key design parameters on the predicted behavior of the LEU-CD core regarding performance parameters such as test-fuel power coupling factors, core available reactivity, temperature feedback reactivity, and control-rod shutdown margins. In addition, a simple study of fuel thermal expansion was performed, in order to confirm that thermal expansion has a negligible effect in the TREAT core. The work performed provides additional understanding on how certain design parameters and fuel element properties affect the predicted behavior of the TREAT LEU core. Further

refinement of the LEU conversion requirements would be necessary to fully evaluate and optimize the LEU fuel design. At the time of publication of this report, the project is entering a cold standby.

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