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Neutronics and Transient Calculations for the Conversion of the Transient Reactor Test Facility (TREAT)

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ABSTRACT

The Transient Reactor Test Facility (TREAT) is a graphite-reflected, graphite-moderated, and air-cooled reactor fueled with 93.1% enriched UO_2 particles dispersed in graphite, with a carbon-to-^{235}U ratio of ~10000:1. TREAT was used to simulate accident conditions by subjecting fuel test samples placed at the center of the core to high energy transient pulses. The transient pulse production is based on the core's self-limiting nature due to the negative reactivity feedback provided by the fuel graphite as the core temperature rises. The analysis of the conversion of TREAT to low enriched uranium (LEU) is currently underway. This paper presents the analytical methods used to calculate the transient performance of TREAT in terms of power pulse production and resulting peak core temperatures. The validation of the HEU neutronics TREAT model, the calculation of the temperature distribution and the temperature reactivity feedback as well as the number of fissions generated inside fuel test samples are discussed.

1. Introduction

The Transient Reactor Test Facility (TREAT) is a graphite-reflected, graphite-moderated, and air-cooled reactor fueled with 93.1% enriched UO_2 particles dispersed in graphite, with a fuel carbon-to-^{235}U ratio of ~10000:1 [1]. TREAT was designed to produce high neutron flux transients to investigate the transient-induced behavior of reactor fuels. It was operated from 1959 to 1994 when it was placed on non-operational standby. During the operation of TREAT, hundreds of experiments were conducted investigating the behavior of reactor fuels under accident conditions. Recently, the US Department of Energy (DOE) made the decision to pursue the resumption of transient testing utilizing TREAT. Analysis of the conversion of TREAT for exclusive use of low enriched uranium (LEU) fuel (19.75% enrichment) is currently underway as a collaborative effort between Argonne National Laboratory (ANL), Idaho National Laboratory (INL), and Los Alamos National Laboratory (LANL) under the sponsorship of the DOE National Nuclear Security Administration's Reactor Conversion Program. The goal of the conversion is to design an LEU core which maintains the experimental capabilities of the HEU core, while continuing to operate safely.

This study presents the methods developed to analyze the transient behavior of TREAT using the Monte Carlo code MCNP and the point kinetics code TREKIN, in support of the conversion from HEU to LEU.

2. TREAT Core and Operation

The TREAT fuel assembly is approximately 4"x4" square x 8 ft. long, with a central 4 ft. Zircaloy-clad fuel region and 2 ft. aluminum-clad graphite axial reflectors above and below the fuel. The core region is capable of accommodating a maximum 19 x 19 array of assemblies, and is surrounded by a graphite radial reflector enclosed in a concrete bioshield. The core loading can be change to accommodate different experimental vehicles placed at the center of the core and/or the operation of the hodoscope. The hodoscope was a collection of collimated neutron detectors used to monitor the fuel-test sample and was positioned at the North side of the bioshield. Special assemblies with the central fuel part removed were loaded in the core to provide the hodoscope a viewing slot of the test sample.

TREAT is controlled by twenty B_4C-bearing control rods which are divided in three groups reflecting their different roles: (a) eight transient rods used to introduce the reactivity changes which drive the transients, (b) eight control/shutdown rods used to assist in establishing critical configurations and (c) four compensation rods that are only used to compensate for the reactivity introduced when a central test vehicle is to be removed from the core. TREAT power transients are controlled by the negative reactivity feedback provided by the heating of the fuel graphite. These transients typically fall into two categories: (a) temperature-limited transients, which are fast (<1 second) power bursts initiated by a step reactivity insertion and constrained solely by the temperature reactivity feedback, and (b) shaped transients, which are slower (several seconds) desired power-time histories produced by time dependent transient rod withdrawal. The operation of the HEU core was limited such that the peak fuel temperature had to remain below 600^{o}C and 820^{o}C during normal operation and under accident conditions, respectively. These temperature limits were established to prevent excessive oxidation and phase transformation of the TREAT fuel Zircaloy cladding.

The key parameter in the conversion of TREAT is the total energy deposition (TED) in a fuel-test sample. The TED is related to the total core energy release through a parameter called the power coupling factor, or PCF:

$$\mathrm{PCF} = \frac{\text{Fission energy (or power)per unit mass of test}-\text{fuel sample}}{\text{Total core energy (or power)}}$$

An LEU core design with a lower PCF than the HEU core for a given test sample would require generating more core energy to achieve the same TED and results in higher cladding temperatures. Therefore, it is desirable that the LEU core has equal or similar PCF to the HEU core to match the performance requirements. Additional parameters considered in developing an LEU design include the all-rods-out core excess reactivity and the shutdown margin of each control rod bank. From a safety standpoint, the primary parameter of concern is the peak cladding temperature.

3. Models and Codes

The general-purpose Monte Carlo N-Particle code MCNP5-1.60 [2] is used for the steady-state neutronics calculations of TREAT. The transient simulations are being performed with the point kinetics code TREKIN [3].

3.1. MCNP

A detailed 3D MCNP model of TREAT has been developed including the core, the radial reflector and the concrete bioshield. Figure 1 illustrates a cross sectional view of the MCNP model of the TREAT loading used for the M8CAL experiment series with the viewing slot present. The MCNP model was also used to calculate the set of core-specific parameters needed by TREKIN for transient analysis, as discussed below.

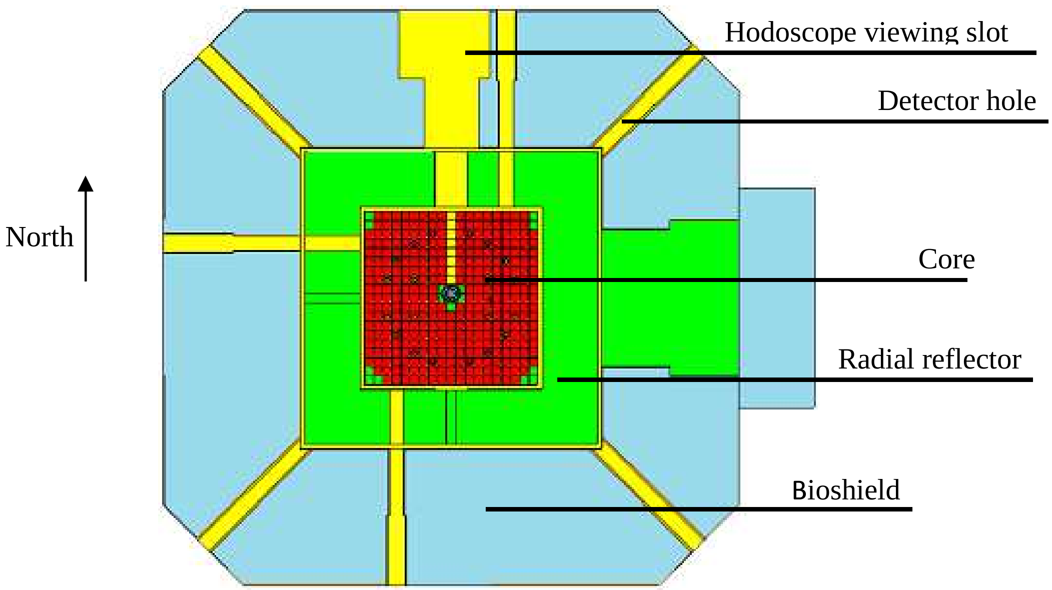

Figure 1. Cross Sectional View of the TREAT MCNP Model

3.2. TREKIN

TREKIN is a point kinetics code that solves the kinetic equations. It uses an Excel-based input-output environment. It was routinely used during TREAT operations to evaluate the transient behavior of planned experiments. TREKIN requires as input data the following set of core-specific properties: the effective delayed neutron fraction, the prompt generation lifetime, the negative temperature reactivity feedback as well as the peak and average fuel temperature as a function of core energy release. During TREAT operations this input data was produced by combining calculations and measurements in such way to get the best predictive capability. Because there will not be LEU measurements available prior to the conversion, a method which relies only on calculations was developed. This method was applied to specific HEU core configurations and validated against measurements.

The prompt generation lifetime and the effective delayed neutron fraction were calculated with MCNP using the KOPTS [4] card, for a cold critical core configuration. The temperature reactivity feedback as a function of core energy is evaluated using MCNP simulations of hot core conditions for a series of increasing energy steps. Because the time duration of a temperature-limited transient is less than one second, the heating of the fuel assemblies is approximated as an adiabatic process.

The temperature distribution for each energy step was estimated using the MCNP-calculated relative power distribution for a cold core with the transient rods fully withdrawn and the control/shutdown rods at their pre-transient position (i.e., the position which held the core at critical with the transient rods inserted). An evaluation of the impact of rod position on power distribution and resulting temperature reactivity feedback is underway.

Using the heat capacity of the fuel-graphite and the MCNP-calculated power distribution, the temperature of each assembly was estimated for increasing total core energy values, ranging from 100 to 5000 MJ, assuming a 26^{o}C initial temperature. Using the clustering algorithm K-Means [5], the fuel assemblies were divided into three groups and the average temperature of each group was calculated. For each group, three axial temperature zones were determined based on the core average relative axial power distribution. For every axial and radial temperature zone, temperature-dependent cross-section libraries were produced using the MCNP utility program Makxsf [6]. Makxsf implements NJOY routines to interpolate cross sections at temperatures between the evaluation temperatures of the distributed cross section libraries. Using the temperature dependent cross sections the temperature reactivity feedback was calculated with MCNP for every total core energy value.

4. Validation

The validation of the TREAT MCNP model and the point kinetics code TREKIN was based on currently-available data from past experiments, including the minimum critical core experiments and the irradiation experiment series performed with the ANCAL and M8CAL core loadings [7].

4.1. MCNP

The MCNP model was validated against critical rod configurations and power coupling factor measurements. Table 1 shows the criticality calculation results for the measured critical control rod configurations and the calculated deviation from criticality. The MCNP calculations were performed using the ENDF/B-VII.0 cross-sections library. Preliminary MCNP calculations showed that the k_{eff} was decreased by approximately 600pcm when switching to the ENDF/B-VII.1 cross section libraries. This reduction is due to the increase of carbon's absorption cross section [8].

Table 1. Criticality Calculations for the M8CAL TREAT MCNP Model and the Deviation from Criticality. The Standard Deviation of the Calculated k_{eff} was 0.0002

Control/Shutdown Rods Withdrawal	Transient Rods Withdrawal	k_{eff}	Deviation from Criticality (pcm)
37.95%	100%	1.00910	910
37.50%	100%	1.00848	848
83.00%	28%	1.00600	600
37.72%	100%	1.00877	877

The PCF was calculated for cold core conditions as the ratio of fission energy deposited in the test sample and the total core energy. Table 2 shows the ratio of the calculated-to-measured PCF for test samples irradiated in the two cores.

Table 2. Calculated-to-Reported Power Coupling Factors (C/R) for Test Samples Irradiated in the M8CAL[10] and ANCAL[11] Cores

Core	Test Sample	PCF C/R
M8CAL	60” wire	0.99
	8” wire	0.97
	8” wire	0.98
	8” wire	0.80
	U-Pu Pin	1.23
	U Pin	1.19
ANCAL w/ SS primary containment	Inner top	1.08
	Inner middle	1.10
	Inner bottom	1.10
	Outer top	1.04
	Outer middle	1.05
	Outer bottom	1.09
ANCAL w/ Al primary containment	Inner top	1.18
	Inner middle	1.17
	Inner bottom	1.20
	Outer top	1.15
	Outer middle	1.15
	Outer bottom	1.16

The measurement uncertainties are currently not known, so the total uncertainty of the measured PCF cannot be assessed. However, the main source of uncertainty is suspected to be the calibration of the detectors which is performed under heat-balance conditions for constant core power and control rod insertion. The measured PCF is essentially the ratio of the number of neutrons reaching the test sample placed at the center of the core to the number of neutrons leaking into the power detectors located inside the bioshield (see Fig. 1). The neutron leakage depends on the control rod insertion (due to shadowing effects) and on the resultant temperature distribution and the neutron spectrum (which is hardened as the core temperature increases). Therefore, for the same core power the response of the detectors maybe different if the control rod insertion and temperature distribution are different than those during the detectors calibration [9]. It has been reported [10] that for equal measured core power the measured PCF differed by approximately 27% for different control rod configurations.

4.2. TREKIN

For every TREAT core loading and before each planned experiment three temperature-limited transients with increasing reactivity insertion were performed. The peak core temperature was measured with thermocouple-bearing fuel assemblies positioned at the places of interest and where the highest temperatures were expected. The results of these measurements were used to estimate the reactivity insertion limits that would result in the peak core temperatures of 600^{o}C and 820^{o}C. The measured temperature limited transients used to evaluate the M8CAL and ANCAL core loadings were used to validate TREKIN. The results of peak power and core energy and of peak core temperature and negative temperature reactivity feedback are shown in Tables 3 and 4, respectively.

TREKIN predicts the hot spot temperature with a calculated-to-reported ratios ranging from 1.00 to 1.08. The measurement error of the thermocouples used to measure the core temperature is reported to be ±2.5% but their exact axial and radial locations during the experiments were not known.

Table 3. Reported (R) and TREKIN Calculated (C) Peak Power and Total Energy

Core	Inserted Reactivity	Peak Power C (MW)	Peak Power R (MW)	Peak Power C/R	Energy C (MJ)	Energy R (MJ)	Energy C/R
M8CAL	1.81%	1031	1292	0.80	684	693	0.99
	3.02%	5330	6242	0.85	1411	1583	0.89
	3.87%	11180	12630	0.89	2018	2287	0.88
ANCAL	1.80%	1353	1345	1.01	799	825	0.97
	2.89%	5635	5683	0.99	1488	1530	0.97
	3.72%	11408	11997	0.95	2107	2257	0.93

Table 4. Reported (R) and TREKIN Calculated (C) Peak Core Temperature and Negative Temperature Reactivity Feedback

Core	Inserted Reactivity (%dk/k)	Peak Core Temperature C (^{o}C)	Peak Core Temperature R (^{o}C)	Peak Core Temperature C/R	Negative Temperature Reactivity Feedback C (%dk/k)	Negative Temperature Reactivity Feedback R (%dk/k)	Negative Temperature Reactivity Feedback C/R
M8CAL	1.81%	240	236	1.02	3.040%	3.246%	0.94
	3.02%	384	378	1.02	5.120%	5.150%	0.99
	3.87%	495	488	1.01	6.470%	6.441%	1.00
ANCAL	1.80%	240	241	1.00	3.169%	3.307%	0.96
	2.89%	401	373	1.08	5.003%	5.087%	0.98
	3.72%	514	486	1.06	6.332%	6.419%	0.99

4.3. LEU Analysis

An LEU core for TREAT must be capable of achieving the same TED with the HEU core, without exceeding the temperature limits. Development of an LEU design is concentrated on identifying features which (1) optimize the PCF and (2) minimize peak cladding temperature. LEU analysis is currently focused on evaluation of the core under a reactivity insertion accident with zero air coolant flow, which presents the maximum temperature the fuel assemblies must be able to withstand. For the HEU core, this temperature is the 820°C accident temperature limit. Operationally, this was imposed as a constraint on the allowable available reactivity, or allowable pre-transient position of the transient rod bank. For the HEU M8CAL half-slotted core, this reactivity limit was 5.95% dk/k.

The corresponding LEU maximum accident scenario temperature is evaluated by calculating the LEU shaped transient needed to match the TED achievable in the HEU with the maximum allowable reactivity insertion of 5.95% dk/k. The HEU shaped transient is evaluated using the TREKIN period-driven mode with 0.3s initial period until a power of 75W is reached followed by an 8s period (see Figure 2). The LEU shaped transient necessary to achieve equal TED is estimated by scaling the HEU shaped transient power-time history by a multiplying factor equal to the ratio of the PCFs in the two cores. The resultant LEU power-time history is evaluated using the TREKIN power-driven mode to determine the pre-transient reactivity (i.e., pre-transient rod position) needed. Finally, the LEU accident scenario is calculated assuming a step insertion of this reactivity. The LEU accident peak temperature is directly linked to the power coupling factor – a higher PCF leads to lower peak temperatures.

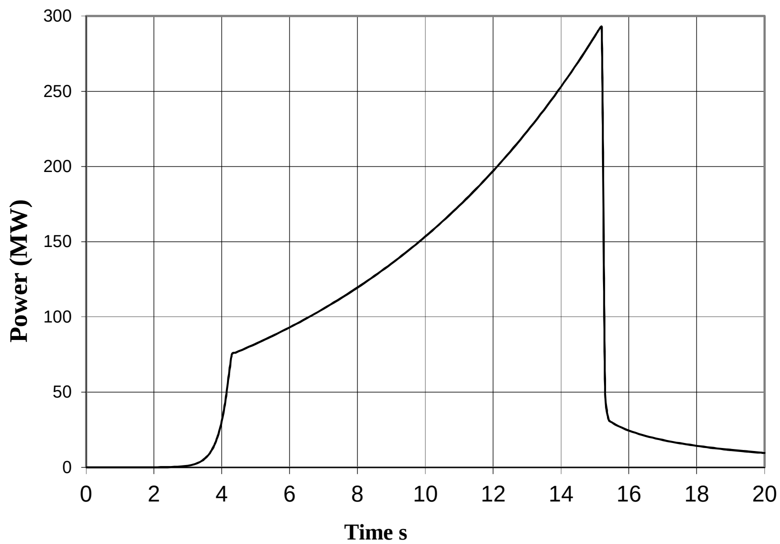

Figure 2: HEU Two-Period Driven TREKIN Calculated Core Power-Time History

For the same outer and inner fuel assembly dimensions as the HEU, various LEU fuel compositions were analyzed by calculating the excess reactivity and PCF. The LEU core should have enough excess reactivity to perform the most demanding experiment (which would produce the highest core temperature and consequently present the highest negative reactivity feedback) and a similar (or equal) PCF to the HEU core. The impurities content of the HEU and LEU fuels are not expected to be identical. For this study the LEU fuel was assumed to have an impurity content equivalent of 2ppm of natural boron. For these preliminary calculations the graphite-fuel density was set at 1.85g/cm^3 and the graphitization at 85%. Three LEU fuel compositions were analyzed by increasing the C/U ratio (keeping the graphite-fuel density constant)and calculating the excess reactivity, the PCF, the prompt neutron generation lifetime, the transient rods worth and the temperature reactivity feedback for a uniform temperature distribution (all the fuel assemblies were at the same temperature). The calculation results are presented in Table 5.

Table 5. Neutronics Characteristics of the HEU and the LEU Core Loadings Analyzed

Parameter	HEU	LEU-A	LEU-B	LEU-C
C/U	10,000	1962	2195	2470
Excess reactivity (k-1/k)	7.8%	8.8%	7.2%	5.1%
PCF relative to HEU	100%	89%	95%	105%
l_p (μs)	868 ± 1.1	890 ± 1.2	973 ± 1.3	1072 ± 1.4
Transient Rods Worth	9.1%	8.3%	8.9%	9.6%
Temp Reactivity Coefficient ($\times10^{-4}$ dk/k/^{o}C)	1.48 ± 0.05	1.45 ± 0.04	1.59 ± 0.04	1.76 ± 0.05

Using the heat capacity of the HEU fuel-graphite, a peak-to-core average temperature of 1.5 and the temperature reactivity feedback calculated for uniform temperature distribution; the inserted reactivity to produce a TED identical to the HEU core was calculated with TREKIN for the three LEU cores. Table 6 shows the relative-to-HEU PCF, the required reactivity insertion to produce an identical TED and the relative-to-HEU peak core temperature.

Table 6. Relative to HEU PCF and Peak Core Temperature for Inserted Reactivity which Produces Equal TED with the HEU Core

Parameter	HEU	LEU-A	LEU-B	LEU-C
PCF relative to HEU	100%	89%	95%	105%
Inserted Reactivity	2.00%	1.91%	1.97%	2.10%
Rel to HEU Peak Temperature	100%	103%	98%	92%

The peak temperature of the LEU core is inversely proportional to the PCF, so the LEU-C composition seems to be the best option. However, LEU-C presents the highest temperature reactivity feedback so the excess reactivity of 5.1% will not be sufficient to perform high demanding experiments possible in the HEU core. LEU-A has higher excess reactivity than the HEU core, but the transient rod worth is not enough to shut down the reactor. Even though LEU-B has a lower PCF, the peak temperature for equal TED is lower than HEU due to the higher fuel density (there is more thermal mass in LEU).

The core performance achievable for the cases presented in Tables 5 and 6 is very closely tied to the fuel density. In earlier analyses, it was not known that a density of 1.85 g/cm3 would be achievable, so lower C/U ratios were calculated leading to lower PCF values and higher core temperatures. Several LEU designs with thicker cladding and larger fuel-to-clad gap were evaluated to accommodate these higher temperatures. Example results for some of the LEU designs considered are presented in Table 7 where the PCF values are expressed relative to HEU. For each case in Table 7, the C/U ratio was selected to obtain an appropriate excess reactivity. As with the results presented in Table 5, the PCF is directly proportional to C/U, i.e., a higher C/U results in a higher PCF.

The designs with the thicker cladding require lower C/U to compensate the reactivity loss due to the increased neutron absorption by the additional Zircaloy. The lower C/U leads to the hardening of the neutron spectrum which results in the decrease of the transient rods worth and the PCF. Even though the thicker cladding would be able to withstand higher temperatures (and hence higher oxidation), the lower PCF would require higher total core energy to achieve an identical TED to the HEU core and consequently, results in higher peak core temperature.

Table 7. Influence of Fuel Assembly Dimensions and Fuel Density on C/U and Core Performance

Parameter	Design A	Design B	Design C	Design D
Density (g/cm^3)	1.77	1.85	1.75	1.85
Clad Thickness (mils)	67	67	25	25
Fuel-Clad Gap (mils)	44	44	50	50
C/U	1110	1400	1452	2150
	Key Results			
Excess Reactivity (dk/k)	6.2%	6.4%	7.8%	7.6%
Transients Worth	7.6%	7.8%	8.3%	8.8%
Rel to HEU PCF	73%	82%	82%	96%

5. Conclusions

Models and analysis methods for evaluation of the TREAT facility have been developed and validated against historic HEU core data in support of the TREAT conversion from HEU to LEU. The goal of the conversion analysis is to establish an LEU design which can maintain the experiment performance of the HEU core while meeting all the safety requirements. Using a combination of the codes MCNP and TREKIN, both steady-state and transient behaviors were calculated, including criticality, test-sample-to-core power coupling, and transient power-time histories. The methods for temperature-limited transient analysis have been validated against measurements from the M8CAL and ANCAL experiment series, and are now applied in the evaluation of the LEU core designs.

Several LEU designs have been evaluated, and selected results have been presented to illustrate the impact of key design parameters on the core behavior. In particular, the performance of the core is closely connected with the C/U ratio that also determines the excess reactivity of the core. For the same fuel density, a higher C/U ratio improves the core performance (higher PCF) but at the same time lowers the core excess reactivity. Therefore, the choice of a C/U ratio is also connected with other fuel design parameters which affect the excess reactivity. For example, thicker cladding or smaller fuel volume will require lower C/U ratios to compensate for the reactivity loss, and consequently higher core energy will be needed to achieve identical TED with the HEU core.

The results of this on-going study, combined with structural analyses and testing, materials testing and LEU fuel manufacturing evaluations will be used to design a TREAT LEU fuel assembly to meet the performance and the safety requirements.

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