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**THE EFFECT OF CARBON CRYSTAL STRUCTURE ON
TREAT REACTOR PHYSICS CALCULATIONS**

R. W. Swanson and L. J. Harrison
Argonne National Laboratory-West
P.O. Box 2528
Idaho Falls, ID 83403-2528
(208) 526-7167

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R. W. Swanson and L. J. Harrison

Argonne National Laboratory-West
Idaho Falls, ID 83403-2528, U.S.A.

ABSTRACT

The Transient Reactor Test Facility (TREAT) at Argonne National Laboratory-West (ANL-W) is fueled with urania in a graphite and carbon mixture. This fuel was fabricated from a mixture of graphite flour, thermax (a thermatomic carbon produced by "cracking" natural gas), coal-tar resin and U_3O_8 . During the fabrication process, the fuel was baked to dissociate the resin, but the high temperature necessary to graphitize the carbon in the thermax and in the resin was avoided. Therefore, the carbon crystal structure is a complex mixture of graphite particles in a nongraphitized elemental carbon matrix.

Results of calculations using macroscopic carbon cross sections obtained by mixing bound-kernel graphite cross sections for the graphitized carbon and free-gas carbon cross sections for the remainder of the carbon and calculations using only bound-kernel graphite cross sections are compared to experimental data. It is shown that the use of the hybridized cross sections which reflect the allotropic mixture of the carbon in the TREAT fuel results in a significant improvement in the accuracy of calculated neutronics parameters for the TREAT reactor.

INTRODUCTION

The primary function of the Transient Reactor Test Facility (TREAT) at Argonne National Laboratory-West (ANL-W) is the irradiation of reactor fuels under simulated reactor accident conditions. As part of the design and planning for such experiments, it is necessary that the experiment-dependent neutronics parameters be determined. The eventual success or failure of the experiment may depend on the quality of these determinations. There are two parameters which fall in this category that are of primary importance for all experiments. The first is the ratio of test-fuel power density to reactor power (defined here as power coupling). The second is the excess reactivity available in the reactor with the experiment in place. The reliability of the results of calculations performed to determine these parameters is dependent on the ability to properly calculate the neutron spectrum which is extremely sensitive to the carbon scattering function. The carbon scattering

function is itself a function of the allotropic form in which the carbon is present.

The TREAT fuel was made by mixing graphite flour, thermax (a thermatomic carbon produced by "cracking" natural gas), coal-tar resin and urania (U_3O_8). During the fabrication process, the mixture was baked to dissociate the resin, but the high temperature necessary to graphitize the carbon in the thermax and in the resin was avoided since it conceivably could have resulted in the volatilization of the urania. During the baking process the U_3O_8 was converted to UO_2 . Therefore, the fuel structure is a complex mixture of crystalline graphite particles in a nongraphitized elemental carbon matrix. The scattering kernels representing graphite and free-gas carbon are of course quite different, and prediction of certain neutronic parameters would be expected to be sensitive to the distribution of carbon between the two forms. Determination of the ratio of graphite to total carbon in the TREAT fuel and the use of a scattering function appropriate for the actual composition of the TREAT fuel should substantially improve the calculational results for TREAT.

Although the TREAT reactor began operation in 1959, the specific composition of the graphite and carbon was treated as proprietary by the manufacturer of the fuel until just recently. Accordingly, past calculations of the TREAT core have employed either free-gas carbon or graphite cross sections. While such modeling worked acceptably overall, there were some persistent discrepancies.

For whatever reason, the fuel fabricator, Great Lakes Carbon Corporation, has now released the information needed to improve the calculation model. The TREAT fuel was 75 parts graphite flour, 25 parts thermax and 29.4 parts Koppers coal tar by weight. Using a weight fraction of 0.913 for carbon in coal tar a ratio of graphitized carbon to total carbon of 0.59 was obtained.

This paper will present the results of a study performed to evaluate the use of hybridized macroscopic carbon cross sections. The hybridized cross sections were obtained by mixing carbon cross sections having a scattering function appropriate for graphite for the graphitized carbon and free-gas carbon cross sections for the remainder of the carbon.

DESCRIPTION OF TREAT

The basic TREAT fuel element is a 2.4-m (8-ft)-long, 10.2-cm (4-in.)-square assembly. The central 1.2 m (4 ft) contains the fuel mixture which contains 0.009 at. % of finely divided highly ^{235}U -enriched uranium oxide. This central section is canned in Zircaloy-3. The upper 0.6 m (2 ft) and the lower 0.6 m (2 ft) of the assembly which contain aluminum canned graphite form the axial reflector. Modifications of this basic design result in a variety of special assemblies. Among these are instrumented assemblies to monitor core temperature, Zircaloy-clad reflector assemblies to fill unfueled

positions, control rod assemblies through which the control rods move and viewing slots used in conjunction with neutron-detecting instrumentation for observing fuel motion. These various assemblies are arranged in a 19 x 19 matrix which rest on a grid plate and are clamped at the top of the assemblies. A 0.6 m (2 ft) radial graphite reflector surrounds the assembly matrix. This radial reflector is covered with aluminum. More detailed information about TREAT is given in Ref. 1.

EXPERIMENTAL INFORMATION

During a recent calibration experiment, irradiations of test fuel were performed in two distinctively different core loadings. Figure 1 shows a plan view of the first core configuration, TREAT core loading number 1341, which contained a calibration vehicle and a large radial viewing slot. The locations of the calibration vehicle, the control rods and unfueled Zircaloy-clad reflector assemblies are indicated in Fig. 1.

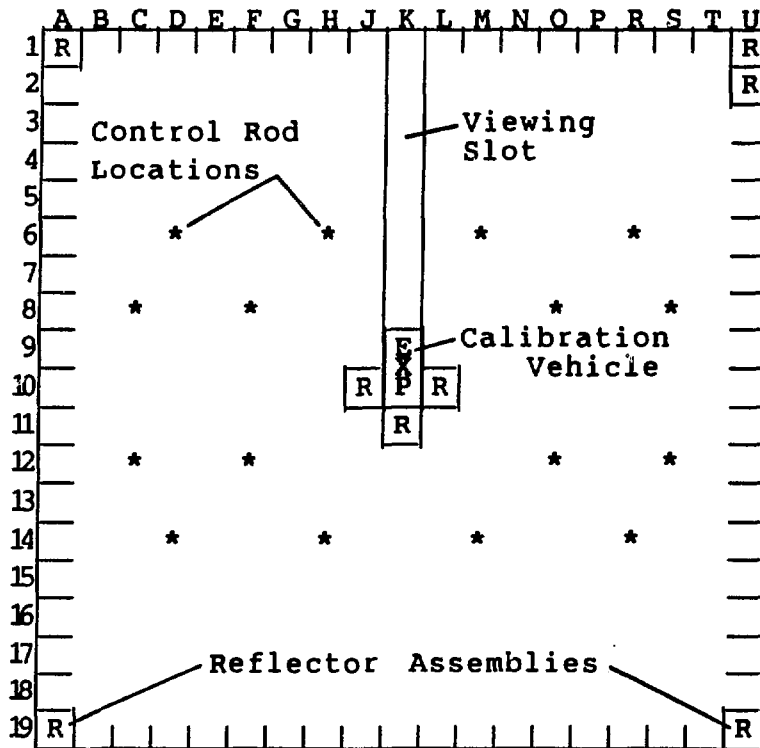


Fig. 1. TREAT core loading number 1341 — plan view.

The calibration vehicle, which consists of an outer and an inner containment, occupied two standard fuel assembly positions. The outer containment consisted of a 0.10 m (4 in.) by 0.20 m (8 in.) type 304 stainless-steel can having a wall thickness of 1.27 mm (0.050 in.). The

inner containment, in which the test fuel was located, consisted of several concentric cylindrical containments composed of Inconel and stainless steel. The test fuel was Zircaloy-clad 5.5% ^{235}U -enriched UO_2 .

Figure 2 shows a plan view of the second core configuration, TREAT core loading number 1343, which contained the same calibration vehicle, but the radial viewing slot was filled with TREAT fuel and additional reflector elements were placed around the outside of the core.

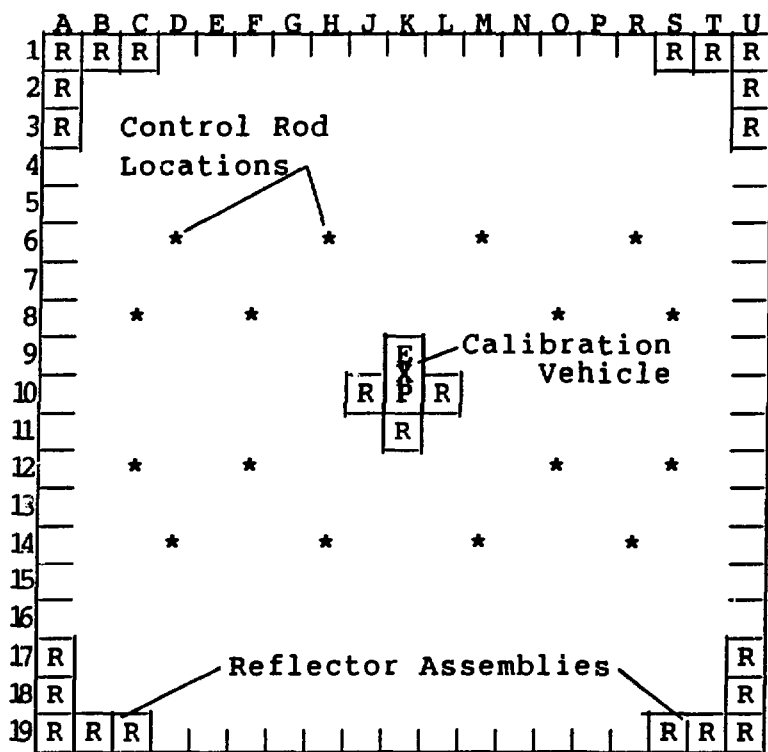


Fig. 2. TREAT core loading number 1343 — plan view.

The ratio of test-fuel fission density to the TREAT-fuel fission density at the peak power location was experimentally determined for core loading number 1343. This was accomplished by placing a 0.762 mm (0.030 in.) diameter 3.5 wt % highly ^{235}U -enriched U/Zr monitor wire at the TREAT core peak power location during the irradiation of the test fuel. This fission density ratio from which power coupling can be obtained lends itself to calculation more readily than does the actual value of power coupling. From radiochemical analysis of the test-fuel and the monitor wire, the ratio of the test fuel fission density to the fission density in TREAT at the peak power location was determined to be 40.4 ± 1.2 for core loading number 1343 at the one-sigma confidence level. This information combined with the critical control rod configurations provides the necessary experimental information needed

configurations provides the necessary experimental information needed for this evaluation.

CALCULATIONAL APPROACH

The cross-section set used for this study is a 50-group neutron cross-section set generated using the AMPX system from an ENDF/B-IV source library.² The multigroup energy structure of this set is described in Table I. An evaluation of ENDF/B-IV cross sections contains several calculated values of k-effective for Cross Section Evaluation Working Group (CSEWG) uranium-graphite critical assemblies.³ The calculated values of k-effective for these assemblies vary from 0.9965 to 1.0055. A previously reported study of temperature effects on power coupling in the TREAT reactor used similar cross sections with excellent results.⁴

TABLE I
Fifty-group Energy Structure

Group	Energy Range, Upper Limit (eV)	Group	Energy Range, Upper Limit (eV)
1	20.00 X 10 ⁶	26	0.700
2	3.00 X 10 ⁶	27	0.600
3	0.60 X 10 ⁶	28	0.550
4	100.00 X 10 ³	29	0.500
5	17.00 X 10 ³	30	0.450
6	1.15 X 10 ³	31	0.400
7	0.21 X 10 ³	32	0.375
8	100.000	33	0.350
9	61.000	34	0.325
10	41.000	35	0.300
11	30.000	36	0.275
12	20.000	37	0.250
13	12.900	38	0.225
14	8.100	39	0.200
15	6.000	40	0.175
16	4.000	41	0.150
17	2.570	42	0.100
18	2.000	43	0.080
19	1.590	44	0.070
20	1.350	45	0.060
21	1.200	46	0.050
22	1.090	47	0.040
23	1.000	48	0.030
24	0.925	49 ^a	0.0253
25	0.800	50 ^a	0.010

^aThe lower limit of this group is 0.0.

For the purpose of evaluating calculated values of k-effective, detailed full-core Monte Carlo calculations were performed for both critical core configurations (loadings 1343 and 1341) with TREAT-fuel cross sections appropriate for 100% graphite and 59% graphite. The calculations of the critical core configurations were performed using the Monte Carlo code KENO-IV.⁵ Each calculation processed approximately 30,000 neutron histories.

Cell Monte Carlo calculations were performed to determine the fission density ratio of the test fuel to the TREAT peak power location in core loading number 1343 with TREAT-fuel cross sections appropriate for 100% graphite and 59% graphite. These calculational results can then be compared to the experimentally obtained results. The cell calculations were performed using the Monte Carlo code MORSE with combinatorial geometry as modified by Scientific Applications.⁶ The size of the cell was chosen such that the specular reflecting boundary was located at the TREAT peak power location.

CALCULATIONAL RESULTS

The calculated k-effective values of the full-core KENO-IV calculations of the critical configurations are presented in the Table II. The statistical uncertainty represents the Monte Carlo one sigma confidence interval. The "100% Graphite" refers to using the scattering function appropriate for graphite alone and the "59% Graphite" refers to using a hybridized scattering function appropriate for 59% graphite and 41% free-gas carbon.

Table II

Calculated Values of k-effective

<u>Calculational Description</u>	<u>k-effective</u>
Loading 1341 100% Graphite	0.9724 \pm 0.0021
Loading 1341 59% Graphite	0.9921 \pm 0.0012
Loading 1343 100% Graphite	0.9707 \pm 0.0024
Loading 1343 59% Graphite	0.9922 \pm 0.0017

This study also explains the results of previously performed analysis in which calculations using free-gas carbon cross sections yielded values of k-effective which were greater than experiment while calculations using carbon cross sections appropriate for graphite yielded values of k-effective which were less than experiment.

The calculated fission density ratios obtained from the MORSE cell Monte Carlo calculations of a calibration experiment are compared to the experimentally determined value in Table III. The statistical uncertainty represents the Monte Carlo one-sigma confidence interval.

Table III

Calculated Fission Density Ratios

<u>Calculational Description</u>	<u>Calculated Fission Density Ratio</u>	<u>Calc.-Exp. Exp.</u>
100% Graphite	43.2 \pm 1.4	+6.9%
59% Graphite	39.4 \pm 1.2	-2.5%

SUMMARY

The use of hybridized cross sections which reflect the allotropic mixture of the carbon in the TREAT fuel results in a significant improvement in the accuracy of calculated values of k-effective for the TREAT reactor. The ability to properly calculate the fission density ratio between test fuel and the reactor has also been improved.

ACKNOWLEDGEMENTS

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