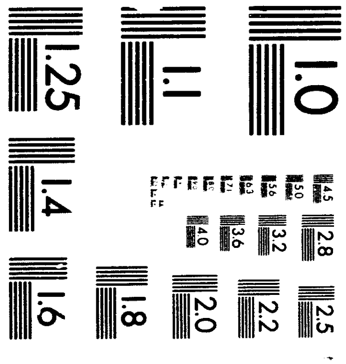
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Conf-910414--43

WAPD-T-2949

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To Be Submitted to

American Nuclear Society
International Topical Meeting
Advances in Mathematics, Computations, and Reactor Physics
Pittsburgh PA
April 1991

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ABSTRACT

Several clean critical experiments were analyzed with ENDF/B-VI data to assess the adequacy of the data for U^{235}, U^{238} and oxygen. These experiments were 1) a set of homogeneous U^{235}-H_2O assemblies spanning a wide range of hydrogen/uranium ratio, and 2) TRX-1, a simple, H_2O-moderated Bettis lattice of slightly-enriched uranium metal rods. The analyses used the Monte Carlo program RCP01, with explicit three-dimensional geometry and detailed representation of cross sections. For the homogeneous criticals, calculated k_{crit} values for large, thermal assemblies show good agreement with experiment. This supports the evaluated thermal criticality parameters for U^{235}. However, for assemblies with smaller H/U ratios, k_{crit} values increase significantly with increasing leakage and flux-spectrum hardness. These trends suggest that leakage is underpredicted and that the resonance eta of the ENDF/B-VI U^{235} is too large. For TRX-1, reasonably good agreement is found with measured lattice parameters (reaction-rate ratios). Of primary interest is rho28, the ratio of above-thermal to thermal U^{238} capture. Calculated rho28 is 2.3 (± 1.7) % above measurement, suggesting that U^{238} resonance capture remains slightly overpredicted with ENDF/B-VI. However, agreement is better than observed with earlier versions of ENDF/B.

INTRODUCTION

To upgrade cross section data, two types of benchmark critical experiments have been analyzed with cross sections from Version VI of the Evaluated Nuclear Data File (ENDF/B-VI): 1) a set of homogeneous U^{235}-H_2O assemblies, and 2) TRX-1, an H_2O-moderated Bettis lattice of aluminum-clad, slightly-enriched uranium rods. In the analyses, which employed the RCP01 Monte Carlo program[1], the assemblies were modeled explicitly in three-dimensions, and cross sections were represented in fine detail. The purpose of this work was to assess the adequacy of the ENDF/B-VI data evaluations for U^{235} (including the fission spectrum), U^{238}, and oxygen.

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*Work supported by Department of Energy Contract DE-AC11-88PN38014.

CROSS SECTION PROCESSING

Detailed elastic scattering, capture and (when appropriate) fission cross section profiles were constructed from 0.0005 eV to 21.17 MeV using a Bettis processing program which contains elements of the NJOY[2] and RCPL1[3] computer codes. For each nuclide, energy mesh generation (and subsequent thinning) followed the default guidelines for the NJOY program and resulted in a variable energy mesh with cross sections that were (generally) linearly interpolable to an accuracy within 1%. Subsequently, the profiles for all nuclides in the cross section library were interpolated onto a common energy mesh, containing in excess of 40000 energy points, for use by RCP01.

Elastic scattering angular distributions and inelastic cross sections were collapsed into a group structure. This structure contains 28 groups from 5.5 keV to 21.17 MeV. The elastic center-of-mass angular distributions were approximated by a group-averaged P_3 Legendre expansion. Below 5.5 keV, elastic scattering is assumed isotropic. The group-averaged inelastic cross sections and group-to-group transfer probabilities were calculated from the appropriate cross-section and secondary-energy-distribution data in the ENDF/B file.

ANALYSIS OF HOMOGENEOUS U^{235}-H_2O ASSEMBLIES

Homogeneous critical assemblies have been used extensively in the past to test cross section data for U^{235} and H_2O. The following experiments were chosen for the present study:

1) Four Gwin-Magnuson assemblies - relatively dilute aqueous solutions of uranyl nitrate in large spherical and cylindrical aluminum containers, unreflected[4].

2) Six small Oak Ridge assemblies[5,6] with lower H/U ratios (designated L5 - L10) - uranyl fluoride solutions in cylindrical and spherical aluminum containers, mostly unreflected (but some reflected with H_2O).

3) Seven Rocky Flats experiments - uranyl nitrate solutions in cylindrical aluminum containers, unreflected. These supplement the small ORNL assemblies. They appear to have been run with painstaking attention to detail, and are thoroughly documented[7].

In the Monte Carlo analyses, the assemblies were described explicitly in three dimensions, in most cases including the vessel. However, some assemblies are specified without the container and have correspondingly small experimentally-determined k_{crit} corrections. The models for the Rocky Flats assemblies included the container and a portion of the filling pipe.

The Monte Carlo analyses were run on the Bettis Cray YMP computer and were highly converged. There were usually at least four independent calculations of one million histories each. Final k_{crit} uncertainties were typically around 0.1% or less (95% confidence interval).

Most of these calculations were done with preliminary ENDF/B-VI data sets, as indicated in Table 1. Subsequently, the U^{235} evaluation (MAT 9228) was modified, and a new oxygen evaluation (MAT 825) was adopted for the final ENDF/B-VI. In addition, the U^{235} fission spectrum was a Bettis evaluation that is very close to ENDF/B-VI. In all cases, however, comparisons were subsequently made with final ENDF/B-VI data to evaluate the differences.

At the large-H/U limit (highly thermalized, low-leakage assemblies), calculated k_{crit} values are primarily sensitive to the thermal criticality parameters of U^{235}. Inclusion of assemblies with lower H/U introduces sensitivity to above-thermal leakage and above-thermal U^{235} fission rate (flux spectrum hardness).

Calculated K_{crit} results are shown in Table 2 along with values of fast leakage and above-thermal U^{235} fission rate.

The results of a least-squares (LS) fit in terms of these variables are shown in Figures 1 and 2. These figures display separately the leakage and flux-spectrum-hardness components of the observed k_{crit} trend, as determined in the least-squares fit. Specifically, the k_{crit} for the ith assembly can be written:

$$k_i = A + BxL + CxF_{25} + dk_i$$

where L = fast leakage
F_{25} = above-thermal fission
k_i = calculated k_{crit} for assembly i
dk_i = difference of k_i from the LS-fit prediction

and A, B and C are parameters determined in the LS fit.

The "projected k_{crit}" is

$$projk_i = k_i - CxF_{25} \qquad \text{(vs fast leakage)}$$

$$= k_i - BxL \qquad \text{(vs above thermal fission)}$$

in Figures 1 and 2 respectively. (The number beside a plotted point identifies the particular assembly, for example, Gwin-Magnuson assembly ORNL10).

The ENDF/B-VI data, primarily the thermal criticality parameters of U^{235} (preliminary Mat 9228), give a good k_{crit} value at the dilute, highly-thermal limit (0.9993 for ORNL10). A modified version of Mat 9228, having a drooping eta below 0.0253 eV, also was found to give a good k_{crit} (0.9982 for ORNL10). The modified version was adopted for ENDF/B-VI.

The effect of using the ENDF/B-VI fission spectrum for U^{235} appears to be small. For assembly L7, which has the most leakage, use of the ENDF/B-VI spectrum increased k_{crit} by 0.0012 ± 0.0013.

The k_{crit} values in Figure 1 show a systematic increase with above-thermal leakage. Part of this trend (perhaps 0.003 at the high leakage end) is due to the multigroup elastic scattering angular representation in RCP01, which can be improved with new coding. In addition, there are two major data sensitivities: the U^{235} fission spectrum (mean energy and shape), and the oxygen high energy scattering cross sections and angular distributions. The oxygen data set for these calculations is ENDF/B-V, Mat 1276. Subsequently, k_{crit} results were obtained with Mat 825, the oxygen evaluation adopted for ENDF/B-VI. These yielded a net decrease of 0.0030 ± 0.0014 Δk for L7 compared to ORNL10, indicating that deficiencies in the Mat 1276 oxygen evaluation are a significant contributor to this trend.

The k_{crit} values in Figure 2a show a systematic increase with above-thermal U^{235} fission rate (flux spectrum hardness). The major data sensitivity here is the resonance alpha (capture/fission ratio) of U^{235}, which is 0.477 for Mat 9228. As an illustration of this sensitivity, an alternate data set with U^{235} resonance alpha of 0.512 exhibits negligible slope versus above-thermal fission rate. These results are displayed in Figure 2b.

Before attempting to draw some conclusions from Figures 1 and 2, it is necessary to try to form some idea of the uncertainties of k_{crit} stemming from uncertainties of the materials content and dimensions of the critical assemblies. While it is difficult to reach any quantitative judgment on this question, some observations are pertinent:

- In the LS fit, the overall residual scatter of individual k_{crit} values is approximately 0.0025 (standard deviation).

- The limiting k_{crit} at the low-leakage, soft-spectrum end (based on the mean of all the large Gwin-Magnuson assemblies) is thought to be well known.

- The Rocky Flats assemblies are well documented and appear to have been run with painstaking attention to detail. They show good agreement with the ORNL assemblies.

The leakage trend (Figure 1), which involves the limiting k_{crit} on one end and all the Rocky Flats assemblies at the other, appears to be well established.

The spectrum-hardness trend (Figure 2) depends strongly on two of the small assemblies: ORNL L5 and L6. Several sensitivity calculations were made for these assemblies, with results shown in Table 4. The primary sensitivity is to overall solution density. Although there is some question as to its precision, the specific gravity appears to be well determined[6]: quoted values are 2.013 for the H/U=27.1 solution and 1.661 for the H/U=44.3 solution (used in L5 and L6 respectively). In comparison, the precision of specific gravity determinations for the Rocky Flats assemblies is 0.06% on average.

A reasonable overall uncertainty on k_{crit} for individual assemblies is judged to be .003 (standard deviation).

ANALYSIS OF TRX-1 CRITICAL EXPERIMENTS

The TRX-1 critical assembly was a simple H_2O-moderated and reflected lattice of slightly-enriched uranium metal rods clad in aluminum. Among the experiments carried out in this assembly were measurements of lattice parameters (i.e., reaction-rate ratios) such as rho28, the ratio of above-thermal to thermal U^{238} capture[8]. TRX-1 is one of the thermal reactor benchmarks of the Cross Section Evaluation Working Group[9]. A full-core model of TRX-1 was used previously to calculate measured lattice parameters with ENDF/B-IV data[10]. The calculation used the RCP01 Monte Carlo program, and described cross sections and the lattice geometry in explicit detail. As part of the CSEWG data testing effort, the old ENDF/B-IV calculation has been repeated with ENDF/B-VI data as shown in Table 1, including MAT 9237 for U^{238}.

Calculated lattice parameters are summarized in Table 4. These are obtained from reaction rates edited for the central, asymptotic portion of the lattice. These are (with a thermal-cut energy of 0.625 eV):

Rho28 = Above-thermal U^{238} capture/Thermal U^{238} capture

Delta25 = Above-thermal U^{235} fission/Thermal U^{235} fission

Delta28 = U^{238} fission/U^{235} fission

There is generally good agreement with experiment, within the uncertainties, although calculated rho28 is slightly high and k_{crit} low.

In a second RCP01 calculation, the ENDF/B-VI U^{238} was replaced with Version V (MAT 1398). The value of rho28 changed to 1.373 ± 0.006 and k_{crit} to 0.9940 ± 0.0008. This shows explicitly the effects of the difference in U^{238} evaluations. One of the major differences is extension of the resolved resonance range up to 10 keV in Version VI, from 4 keV in the earlier versions.

There has been a long-standing problem that ENDF/B U^{238} data overpredicted resonance capture in U^{238} and consequently produced low k_{crit} values and high conversion ratios[11]. This is illustrated for TRX-1 in Figure 3, which shows the RCP01 results obtained with ENDF/B-IV and ENDF/B-VI. Also shown is a calculation with ENDF/B-V data performed by P. F. Rose and E. Schmidt at Brookhaven National Laboratory with the SAM-CE Monte Carlo Program[11]. In addition, the RCP01 point with Version V U^{238} is shown (labeled "ENDF/B-V"). Although rho28 is still slightly high, and k_{crit} low, Version VI provides improved agreement with experiment relative to the earlier versions.

CONCLUSIONS

In summary, these studies of ENDF/B-VI data sets indicate that:

1) The U^{235} thermal criticality parameters perform well.

2) There is a residual trend of k_{crit} with above-thermal leakage, but use of Mat 825 (ENDF/B-VI oxygen) in place of Mat 1276 (ENDF/B-V oxygen) significantly reduces this trend.

3) There is a strong trend of k_{crit} with above-thermal fission rate. This suggests that the resonance alpha of ENDF/B-VI U^{235} (Mat 9228) is too low.

4) For TRX-1, calculated lattice parameters are in reasonably good agreement with experiment. Of primary interest, rho28 calculated with ENDF/B-VI Mat 237is 2.3 (± 1.7) % above measurement. This is better agreement than was found with earlier versions of ENDF/B.

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Table 1. ENDF/B Material ID's used in the Analyses

Nuclide	MAT No.
U235	Prel. 9228
U238	1398 (9237)
U234	1394
U236	1396
H	125
O	1276 (825)
Al	1313
N	1275
F	1309

Table 2. Calculated Kcrit Results for Homogeneous Critical Assemblies

Assembly	Kcrit	Fast Leakage	Above-thermal Fission
Gwin-Magnuson Assemblies:			
ORNL 1	0.9996 ± 0.0005	0.1418	0.0084
ORNL10	0.9993 ± 0.0003	0.0533	0.0070
ORNL12	1.0009 ± 0.0006	0.0958	0.0076
ORNL22	0.9982 ± 0.0004	0.0215	0.0066
Small Oak Ridge Assemblies			
L5	1.0171 ± 0.0008	0.4350	0.1830
L6	1.0128 ± 0.0008	0.4416	0.1300
L7	1.0087 ± 0.0009	0.5566	0.0673
L8	1.0074 ± 0.0012	0.1957	0.0098
L9	1.0030 ± 0.0008	0.1397	0.0084
L10	1.0022 ± 0.0011	0.1956	0.0085
Rocky Flats Assemblies			
RF1	1.0063 ± 0.0009	0.4391	0.0933
RF4	1.0063 ± 0.0009	0.4129	0.0397
RF6	1.0036 ± 0.0008	0.3339	0.0181
RF7	1.0088 ± 0.0008	0.3424	0.0195
RF8	1.0098 ± 0.0009	0.4136	0.0411
RF9	1.0064 ± 0.0008	0.4157	0.0418
RF10	1.0100 ± 0.0009	0.4366	0.0936

Note: Uncertainties are 95% confidence intervals from Monte Carlo statistics.

Table 3. Kcrit Sensitivities for Homogeneous Critical Assemblies

Case	Calculated Kcrit
Assembly L5:	
Base	1.0171 ± 0.0008
Reduce all atomic number densities by 1%	1.0078 ± 0.0014
Reduce critical height by 1%	1.0156 ± 0.0014
Reduce N(U235) by 1%	1.0168 ± 0.0019
Assembly L7:	
Base	1.0087 ± 0.0009
Reduce all atomic number densities by 1%	1.0021 ± 0.0019

Table 4. Lattice Parameters in TRX-1: Comparison of Measurement and ENDF/B-VI Calculations

Parameter	Measurement	Calculation
Rho28	1.320 ± 0.021	1.350 ± 0.008
Delta25	0.0987 ± 0.0010	0.0992 ± 0.0009
Delta28	0.0946 ± 0.0041	0.0993 ± 0.0005
kcrit	1.0000 ± 0.0020	0.9946 ± 0.0009

Note: Measured values embody corrections and uncertainties (standard deviations) as evaluated by Sher (Ref. 11). Calculational uncertainties are 95% confidence intervals reflecting Monte Carlo statistics.

Figure 1. Homogeneous Benchmark Values of Projected Kcrit versus Above-Thermal Leakage

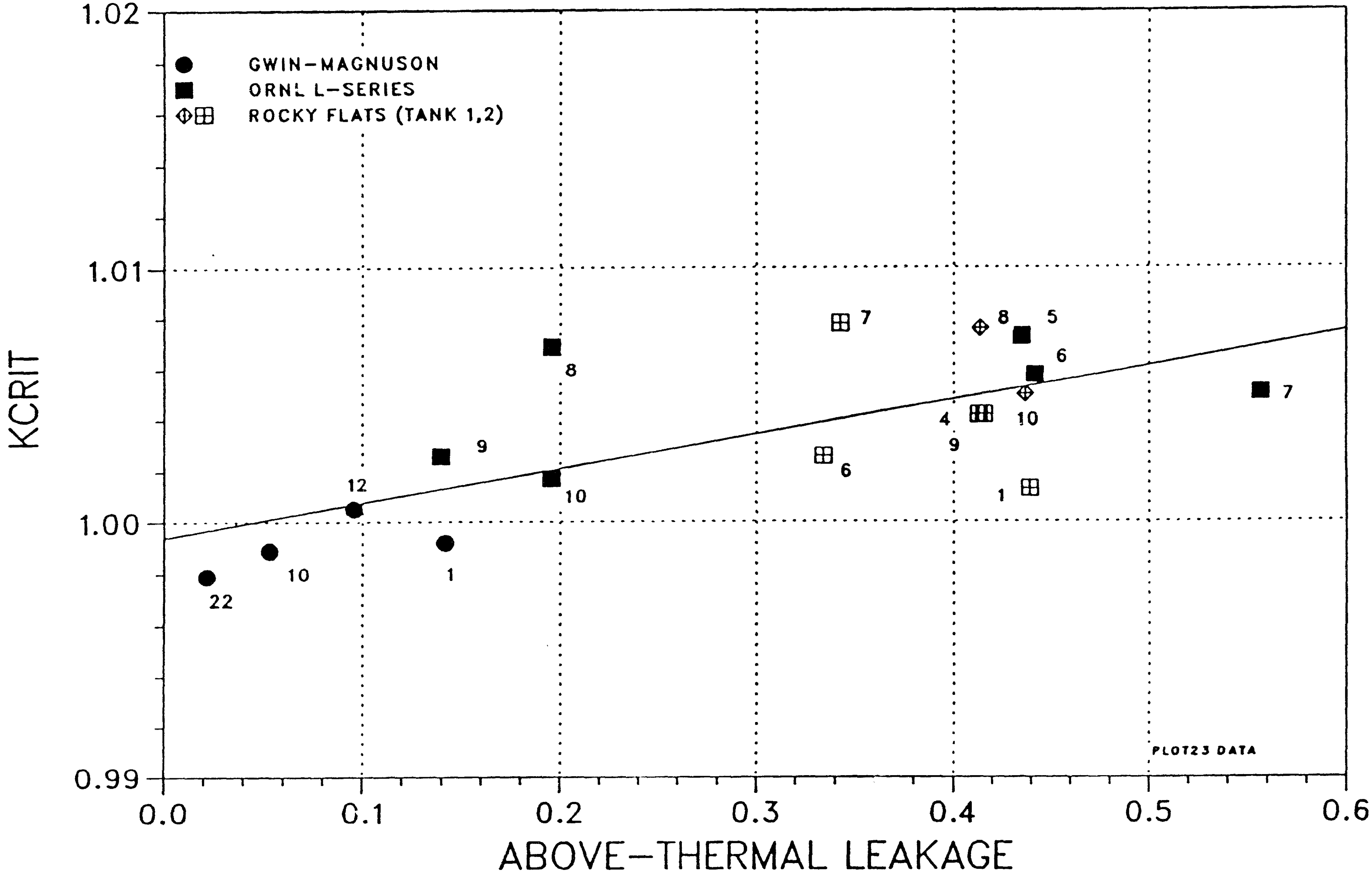


Figure 2. Homogeneous Benchmark Values of Projected Kcrit versus Above-Thermal Fission Rate

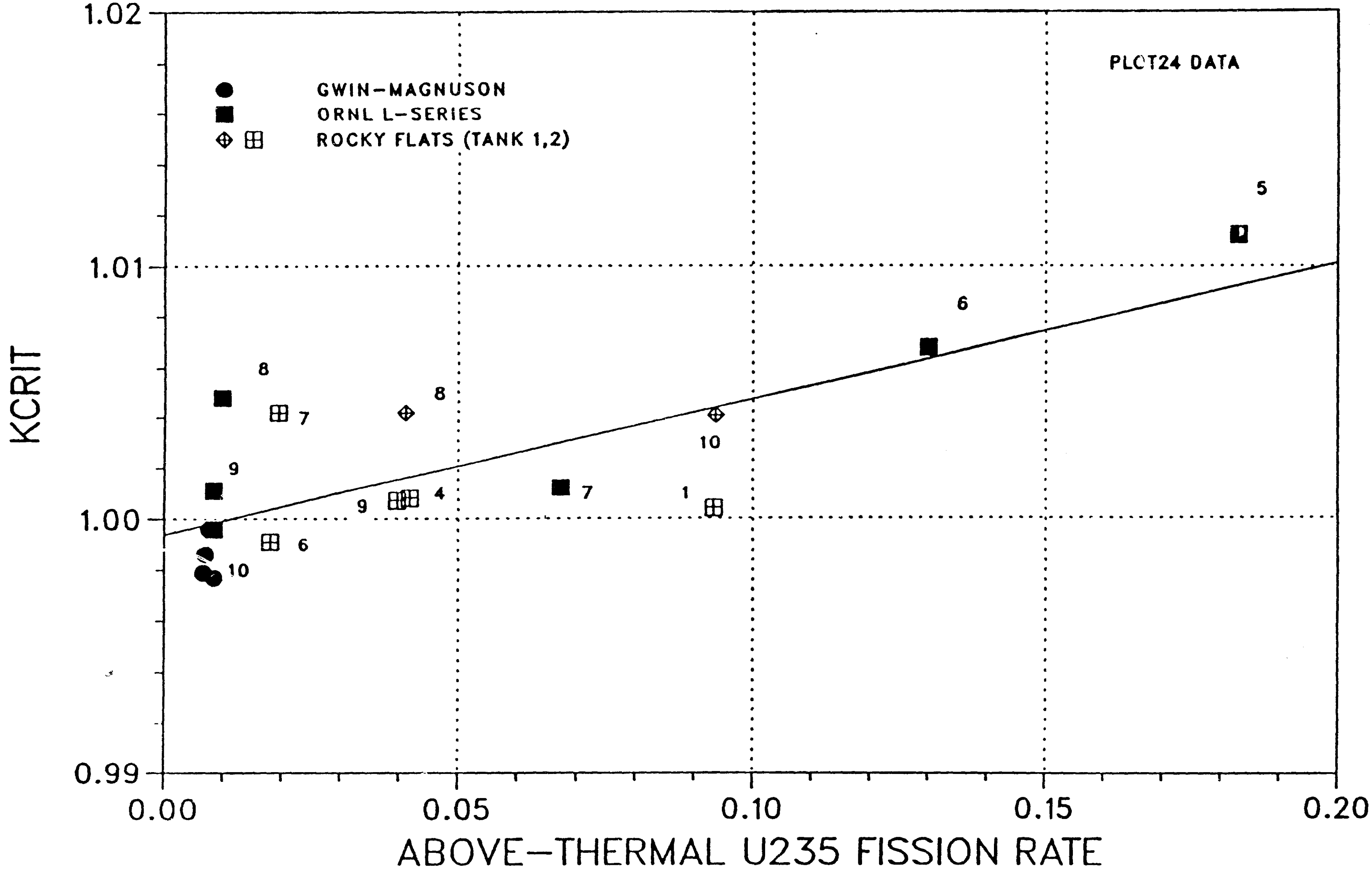


Figure 3. Homogeneous Benchmark Values of Projected Kcrit versus Above-Thermal Fission Rate (Alternative data set with resonance alpha = 0.512)

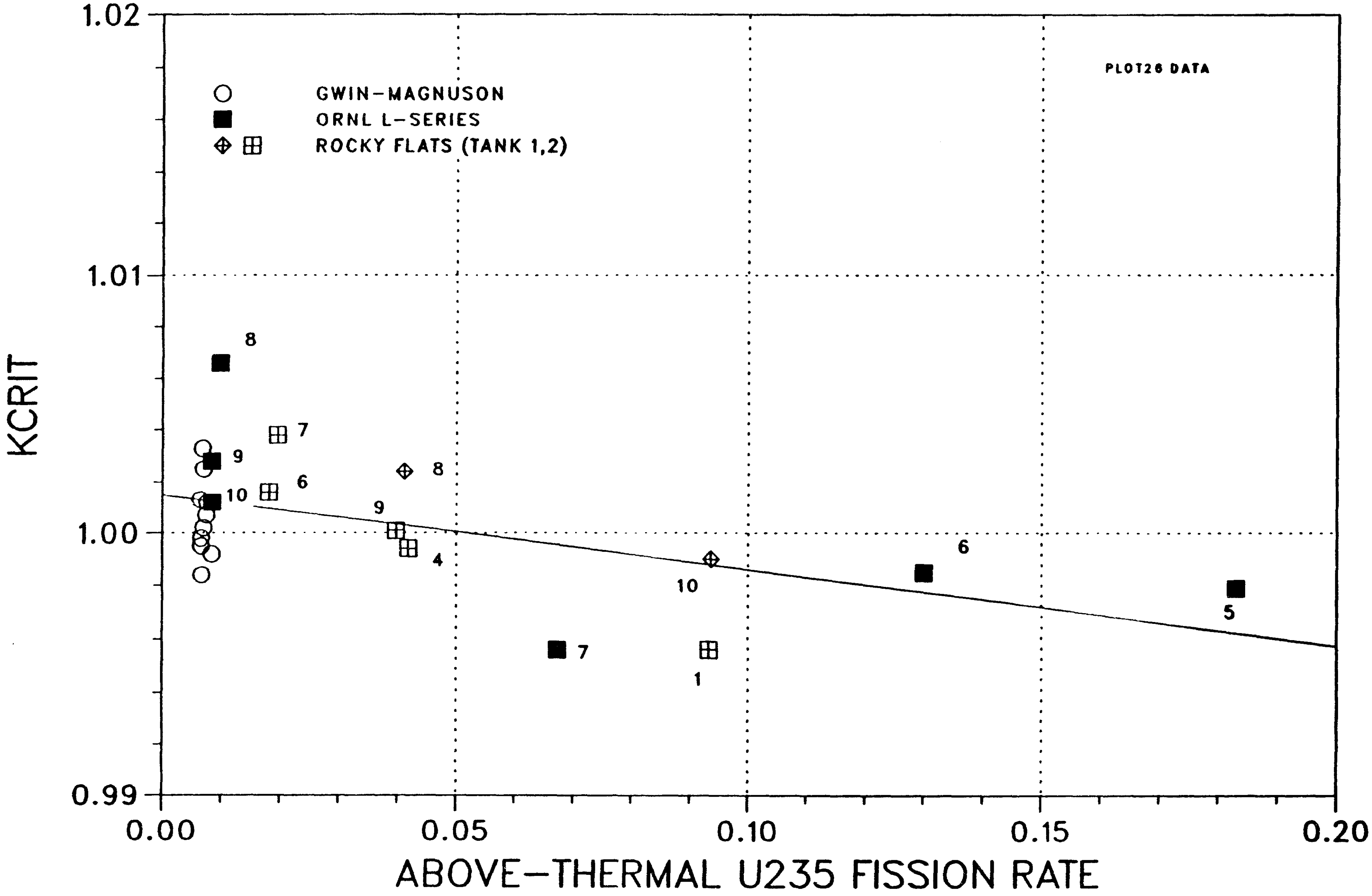
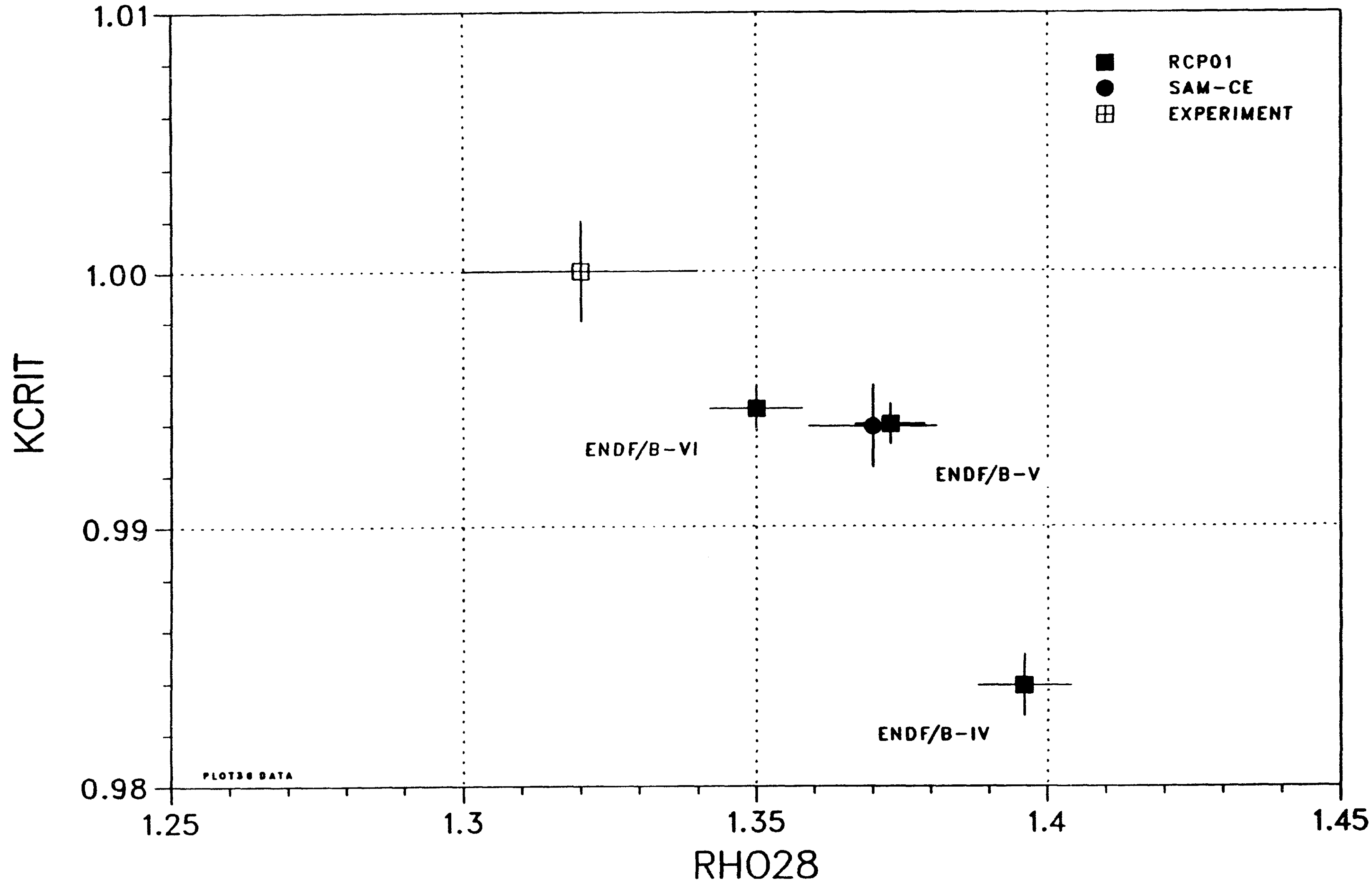


Figure 4. Kcrit vs. Rho28 for TRX-1



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