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Conf-930907--5

UCRL-JC-112934
PREPRINT

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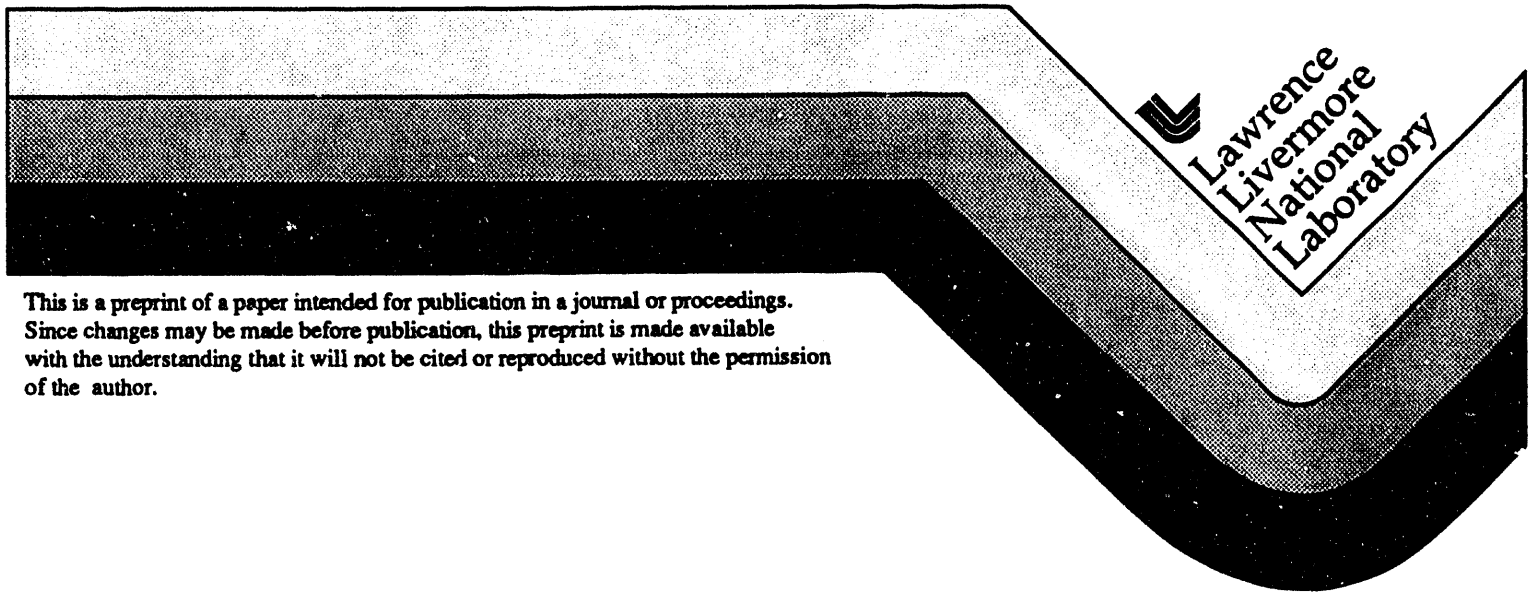
Prepared for Submittal to:
American Nuclear Society1993 Topical Meeting on
Physics and Methods in Criticality Safety
Nashville, Tennessee
September 19-23, 1993

March 1, 1993



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ABSTRACT

For several years, we have been conducting criticality benchmark calculations with COG. COG is a point-wise Monte Carlo code developed at Lawrence Livermore National Laboratory (LLNL). It solves the Boltzmann equation for the transport of neutrons and photons. The principle consideration in developing COG was that the resulting calculations would be as accurate as the point-wise cross-sectional data, since no physics or computational approximations were used.

The objective of this paper is to report on COG results for criticality benchmark experiments in concert with MCNP comparisons which are resulting in corrections and upgrades to the point-wise ENDL cross-section data libraries.

Benchmarking discrepancies reported here indicated difficulties in the Evaluated Nuclear Data Livermore (ENDL) cross-sections for U-238 at thermal neutron energy levels. This led to a re-evaluation and selection of the appropriate cross-section values from several cross-section sets available (ENDL, ENDF/B-V). Further cross-section upgrades are anticipated.

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1.0 INTRODUCTION

1.1 Background

For several years, we have been conducting criticality benchmarking calculations [1-3] of the LLNL developed Monte Carlo particle transport code COG.[4] The principle consideration in developing COG was that the resulting calculations would be as accurate as the point-wise cross-sectional data, since no physics or computational approximations were used. Indeed, the process of criticality benchmarking itself is reduced to errors in only one of three areas; (1) the model, (2) the code itself, or (3) the point-wise data. As part of the benchmarking process, we have compared COG calculations to both critical experiments and other code calculations including MCNP,[5] KENO,[6,7] SAN,[8] and MORSE.[9] Throughout the process, we have identified a number of discrepancies between various code calculations and experimental results. [1-3]

Many of the discrepancies identified code correction required by COG or inherent problems with other codes or approximations. In Alesso,[2] we discussed the unsatisfactory state of affairs in general, for some specific isotopes. In Alesso,[3] we

* This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

identified a particularly troubling discrepancy between calculation and experiment. In Heinrichs,[10] a definitive effort was made to identify the problem. Heinrichs[10] found that by using COG with ENDL[11] and MCNP with ENDF/B-V[12] a consistent 5 per cent under prediction was produced. Recently, this discrepancy was resolved in Cullen[13] as a result of errors in nuclear data in the ENDL cross-section library.

1.2 Objective

The objective of this paper is to report on COG and MCNP results for a criticality benchmark experiment using two different cross-section sets: the LLNL ENDL92 set and the ENDF/B-V set.

The LLNL ENDL92 cross-section set was developed primarily for neutrons in the fast spectrum. COG and ENDL92 have been used successfully in past benchmarking activities in which the neutrons were primarily in the fast spectrum.[1] In this work, testing with a critical experiment having neutrons primarily in the thermal spectrum is attempted.

The ENDF/B-V cross-section set and MCNP have demonstrated good comparisons with critical experiments for neutrons in the thermal spectrum.[19]

Results from this work, along with future benchmarking work of this type may provide criteria for unifying data from evaluated cross-section sets into a single nuclear data library.

Future plans hopefully include a significant LLNL unification of our cross-section libraries by merging data from international libraries, JEF,[14] JENDL,[15] ENDF/B, and BROND.[16]

1.3 Summary of Results

Discrepancies in results of criticality benchmarks of COG with experiment and with calculations from other codes led to the possibility that the cause of the discrepancies could be due to inconsistencies in nuclear data in the cross-section libraries. Subsequent benchmarks to confirm this possibility led to the task to compare cross-section libraries, which ultimately unveiled the fact that ENDL has a 10 percent larger U^{238} capture cross-section than that found in ENDF/B. This high ENDL cross-section is expected to be responsible for the COG benchmarking discrepancies, and work is in progress to both update the cross-section libraries and to repeat the COG benchmarks with this new library.

We found that the process of using a point-wise code with no physics or computational approximations strongly facilitated identification and resolution of benchmark descrepencies that required exploration of (1) modeling errors, (2) code errors, and (3) cross-section errors.

2.0 MONTE CARLO CODE BENCHMARKS

2.1 Overview

Assurance of subcriticality is the most important element in any nuclear operation. A good understanding of the detailed nuclear fission process is the only way to assure subcriticality. Today, this assurance is provided by using an analytical computational tool to evaluate and analyze all possible scenarios and geometries. The reliability of the evaluation results depends upon how accurately the computational tool represent the realistic condition of the operation in question. Proof of the accuracy of the computational tool again depends upon the proper benchmarking of the code against the actual nuclear fission process experiments (criticality experiments). The applicability of a code to a specific geometry and condition relies on whether a benchmark has been done for a similar type of experiment.

The COG code was developed at LLNL and uses the ENDL cross-sections evaluated by LLNL. The ENDL92 cross-section set was originally developed primarily for neutrons in the fast spectrum.

The principle consideration in developing COG was that the resulting calculation was to be as accurate as the input data given to the code. Cross-section data was presented by evaluators in the 1980's as point-wise data (i.e., a series of cross-section points as a function of neutron energy with the understanding that interpolation between adjacent points produces results as good as the data). COG was written to use this form of the cross-section data directly. The angular scattering data are likewise presented and used as the evaluators present them. No physics or computational approximation has been made that would compromise the accuracy of these data. COG has been run using the point-wise cross-sections of the LLNL ENDL.

Several other well known codes have been used in our benchmarking. These include:

KENO-IV[6] and KENO-Va[7] are multigroup Monte Carlo codes developed at ORNL which are part of the package of codes called SCALE.[7] Both versions have been extensively used in the criticality safety field.

MCNP[5] is another point-wise Monte Carlo code developed at Los Alamos National Laboratory (LANL). The code's standard point-wise cross-sections based on ENDF/B-V[12] were used.

MORSE-C[9] is a LLNL code based on the ORNL code MORSE.[9] It is a multigroup Monte Carlo code.

SAN[8] is a discrete ordinates code. Developed at LLNL, it is a version of the ANISN code. SAN was run on a CRAY computer using the N92GRP multigroup cross-section set.

2.2 Benchmark

A critical experiment containing 1.43 atomic per cent enriched U-235 in uranium in a UF4/paraffin wax mixture is presented in Reference 17. The dimensions of the uranium-paraffin mixture are 86.8 cm square by 174.4 cm high. The assembly was not reflected.

Models were prepared as input to COG and MCNP. The ENDL92 cross-sections were used with both MCNP and COG. The ENDF/B-V cross-sections in their parameterized form were used with MCNP. These models were run on an LLNL Cray computer.

The MCNP code provides two different methods for estimating k_{eff} values: the absorption method and the collision method. Results for both methods are presented here.

$S(\alpha,\beta)$ treatment deals with the scattering of low energy neutrons in moderators in which scattering isotopes (hydrogen, for example) are bound to a molecule. An $S(\alpha,\beta)$ scattering model for such a moderator often results in a k_{eff} value that is significantly different than a free gas scattering model for such a moderator.

Two different $S(\alpha,\beta)$ treatment models, the Poly.01t model and the lwtr.01t model, are provided in MCNP. Results for both models are presented here.

The MCNP and COG results are shown in Table 1.

The results in Table 1 show the k_{eff} values to be about 5 percent low for the critical experiment when the ENDL92 cross-sections are used with either COG or MCNP. The k_{eff} values for MCNP and the ENDF/B-V cross-section set are close to 1.0, except for the collision estimator without the $S(\alpha,\beta)$ treatment.

The wax is $C_{25}H_{52}$. The $S(\alpha,\beta)$ treatment available in COG on the Cray computer is for CH_2. This results in 3.85 w/o hydrogen in the wax mixture that has no $S(\alpha,\beta)$ treatment in COG for this calculation.

To resolve the differences in k_{eff} values in Table 1, differences in nuclear data for ENDL92 and ENDF/B-V were examined. Cullen[13] investigated differences between carbon and fluorine cross-sections, ^{235}U nu-bar values, ^{235}U fission cross-sections, and ^{238}U capture cross-sections. The ^{238}U capture resonance

integral in ENDL92 was found to be about 10 percent higher than that for ENDF/B-V and for ENDF/B-VI. It was further determined that the high ^{238}U capture all by itself was sufficient to account for the low k_{eff} values found using ENDL92 in Table 1. With proper treatment of the thermal range that includes both Doppler broadened cross-sections and sampling that includes relative speed, $S(\alpha,\beta)$ treatment should not be needed for this critical experiment model.

COG uses cross-sections in a point-wise format. ENDF/B-V is presented in a parameterized format. The decision was made to convert ENDF/B-V to a point-wise format. Methods for performing a conversion of this type are described in Reference 18. Some results of the conversion are discussed in Reference 18.

In Reference 19, preliminary benchmark calculations using TART[20] and the ENDF/B-V point-wise cross-section set for some ^{235}U spherical fast critical assemblies with various reflectors show the average k_{eff} to be 1.013+0.010 as compared to TART and ENDL92 giving 1.003+0.007.

Models were run on a Hewlett Packard 9000/730 work station using COG with ENDL92 and the ENDF/B-V point-wise cross-section sets. These models were identical to those run for Table 1 using a LLNL Cray computer. $S(\alpha,\beta)$ treatment was used, and COG was corrected to handle the $C_{25}H_{52}$ material properly. The results are shown in Table 2.

The results in Table 2 show the k_{eff} values using COG and the ENDF/B-V point-wise cross-section set to have a mean value bias of 0.09 percent using $S(\alpha,\beta)$ treatment and 0.26 percent for no $S(\alpha,\beta)$ treatment. These results are in agreement

with the MCNP k_{eff} results in Table 1 using the parameterized ENDF/B-V cross-sections, except for the collision estimator k_{eff} without S(α,β) treatment.

The results in Table 2 show the k_{eff} values using COG and the ENDL92 point-wise cross-section set to have a mean value difference of 0.76 percent using S(α,β) treatment and 0.16 percent for no S(α,β) treatment compared to values in Table 1.

Table 1. 0 K_{eff} Calculations for UF_4/Paraffin Wax Mixture

Run No.	1	2	3	4	5	6	7	8
Code	MCNP-3b	MCNP-3b	MCNP-3b	MCNP-3b	MCNP-3b	MCNP-3b	COG	COG
X-S	ENDF/B-V	ENDF/B-V	ENDF/B-V	ENDL	ENDL	ENDL	ENDL	ENDL
S (α, ß)	Poly.01t	lwtr.01t	none	Poly.01t	lwtr.olt	none	CH_2*	none
K_{eff} (Collision) ± 1σ	1.001946 ±.0065	1.007694 ±.0069	.976350 ±.0058	.943892 ±.0064	.942531 ±.0068	.946061 ±.0069	.9546 ±.0048	.9416 ±.0058
K_{eff} (Absorption) ± 1σ	.994099 ±.0049	1.002738 ±.0052	.994257 ±.0052	.932620 ±.0053	.946839 ±.0050	.951768 ±.0050		

* 3.85 w/o H has no S (α, ß) treatment.

Table 2.0 COG can now be run with ENDF/B or ENDL

Cross-Section Library	S(α, ß)	Keff± 1σ
ENDL	None	.9432 ± .0047
ENDF	None	.9974 ± .0048
ENDL	H & Poly	.9470 ± .0047
ENDF	H & Poly	.9991 ± .0048

Where do we go from here?

3.0 CROSS-SECTION UNIFICATION

The formats of the Livermore libraries (ENDL) and the U.S. libraries (ENDF/B) are completely different. In the ENDF/B system, the data are expressed in many different formats employing multiple interpolation regions and the possibility of six different interpolation schemes. The energy distributions are described by a combination of both an arbitrary tabulated function and an evaporation spectrum.[12]

Before using an evaluation in the ENDF/B format, White[19] preprocessed the information into point-wise form. The output is then passed through an additional set of codes and translated into the ENDL format.

In Figure 1 is a diagram showing the overall picture of the use of nuclear data in applications codes.

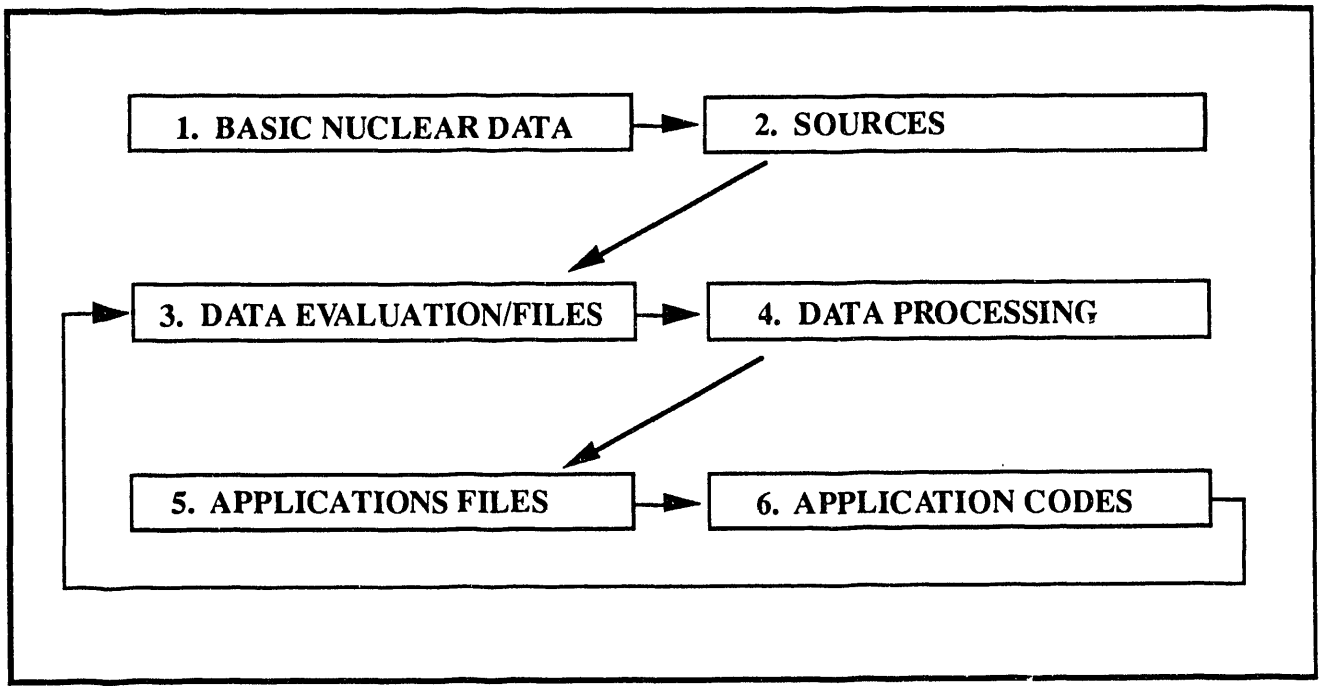

Figure 1. Diagram showing the flow from basic data to applications codes.

LLNL has current plans to unify ENDL cross-section for all isotopes by utilizing benchmarked data from libraries from many sources. The fast spectrum from ENDL for most isotopes is expected to remain unaffected, but thermal spectrums for various isotopes may be changed.

The process of using a code like COG with no physics or calculational approximations should make the benchmarking process for both the point-wise data and the code COG most effective.

4.0 CONCLUSION

In this paper, we presented a criticality benchmark process and results that may lead to upgrades in the ENDL cross-section set. In addition, we have discussed future cross-section upgrades to follow in concert with a benchmarking process that utilizes a point-wise code without physics or calculation approximations to facilitate descrepancy resolution.

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