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THE EFFECT OF RESONANCE STRUCTURE
ON 14-MeV MONTE CARLO NEUTRON TRANSPORT
IN NITROGEN AND AIR

MASTER

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Laboratory

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THE EFFECT OF RESONANCE STRUCTURE ON 14 MeV
MONTE CARLO NEUTRON TRANSPORT IN NITROGEN AND AIR

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ABSTRACT

The results of Monte Carlo calculations can be sensitive to methods used to treat cross sections. This sensitivity can be emphasized by studying one isotope of an element or material that has a resonance region. Very few naturally occurring materials exist in a mono-isotopic form, but when such a material is an important part of a problem, care should be exercised in the selection of a code to be used for the calculations. It is recommended that the ALICE code, that uses a multiband treatment for cross sections, be used at LLNL for neutronic and neutron-induced photonic problems.

INTRODUCTION

Monte Carlo Neutron/Photon transport codes at LANL and LLNL have been used to calculate neutron and photon leakage from nitrogen spheres of various radii. The LANL Monte Carlo code, MCNP, uses a continuous energy representation for both particle tracking and cross section data. The LLNL code, TART, uses continuous energy for particle tracking and 175 energy group representations of the neutron cross sections. Another LLNL Monte Carlo transport code, ALICE, uses continuous energy for particle tracking and a multiband treatment of cross sections in the same energy group structure as is used by the TART code.

DISCUSSION

The two problems compared by the laboratories are specified in Table 1. The primary information compared was the neutron surface current and flux leaking from the problems. The results of these calculations are presented in Tables 2 and 3.

The calculated results for Problem 1 are all in agreement, independent of methods of data treatment by the codes. This is because the thickness of material is not sufficient to show the effect of the methodological differences. References 1 and 3 have examples that demonstrate the effect. The ENDL76 and ENDL80 data sets (evaluated neutron cross section library of microscopic data used to derive code data) are essentially the

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Table 1. Computational model specifications.

Geometry	Problem 1	Problem 2
	Spherical	Spherical
Radius (cm)	1.89×10^4 (1 mfp)	13.23×10^4 (7 mfp)
Material	Nitrogen	Nitrogen
Density (g/cm ³)	1.2497×10^{-3}	1.2497×10^{-3}
Source energy	13.86 - 14.13	13.86 - 14.13
Source location	center of sphere	center of sphere

Table 2. Calculated neutron and photon leakage currents and flux for Problem 1.

Code/data set	Neutron		Photon	
	Current	Flux	Current	Flux
MCNP/ENDL76	$.773 \pm .0014$	$(2.04 \pm .007) \times 10^{-10}$	$.373 \pm .004$	$(1.09 \pm .01) \times 10^{-10}$
TART/ENDL80	$.772 \pm .002$	$(2.05 \pm .008) \times 10^{-10}$	$.376 \pm .004$	$(1.10 \pm .01) \times 10^{-10}$
ALICE/ENDL80	$.771 \pm .001$	$(2.05 \pm .002) \times 10^{-10}$	$.374 \pm .001$	$(1.10 \pm .003) \times 10^{-10}$

Table 3. Calculated neutron and photon leakage currents and flux for Problem 2.

Code/data set	Neutron		Photon	
	Current	Flux	Current	Flux
MCNP/ENDL80	$.0268 \pm .0003$	$(1.918 \pm .021) \times 10^{-13}$	n/a	n/a
TART/ENDL80	$.0244 \pm .0006$	$(1.750 \pm .044) \times 10^{-13}$	$.0626 \pm .0014$	$(3.948 \pm .086) \times 10^{-13}$
ALICE/ENDL80	$.0273 \pm .0006$	$(1.944 \pm .045) \times 10^{-13}$	$.0623 \pm .0013$	$(3.939 \pm .082) \times 10^{-13}$

same for nitrogen. The results of calculations for Problem 2 clearly indicate there are problems with methods of cross section treatment. The thickness of the material in Problem 2 is 7 times that in Problem 1.

In calculations using a single isotope with thicknesses of material greater than a few mean-free-paths, the errors resulting from cross section treatments are apparent. Table 3 presents the results of calculations by LLNL and LANL showing that ALICE and MCNP are in agreement. The MCNP code treats resonance self shielding effects exactly. From the agreement one may conclude that the ALICE code treats those effects adequately.

Figure 1 presents the nitrogen total and elastic cross sections. Note that the resonance structure of the elastic cross section is tracked by the total cross section. This indicates that while the other reactions affect the value of the total cross section, they do not add significantly to the resonance structure.

FIG. 1

The TART code results are clearly different than those calculated by MCNP and ALICE. This type of disagreement has been reported in Refs. 1, 2, and 3. The significance of the differences observed are: the multiband code, ALICE, calculates as accurately as the point-wise Monte Carlo code, MCNP; and TART is less accurate because of its cross section representation.

Some additional calculations have been completed with both TART and ALICE but not with MCNP, i.e., the 7.7 mean-free-path liquid nitrogen pulsed sphere experiment and a 1.32 km air sphere. Table 4 gives the experimental and calculated counts for specific time intervals for the pulsed sphere. The ALICE code agrees better with the experimental data than TART, as would be expected.

Table 4. Experimental and code calculated counts for the 7.7 mfp sphere.

	Counts in time interval 0-200 n/sec	Counts in time interval 200-400 n/sec	Total counts 0-460 n/sec
Experimental	.01760	.04623	.06383
ALICE	.01458	.04725	.06183
TART	.01350	.04524	.05874

Calculations were done for a sphere of air (as specified below) in order to address the question of what differences in neutron and photon flux and current can be expected using the techniques of TART and ALICE. The spherical air problem had a density of $1.2757 \times 10^{-3} \text{ g/cm}^3$, a radius of $13.23 \times 10^4 \text{ cm}$, and source energies in the range from 13.86 to 14.13 MeV. The density and composition were adjusted such that the mean-free-path at the source energy was identical to the large nitrogen sphere problem that both LANL and LLNL studied. The results of the ALICE and TART calculations are given in Table 5. The calculated spectra in the resonance region for both TART and ALICE are shown in Fig. 2. ALICE has a larger total neutron current and in the resonance region the group currents calculated with ALICE are consistently slightly larger than those from TART. It is important to note that TART and ALICE results disagree by only 3.6% at 1.32 Km of air. This disagreement is the result of the method of cross section treatment, and is as small as it is because the dilution of nitrogen with oxygen (both of which have resonance structures above .4 MeV), reduces the effects of resonance self

shielding considerably. The difference in the results at 1.3 Km of air attributed to method of cross section treatment, is about the same as the intrinsic uncertainty in the measured cross section (compare Tables 3 and 5).

Table 5. Results of calculations by LLNL on fictitious air.

Code/data set	Neutron		Photon	
	Current	Flux	Current	Flux
TART/ENDL80	.0268 $\pm$.0004	(1.930 $\pm$.025) $\times 10^{-13}$	.0524 $\pm$.0008	(3.358 $\pm$.064) $\times 10^{-13}$
ALICE/ENDL80	.0278 $\pm$.0005	(2.003 $\pm$.038) $\times 10^{-13}$	.0561 $\pm$.0013	(3.528 $\pm$.073) $\times 10^{-13}$

CONCLUSION

The TART and ALICE codes calculate similar results when resonance self shielding is not important. The ALICE code should be used for problems when either one isotope with resonance structure is present or the predominant isotope in a material has resonance structure, and the thickness of material is greater than one mean-free-path.

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 DMIN = 7.00196E-02 DMAX = 1.51857E+01 DIST MIN = 2.74376E-04 DIST MAX = 1.55174E-02

FIG. 2.

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