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# APPLICATIONS OF EVALUATED NUCLEAR DATA IN THE LAHET<sup>TM</sup> CODE LA-UR-97-1744

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#### Abstract

We investigate the use of evaluated cross section data to define the nonelastic interaction rate for reactions described by the intranuclear cascade code in  $LAHET^{TM}$ . We find that improved predictions of total neutron production within stopping-length target assemblies are obtained.

#### 1 Introduction

The total neutron production (n/p) from protons incident on a thick stopping target is a key parameter in accelerator technologies that utilize spallation neutrons. Recent measurements of (n/p) have been performed through a USA-France collaboration at Saturne for various targets (including Pb and W), for protons with energies varying from 400 MeV to 2 GeV. LAHET<sup>TM</sup> [1]-MCNP<sup>TM</sup> [2] calculations of the total neutron production were found to describe these measurements well, except at the lowest proton energies. In this paper we compare the total nonelastic cross section determined by the Bertini intranuclear cascade model within LAHET with measured data, and find that the Bertini model underpredicts these measurements below a few hundreds of MeV, since an optical model is not used. We describe how the use of evaluated nonelastic cross section data, to constrain the INC calculations, leads to more accurate predictions of (n/p).

The work described here tests the concept for use in the merged LAHET-MCNP code presently under development, where it will be used in conjunction with the 150 MeV proton-neutron libraries being created for certain isotopes.

#### 2 Evaluated Nonelastic Cross Sections

We have evaluated the total nonelastic cross sections for neutrons and protons incident on three of the most important isotopes in accelerator-driven technologies: Fe, W, and Pb (tungsten and lead are potential target and blanket materials). The proton evaluations cover energies from threshold to 2 GeV; the neutron evaluations from 20 MeV to 2 GeV.

Below 150 MeV, the nonelastic cross section evaluations were taken from the new 150 MeV Los Alamos evaluations [3]. These evaluations were based primarily on optical model calculations, though in some cases small adjustments to better describe measurements were made. For protons with energies between 150 MeV and 400 MeV, our evaluations follow Madland's medium energy optical model calculations. For neutrons above 150 MeV, and protons above 400 MeV, our evaluations represent an eye-guide fit to measurements.

Experimental data were obtained from the compilations of Carlson, Barashenkov, and the National Nuclear Data Center [4]. In the case of tungsten, only one (proton-induced) measurement exists above 20 MeV. Therefore, as shown by the "systematics" data points in Fig. 1, we interpolate values from measurements on other targets, using a fit of the type  $aA^{2/3} + b$ .

Our evaluations, shown as the full line in Fig. 1, are seen to account for the experimental data well. But the predictions obtained from the Bertini INC model within LAHET (dashed line in Fig. 1) are seen to underpredict measurements below a few hundred MeV, though they agree well at higher energies, where the nonelastic cross section is similar to the geometric cross section. This is because the semiclassical assumptions in the INC model fail at lower energies.

In the traditional use of the INC, an assumed "geometric" cross section is used to obtain a potential interaction point; a sampled interaction may lead to a "transparency", treated as a nonevent on the particle trajectory. Using evaluated nonelastic data, a definite interaction point is determined; in case of a transparency, the interaction is resampled until a real event is obtained. Therefore, by constraining the INC nonelastic reaction rates with the evaluated nonelastic cross section data, it would be expected that an improved LAHET predictive capability would result.

For comparison, Fig. 1 also shows (dash-dot lines) results based on the phenomenological Wellisch and Axen parameterization for proton reactions [5] Note that errors exist in the formulas presented in their publication; the correct equations used are shown in reference [6]. Generally, this parameterization described measurements well and has considerable predictive capability, though in the case of lead it is seen to underpredict data at lower energies. We are considering using this formula to provide the INC nonelastic cross sections for isotopes where a detailed evaluation does not exist. Although the parameterization in mass is not reliable for nuclei lighter than carbon, mass-specific parameterizations can easily be found to approximate the data for lighter nuclei[6].

# 3 Integral (n/p) LAHET results

The Sunnyside-Saturne series of experiments[7] may be briefly described as a Pb or W target inside a Pb blanket (16.51 cm thickness), the whole inside a cylindrical (127 cm outer radius) water bath containing a solution of  $MnSO_4$ . The Pb target was 12.54 cm in radius, 120 cm long. The W target as 7.62 cm radius, 81.2775 cm long, held in an aluminum sleeve and mounted in the same blanket; it was backed by a Pb beam stop, 12.54 cm in radius, 37.375 cm long. The measured quantity was the <sup>56</sup>Mn production from neutron capture in the solution. At some energies, more that one run was made, sometimes with different Mn concentrations. The experimental results are shown in column 2 of Tables 1 and 2. The analysis of systematic error has not been finalized, but preliminary results [8] indicate a 5% systematic uncertainty below 800 MeV and 10% above.

To test the effect of the cross section evaluations, the tabulated Fe, W, and Pb cross sections were implemented in the developmental version LAHET3.0, the resulting code being designated LAHET3MC. The new tabulations were applied to the three elements to determine the reaction rates as described above; for all other isotopes in the problem, standard LAHET methods were used. The neutron production below 20 MeV, calculated with each version of LAHET, was used as an input source to MCNP to calculate the Mn activation rate. The statistical uncertainty in the calculated values ranged from 0.4% at 400 MeV to 0.2% at 2 GeV. In addition, further calculations were made with LAHET3MC to examine the sensitivity of the results to the use of the ISABEL INC rather than the Bertini model, and to the use of the preequilibrium model.

The results of the calculations for the tungsten target cases are shown in Table 1, as the ration of experiment to calculation; the results for the lead target cases are shown in Table 2. In each case, columns 3 and 4 show very small differences between LAHET2.8 and LAHET3.0. Column 4 shows the LAHET3MC results using the cross section evaluations, but still with the Bertini INC and the preequillibrium model. The effects of changing the INC model and turning off the preequillibrium model may be seen in comparing columns 5 through 8, all of which are calculations with LAHET3MC using the cross section evaluations.

An inspection of Tables 1 and 2 shows that the use of the evaluated cross sections does indeed reduce the discrepancy in the 400 MeV calculations, although at the cost of a small increase at 800 MeV. A more firm conclusion awaits a definitive evaluation of the experimental uncertainties. The evaluated cross section usage only improves the estimation of reaction rate, not secondary particle multiplicity. The variation in multiplicity is reflected in the comparison of columns 4 through 8 which indicate a total spread of about 6%. The averages over all experiments quoted in the tables cannot be taken too seriously, but do indicate the general trend for each model variation.

	Exp.	2.8	3.0	3MC	3MC	3MC	3MC
	Mn-56	$\mathbf{Bert}$	$\mathbf{Bert}$	$\mathbf{Bert}$	$\mathbf{Bert}$	ISAB	ISAB
	per	prq	prq	prq	no prq	$\mathbf{prq}$	no prq
${\rm MeV}$	proton	$\rm E/C$	$\rm E/C$	$\rm E/C$	$\rm E/C$	$\rm E/C$	$\rm E/C$
400	0.0665	1.198	1.194	1.101	1.079	1.136	1.083
800	0.1959	0.959	0.949	0.933	0.912	0.967	0.927
800	0.2117	1.037	1.026	1.008	0.986	1.045	1.001
1600	0.5363	1.044	1.029	1.017	0.996	1.044	1.012
1600	0.5200	1.012	0.997	0.986	0.966	1.012	0.982
<b>2000</b>	0.6717	1.015	1.013	0.990	0.976	1.032	0.985
<b>2000</b>	0.6512	0.984	0.982	0.960	0.946	1.001	0.955
Ave		1.036	1.027	0.999	0.980	1.034	0.992

Table 1: W target calculations with LAHET2.8, LAHET3.0, and LA-HET3MC, with variation from INC model and use of preequilibrium model.

	Exp.	2.8	3.0	3MC	$3 \mathrm{MC}$	$3 \mathrm{MC}$	3MC
	Mn-56	$\mathbf{Bert}$	$\mathbf{Bert}$	$\mathbf{Bert}$	$\mathbf{Bert}$	ISAB	ISAB
	per	$\mathbf{prq}$	$\mathbf{prq}$	$\mathbf{prq}$	no prq	$\mathbf{prq}$	no prq
MeV	proton	$\rm E/C$	$\rm E/C$				
400	0.0576	1.220	1.210	1.108	1.042	1.147	1.075
800	0.1676	0.988	0.984	0.940	0.918	1.012	0.957
800	0.3310	0.993	0.990	0.945	0.923	1.017	0.963
1600	0.8361	1.024	1.044	0.993	0.981	1.057	1.003
2000	0.5459	1.034	1.050	1.020	0.991	1.048	1.018
Ave		1.052	1.056	1.001	0.971	1.056	1.003

Table 2: Pb target calculations, labeled as in Table 1.

## 4 Conclusions

The new evaluated cross sections, as used in LAHET, significantly reduce the observed discrepancies in the simulation of the Sunnyside-Saturne experiments. A somewhat greater improvement may be expected though the use of evaluated data libraries to 150 MeV for protons in a merged LAHET/MCNP code. Sensitivity to the calculational models is small enough that smaller and more definitive experimental uncertainties are needed to guide the code development effort.

This evaluation also partly validates the Wellisch and Axen parameterization[5]. The latter, yet to be tested in LAHET, should provide a more reliable estimate of proton reaction rates, especially at low energies and in the absence of evaluated data. A similar parameterization for neutron cross sections is most desirable.

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Figure 1: Total nonelastic cross section compared with measurements.