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A COMPARISON OF HIGH-ENERGY FISSION MODELS FOR THE HETC TRANSPORT CODE -- PART I: THIN TARGETS

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Abstract:

Calculations have been made to compare results from high-energy fission models which have recently been developed by others for use in the high-energy transport code HETC. The cases considered are proton beam energies of 0.3, 1.0, and 2.9 GeV bombarding thin U-238 targets. Comparisons are given for fission cross sections, neutron production, and fission fragment energies.

1. INTRODUCTION

For high-energy hadrons incident on high-mass target materials (e.g., uranium), the target nucleus may undergo fission during de-excitation. Recently, there have been several high-energy fission models developed /1-4/ for the hadronic transport code HETC /5/, which is used for spallation neutron source studies. The objective here is to investigate the appropriate high-energy fission model for routine HETC calculations for spallation neutron source applications.

All of the calculations made here are for proton beams (0.3, 1.0, and 2.9 GeV) incident on thin U-238 targets, and were made using the Rutherford and Appleton Laboratory (RAL) high-energy fission model developed by Atchinson /1/.* Results for fission cross sections, neutron multiplicities and spectra, and fission fragment recoil energies are compared with available results for the same cases computed by the Oak Ridge National Laboratory (ORNL) model developed by Alsmiller, et al. /2/.

All of the comparisons in this paper are for thin targets -- i.e., for target thicknesses sufficiently small that the secondary particles created escape from the target without undergoing further collisions, so the results are for a single proton collision. Thus, such thin target comparisons are appropriate for identifying basic differences in model predictions. However, to determine the practical importance of such model differences for spallation source applications, thick targets must be considered, whose results represent an average of collisions initiated by primary beam protons and secondary particles (neutrons, protons, and pions) over a wide range of energies. A comparison of different high-energy fission models based on thick targets is given in a companion paper.

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2. HIGH-ENERGY FISSION PROCESS

Without fission, the spallation collisions can be treated as a two-step process: (a) an intranuclear cascade, described by a series of independent particle-particle collisions inside the nucleus, and (b) subsequent de-excitation by a series of particle emissions, which can be described by an evaporation model. For very heavy nuclei, there is competition between evaporation and fission at each step of the de-excitation sequence. The probability of fission at some step during de-excitation in high-energy ($\gtrsim$100 MeV) collisions is proportional to Z^2/A of the target nucleus. For example, $\sigma_f/\sigma_t \approx 0.05$ for lead and $\sigma_f/\sigma_t \approx 0.8$ for uranium.

The information which must be determined by the fission model is the probability of fission at each step and the parameters of the fission fragments immediately after fission, which are then used as input for a post-fission evaporation calculation for each fragment.

If fission occurs, the following quantities are expected to be different compared to spallation without fission: (a) energy deposition, (b) residual mass distributions, (c) neutron multiplicity and (d) neutron spectrum. There are clearly large differences in these first two items if fission takes place. The magnitude and spectral differences in neutron production is not well-determined, and this is the main emphasis of the calculations made here.

3. BASIC FEATURES OF FISSION MODELS

Recently, there have been two high-energy fission models developed for use in the thick-target nucleon-meson transport code HETC: one by Atchinson at Rutherford and Appleton Laboratories (RAL) /1/, and one by Alsmiller, et al. at the Oak Ridge National Laboratory (ORNL) /2/. Also, Takahashi at Brookhaven National Laboratory (BNL) /3/ and Nakahara at the Japan Atomic Energy Research Institute (JAERI) /4/ have developed high-energy fission models for

NMTC transport code /6/, which is an earlier version of HETC. (Barashenkov et al. have also developed a high-energy fission model for use in the Dubna transport code /7/.)

The fundamental basis of all of these models is the statistical model of fission developed by Fong /8/. Basically, the assumption is that the fission process is "slow" (i.e., the nucleus exists in an equilibrium state at any time), so the probability of a particular fission mode (state of the fission fragments) is proportional to the density of quantum states at the time of splitting. From the Fong theory, the fission mode probability is expressed as a function of eleven variables: $N(A_1, A_2, Z_1, Z_2, C, D, k, E, E_1, j_1, j_2)$, where the subscripts denote the fission fragments; A, Z, and j denote mass number, charge number, and angular momentum; and the remaining are energy variables (C, Coulomb; D, deformation; k, translational; E, total; and E_1, excitation).

The high-energy fission models developed differ in the apporoximations made in arriving at a practical implementation of the above general expression and in the physical data used. It is not the purpose here to evaluate these various approximations. Indeed, many of the approximations are interdependent, making judgement of the practical importance of particular assumptions difficult. Therefore, the model comparisons here are in terms of "output" rather than assessment of the intermediate physics. Simple characterizations of the different models are given in Figure 1.

Also given in Figure 1 are the values for the parameter B_0 assumed for the different models, which , as shown later, has an important influence on neutron production. This parameter is involved in the evaporation calculation in the following way. From evaporation theory (e.g., /9/), the probability of particle emission of type i with kinetic energy E is expressed as

$$p_i(E) \propto (2S_i+1)\ m_i E\ \sigma_{ci}(E)\ w(E^*),$$

with S_i = spin, m_i = mass, and σ_{ci} = cross section for compound nucleus formation in the inverse reaction. The level density for excitation energy E^* is given by

$$w(E^*) = w_0 \exp\left[2(aE^*-\delta)^{\frac{1}{2}}\right],$$

where w_0 and a are constants for a given nucleus and δ is the pairing energy. The level density parameter , a, is given by

$$a = A/B_0(1 + Y\ (A-2Z)^2/A^2),$$

and $Y \approx 1.5$. From various analyses, B_0 is in the range from about 8 to 20 MeV (e.g./9/).

4. PREVIOUS VALIDATIONS

Several thick-target calculations, with and without high-enrgy fission taken into account, have been made for neutron production and compared with experimental data (Tables 1 and 2). We conclude from these, and other (e.g., /10,14/), comparisions that the theoretical predictions and measurements that have been made to date agree to within roughly 20 to 30%, and this general magnitude of agreement for neutron production can be obtained by neglecting high-energy fission. It is difficult to isolate the influence of the high-energy fission models in these thick targets comparisons where low-energy fission also contributes to the neutron production.

5. THIN TARGET COMPARISONS

In this section, calculations made here using the RAL fission model are compared with results from Alsmiller et al. /2/ obtained with the ORNL model. All of the comparisons are for protons incident on a thin U-238 target.

Figure 2 shows the fission cross sections calculated by the RAL and ORNL models compared with experimental data. The fission cross section predicted by thE RAL model is about 15-20% lower than for the ORNL model for beam energies below ≈1 GeV, and the energy dependence of the cross section predicted above ≈1 GeV appears to be different for the two models. As is evident, the spread of the experimental data is too large to judge the correctness of either model. Also shown in Figure 2 are the nonelastic cross sections from the two calcualtions, which are in agreement, as expected, since both calculations use the same intranuclear cascade model.

Figures 3 and 4 show comparisons of neutron multiplicity from evaporation only (taken to be $\lesssim$12.5 MeV) and over all energies (evaporation plus intranuclear cascade), respectively. For the standard B_0 values used in the two models (B_0 = 14 for RAL, B_0 = 10 for ORNL), the RAL model predicts lower neutron emission by about 20-25%. These comparisions also show the sensitivity of neutron production to values assumed for B_0 . The variation in neutron production over the range of B_0 parameters suggested as reasonable from present experimental data are about the same as the model differences.

To consider further the influence of B_0, we have calculated the low-energy neutron production spectrum for 1-GeV protons using the RAL model (Figure 5). The integral neutron production below 12.5 MeV is 20% higher for B_0 = 8 than for B_0 = 14. Also, shown in Figure 5 is the neutron spectrum obtained when high-energy fissioning is neglected. With fission included, the neutron production is about 8% higher, and there is evidence of some "spectral hardening" for neutron energies above about 2 MeV. Neutron production above this energy is important because this corresponds approximately to the energy threshold for neutron induced fission for U-238. Thus, while the magnitude of spectral hardening introduced by high-energy fission appears to be small, its influence on total neutron production in thick U-238 targets can be amplified by providing a larger source of neutrons that can cause multiplication via low-energy fissioning.

There are large differences in energy deposition for spallation collisions with and without high-energy fissioning. If fission takes place, the "local" energy deposition at the collision site is mainly from the kinetic energy of the fission fragments which, as in low-energy fission, is expected to be about 170 MeV per fission. (From non-fissioning spallation collisions, the deposition from heavy short-range secondary particles and residual nuclei is, nominally, only about 20-30 Mev per collision.) Thus, the fission fragment kinetic energies predicted by high-energy fission models is important in predicting the target heating for spallation neutron sources. A comparison of the (total) fission fragment energies calculated using the RAL and ORNL models is given in Figure 6, and the agreement is good. As also indicated in Figure 6, this energy is not sensitive to B_0. This is as expected since the fission fragment energy results mainly from the Coulomb repulsion between fragments. Thus, the fragment energies are not sensitive to few-neutron differences of the fragment masses.

6. SUMMARY AND CONCLUSIONS

A summary comparison of the RAL and ORNL high-energy fission models in terms of neutron multiplicities predicted is given in Table 3, from which we conclude: (1) for the standard B_0 values incorporated in the models, the ORNL model predicts about 20% more neutrons, (2) the neutron production is sensitive to the value of B_0 assumed, varying by about 20% over the range of B_0 values inferred from presently available experimental data, (3) for the same assumed B_0 in each model, the ORNL model still predicts more neutrons tham the RAL model, by about 12%, and (4) the effect of high-energy fissioning compared to spallation without fissioning is to increase the neutron production by about 7% (with a somewhat harder spectrum in the enegy region from ≈ 2 to ≈ 15 Mev).

Additional calculations are underway to investigate the isotope production distributions predicted by these spallation models.

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Table 1. Comparison of ORNL Fission Model with FERFICON Data(a)

	Target	Proton E (MeV)	Quantity Compared	Theory/Exp.
1.	Depleted U (3.2ϕ × 30.5 cm)	480	Neutron captures in water bath	11.8/9.6(b) = 1.23(d)
	Depleted U (37 rod array)	480	" "	14.1/17.7(b) = 0.82(d)
2.	Depleted U (10ϕ × 40.6 cm)	800	" "	27.2/25.3(c) = 1.08
	Depleted U (37 rod array)	800	" "	28.6/28.8(c) = 0.99

(a) Calculated results from Alsmiller, et al. /10/.

(b) Fraser, et al., FERFICON measurements at TRIUMF, reported at BNL Symposium /11/.

(c) Russell, et al., FERFICON measurements at LASL, reported at ICANS-IV /12/.

(d) Calculations of Fraser, et al. /11/, using NMTC without high-energy fission give theory/exp. ratios of 1.05 and 0.72 for cylindrical and array targets, respectively.

Table 2. Fission Model Comparisons with (a) Vasil'kov Experiments

Fission Model	Proton E (MeV)	Quantity Compared	Theory/Exp.
JAERI (e)	660	U-238 captures	$\frac{44.9 \pm 5.1}{46 \pm 4} = 0.98$ (b)
BNL (f)	660	" "	$\frac{38.3 \pm 5.2}{46 \pm 4} = 0.83$ (d)
JAERI (e)	400	" "	$\frac{15.96 \pm 4.65}{22.1 \pm 2.4} = 0.72$ (c)
BNL (f)	400	" "	$\frac{15.1 \pm 4.9}{22.1 \pm 2.4} = 0.70$

(a) Very large natural uranium assembly /13/.

(b) Without high-energy fission in model, theory/exp. = 0.72

(c) Without high-energy fission in model, theory/exp. = 0.61

(d) Assuming depleted uranium with 0.33% U-235 in calculations, theory/exp. = 0.88

(e) Ref. /4/.

(f) Ref. /3/.

Table 3. Summary comparison of neutron production predicted by RAL and ORNL high-energy fission models, for proton beams on thin U-238 target.

Case	Beam Energy (MeV)	Ratio	
		neutrons $\lesssim$12.5 MeV	neutrons of all energies
1. $\frac{\text{ORNL}^*}{\text{RAL}}$	300	1.23	1.19
	1000	1.28	1.22
	2900	1.26	1.19
2. $\frac{\text{ORNL } (B_0 = 8)}{\text{ORNL } (B_0 = 15)}$	1000	1.22	1.17
3. $\frac{\text{ORNL } (B_0 = 8)}{\text{RAL } (B_0 = 8)}$	1000	1.14	1.12
4. $\frac{\text{RAL (with Fission)}^*}{\text{RAL (w/o Fission)}}$	1000	1.08	1.07

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*For Standard B_0 Values incorporated in the models (B_0 =10 for ORNL, B_0 =14 for RAL).

Figure 1. Features of Different High-Energy Fission Models

1. Basic Approaches

- RAL
  - empirical formulas used far as possible
- ORNL
  - heavy reliance on empirically derived constants

    NOTE: Fissions neglected for subactinides ($Z < 91$)
- BNL
  - close simulation of Fong's statistical model formulas, minimum reliance on experimental data
- JAERI
  - similar to RAL approach, but different in detail

2. B_0 Values Used in Standard Versions

Model	B_0
RAL	14
ORNL	10
BNL	8
JAERI	8

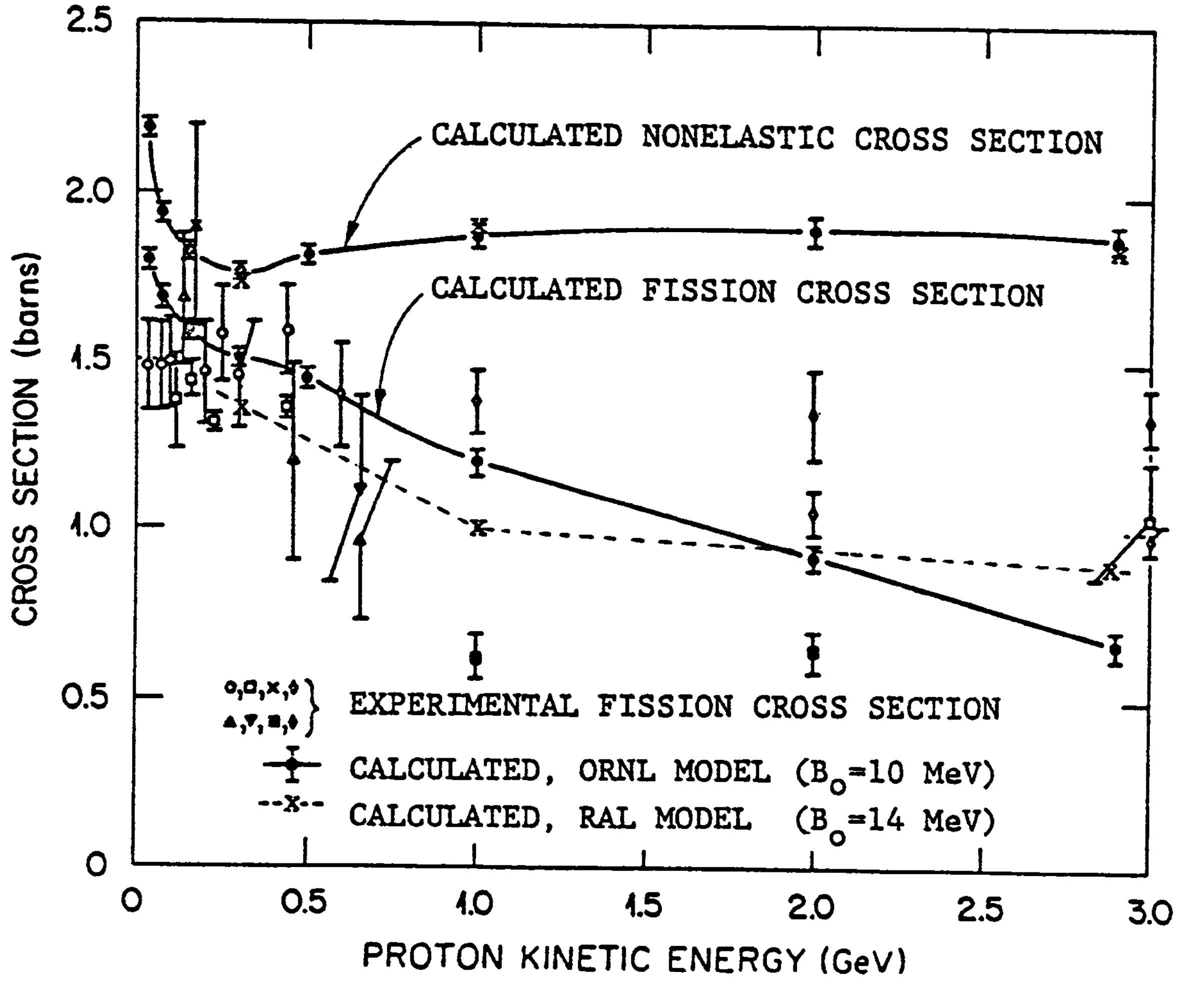

Figure 2. Comparison of calculated cross sections using the RAL and ORNL fission models for the case of protons incident on thin U-238 target. References for experimental data given in /2/.

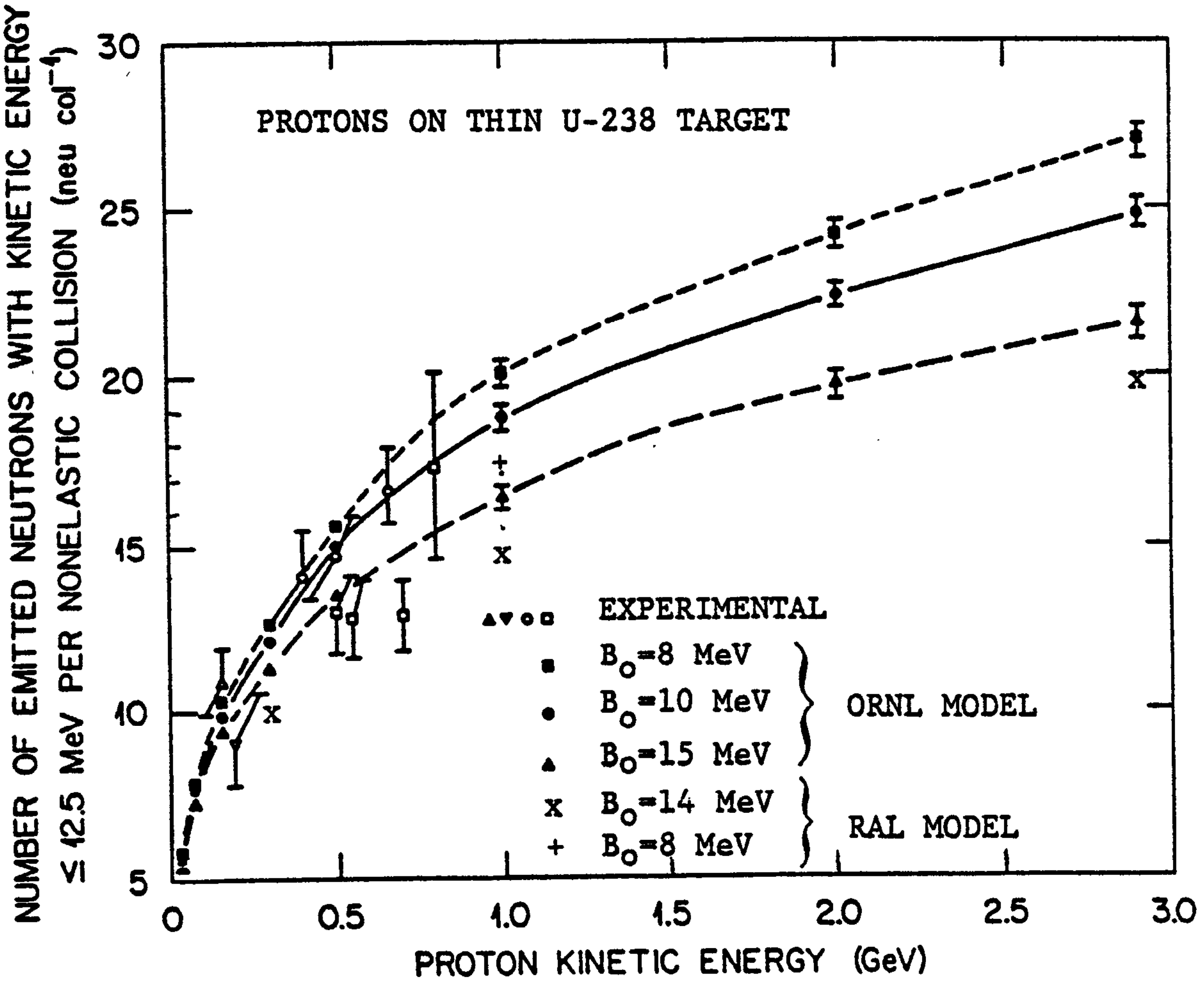

Figure 3. Comparison of RAL and ORNL fission model predictions for neutron production below 12.5 MeV. References for expermental data given in /2/.

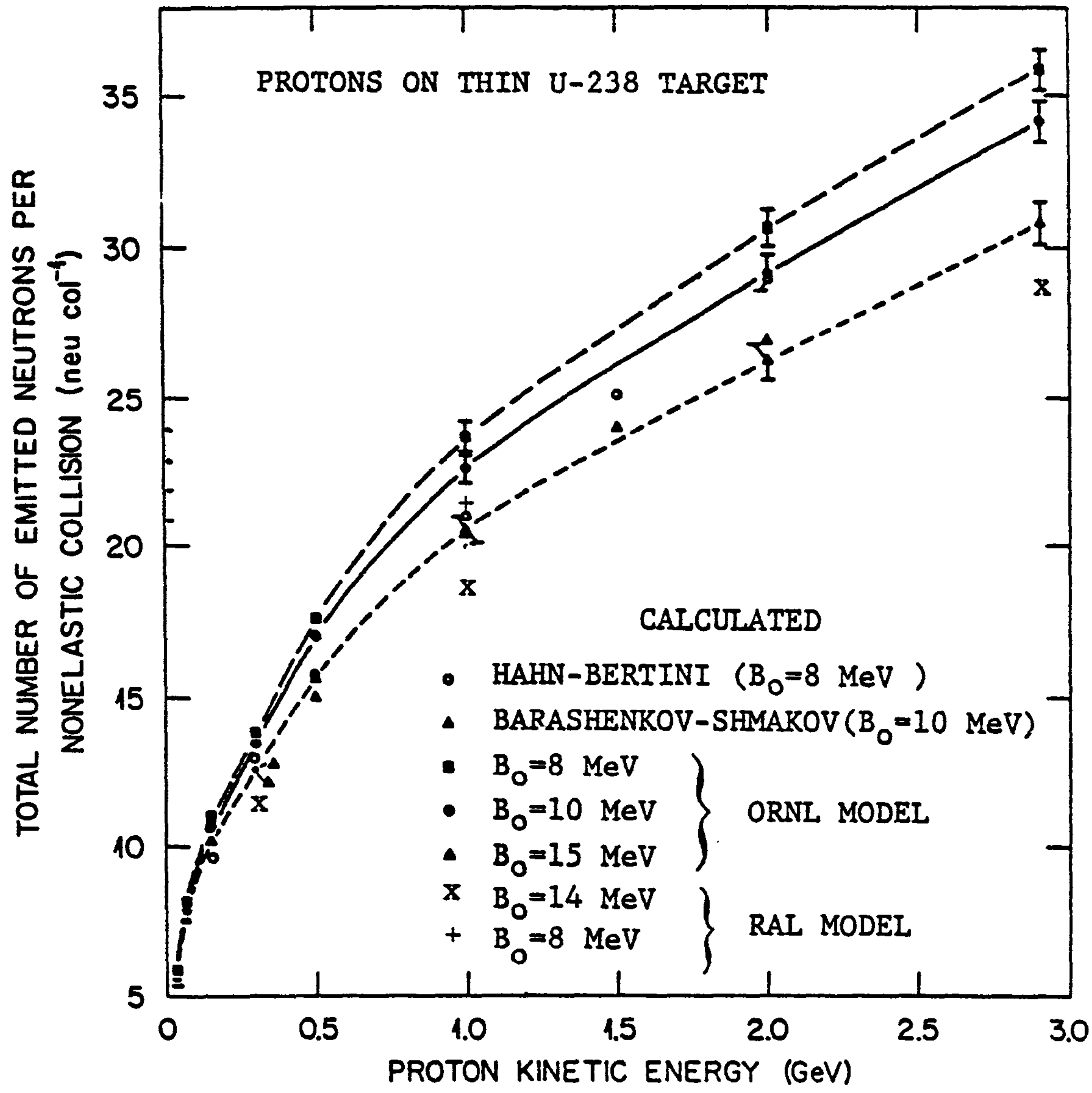

Figure 4. Comparison of total (evaporation plus cascade) neutron production predicted using RAL and ORNL high-energy fission models. Also shown are the results of Barashenkov and Shmakov using the Dubna fission model /15/. The calcualtions of Hahn and Bertini were made neglecting fission /16/.

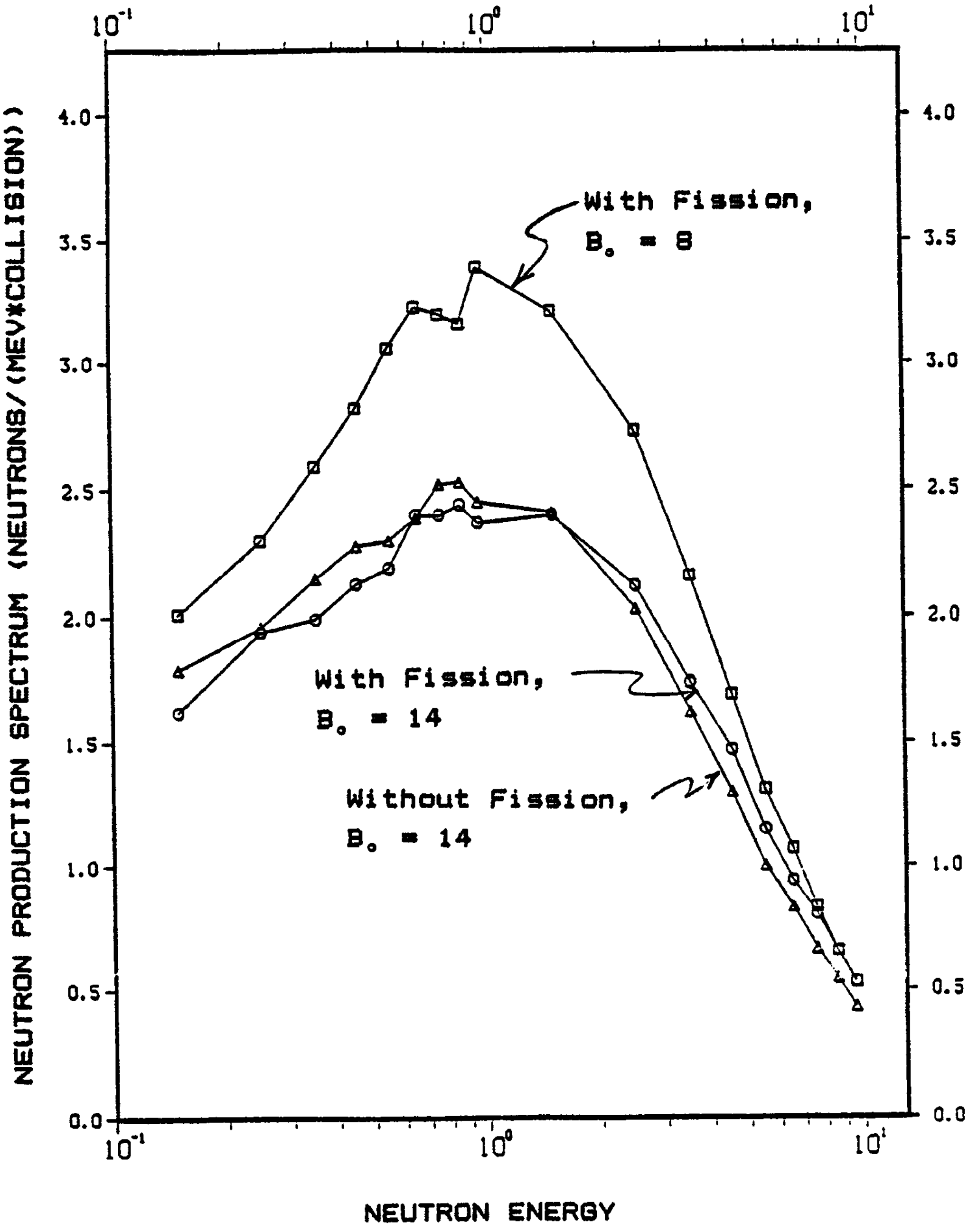

Figure 5. Low-energy neutron production spectrum calculated using RAL fission model, 1-GeV proton beam on thin U-238 target.

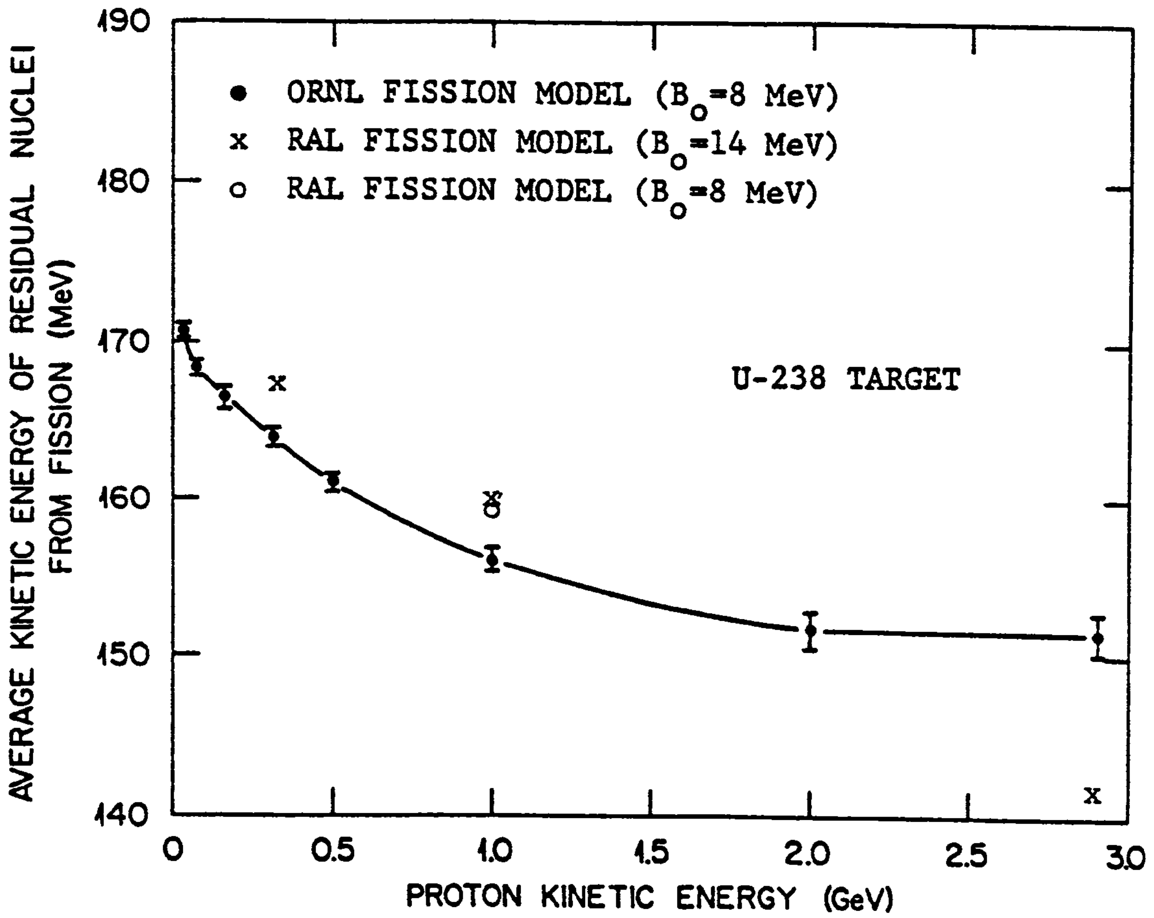

Figure 6. Comparison of fission fragment energies predicted by the RAL and ORNL fission models for protons incident on thin U-238 target.