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Analysis of Fe(n,xγ) Cross Sections Using the TNG Nuclear Reaction Model Code

K. J. McCollam

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Analysis of Fe(n,xγ) Cross Sections Using the TNG Nuclear Reaction Model Code

K. J. McCollam*

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ABSTRACT

Theoretical gamma ray cross sections have been calculated using a nuclear reaction model code. These are compared to experimental gamma ray production cross sections obtained from neutron interactions with ^{56}Fe at incident neutron energies of 1 to 40 MeV. The optical model and nuclear level density parameters in the code have been varied to affect a close agreement between calculations and the data. Present analyses, which focus on incident neutron energies between 17 and 40 MeV, display somewhat better agreement than those previously reported.

1. INTRODUCTION

As detailed in a previous Oak Ridge National Laboratory Report,[1] work at the Oak Ridge Electron Linear Accelerator (ORELA) produced excitation functions for 70 discrete-line gamma-rays, resulting from neutron interactions with an ^{56}Fe-enriched sample at incident energies up to 41 MeV. These gamma-rays indicate energy level transitions in residual nuclei of several reactions: ^{56}Fe(n,n')^{56}Fe, ^{56}Fe(n,p)^{56}Mn, ^{56}Fe(n,α)^{53}Cr, ^{56}Fe(n,2n)^{55}Fe, ^{56}Fe(n,np+pn)^{55}Mn, ^{56}Fe(n,nα+αn)^{52}Cr, ^{56}Fe(n,3n)^{54}Fe, and ^{56}Fe(n,2np+npn+p2n)^{54}Mn.

Subsequent analysis of these gamma-ray data was carried out using the TNG nuclear model code.[2] The calculated cross sections generally showed reasonable agreement with the data, especially below about 20 MeV incident neutron energy.[3] However, above 20 MeV the calculations in some cases differed substantially from the data. This discrepancy prompted further analysis using TNG, detailed here.

This analysis centers on examination of a few specific gamma rays, chosen both for their representation of the various observed reactions and for their relatively large experimental yields. In concentrating on the data for these gamma-rays, it is assumed that agreement between calculations and these specific data represents a successful application of the TNG code.

The original TNG calculations, some of which are given in reference 3, will be referred to as 'original' and are the starting points for all calculations to be described in this paper. The validity of present results will also be judged on how they improve on the original, whether or not they can be made to agree arbitrarily well with the data.

In addition to results for specific reactions, calculations of the total cross section and total reaction (nonelastic) cross section are also considered. It was found that comparison between such calculations using available optical model parameters and data for total yields and total reaction yields for ^{56}Fe are not in good agreement for incident energies greater than 25.0 MeV.

2. ANALYSIS

In the TNG code, both the optical model and the nuclear level density structure are parameterized. The optical model affects calculated results for total cross section, total elastic cross section, and total nonelastic cross section. Level density parameters are characteristic of each residual nucleus and therefore affect results for specific reaction cross sections. All calculations in this analysis were done from 17 to 40 MeV, where the original calculations most warranted improvement.[3]

During the analysis the three optical model sets given in Table 1 were tried. Set A in the table is a reproduction of the original parameters[3] which represented modifications to those presented by Arthur and Young.[4] Set B is composed of Arthur and Young parameters. Set C comprises original values (from Set A) for the neutron and proton models, with Arthur and Young values (from Set B) for the alpha optical model. Results compared to total and nonelastic cross section data for these sets are shown in Figures 1 and 2,

Table 1. Optical model parameters

	Set A (original)		
Neutron:	V(MeV)=49.747-0.43E	r=1.287 fm	a=0.56 fm
	W_{sd}(MeV)=11.8-0.21E	r=1.345 fm	a=0.47 fm
Proton:	V(MeV)=59.185-0.32E	r=1.17 fm	a=0.75 fm
	W_{sd}(MeV)=13.086-0.25E	r=1.32 fm	a=0.585 fm
	W_{vol}(MeV)=-2.7+0.22E	r_c= 1.25 fm	
Alpha:	V(MeV)=50	r=1.641 fm	a=0.576 fm
	W_{vol}(MeV)=10.311	r=1.641 fm	a=0.576 fm
		r_c=1.17 fm	
	Set B (Arthur and Young)		
Neutron:	V(MeV)=49.747-0.4295E-0.0003E^2	r=1.287 fm	a=0.56 fm
	W_{vol}(MeV)=-0.207+0.253E	r=1.345 fm	a=0.47 fm
	W_{sd}(Mev)=8.447-0.325E	r=1.345 fm	a=0.47 fm
Proton:	V(MeV)=58.384 - 0.55E	r=1.25 fm	a=0.65 fm
	W_{sd}(MeV)=13.5 - 0.15E	r=1.25 fm	a=0.47 fm
		r_c=1.25 fm	
Alpha:	V(MeV)=193-0.15E	r=1.37 fm	a=0.56 fm
	W_{vol}(MeV)=21+0.25E	r=1.37 fm	a=0.56 fm
		r_c=1.4 fm	
	Set C (Present)		
Neutron:	Same as Set A		
Proton:	Same as Set A		
Alpha:	Same as Set B		

respectively. None of the three sets agree with the data at incident energies greater than 25.0 MeV. Other variations in the optical model were tried, but did not give good agreement and so were abandoned. Overall, Set C gave the best results for the tertiary reactions and thus this set was chosen for the analysis.

Once the optical model parameters of Set C had been chosen, the analysis was focused on consideration of particular reactions, represented by discrete-energy gamma ray cross sections. TNG results for these rest largely on the choice of level density parameters for the residual nuclei. The calculation is particularly sensitive to the parameter 'a', which in TNG is used to determine three other level density parameters: E_x, E_o, and T.[5]

A TNG run first calculates results for the binary reactions, (n,n′), (n,p), and (n,α), then proceeds to tertiary reactions via one of these binary channels; it can then choose one

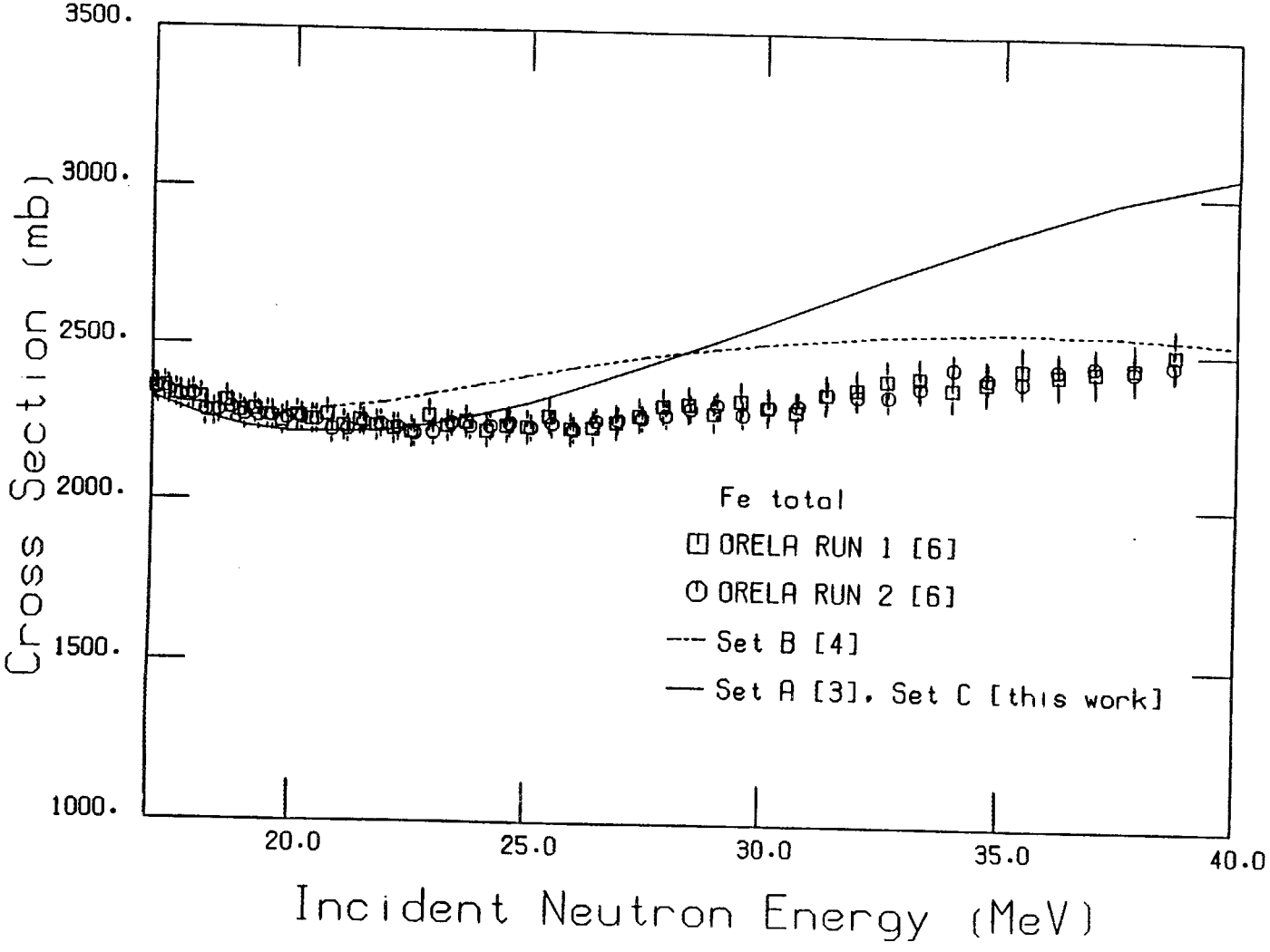

Figure 1. Comparison of calculated total cross section using the optical model parameters from sets A, B, and C with the data of Larson.[6]

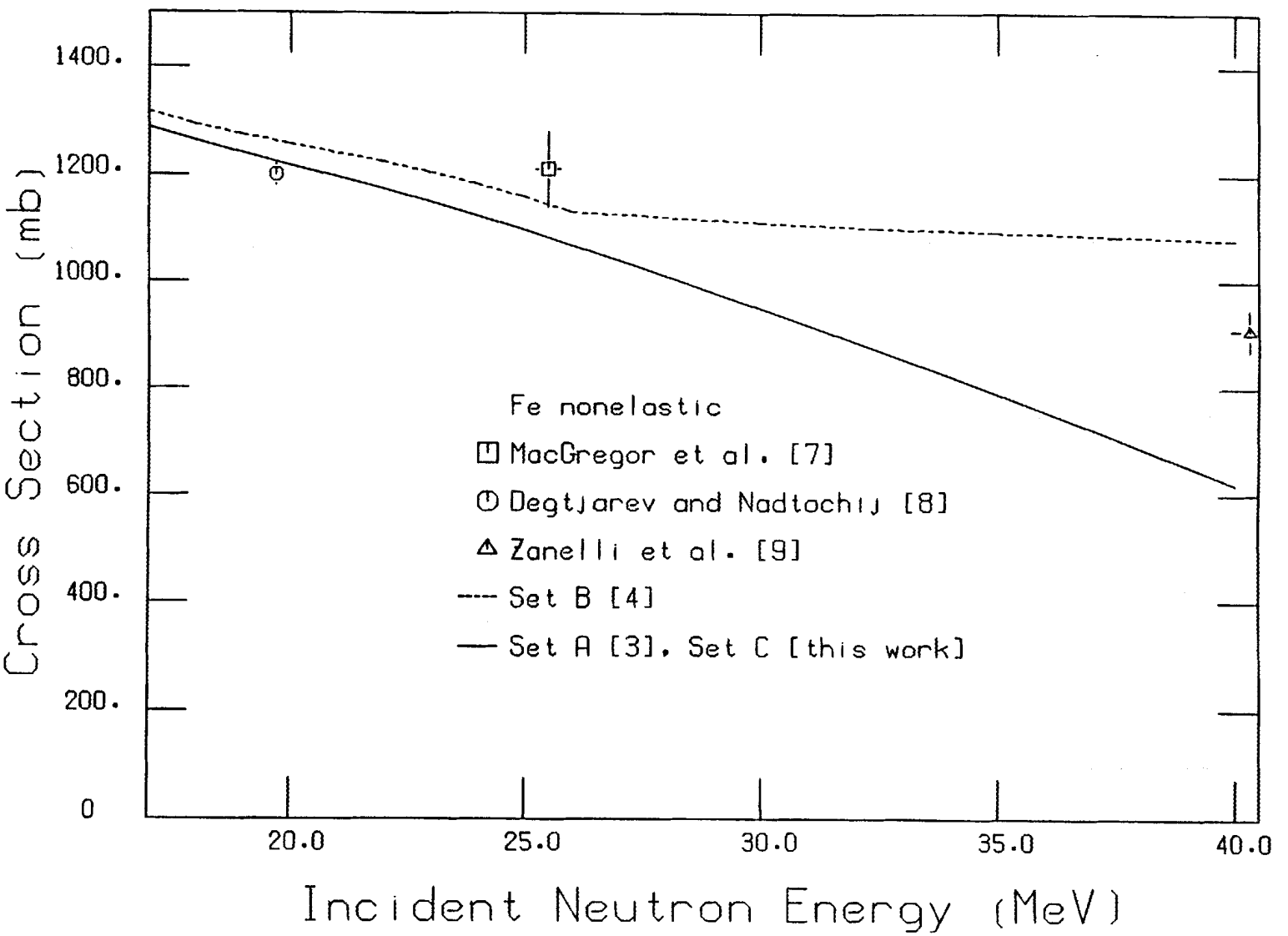

Figure 2. Comparison of calculated nonelastic cross section using the optical model parameters from Sets A, B, and C with measured data.[7,8,9]

tertiary reaction channel from which to go on to quaternary reactions if desired. The binary step affects all subsequent steps so it is convenient to first optimize these reactions, later proceeding to the tertiary and quaternary steps.

The most serious disagreement in the binary step was in $^{56}Fe(n,\alpha)^{53}Cr$, for which the original calculation for the 1289.6 keV gamma ray is shown in Figure 3. Several changes to the level density were used in attempts to bring the tail above 20 MeV to the data. No such changes were able to bring the calculation above ~0.75 mb at the tail. Optimization of the (n,α) calculation was abandoned.

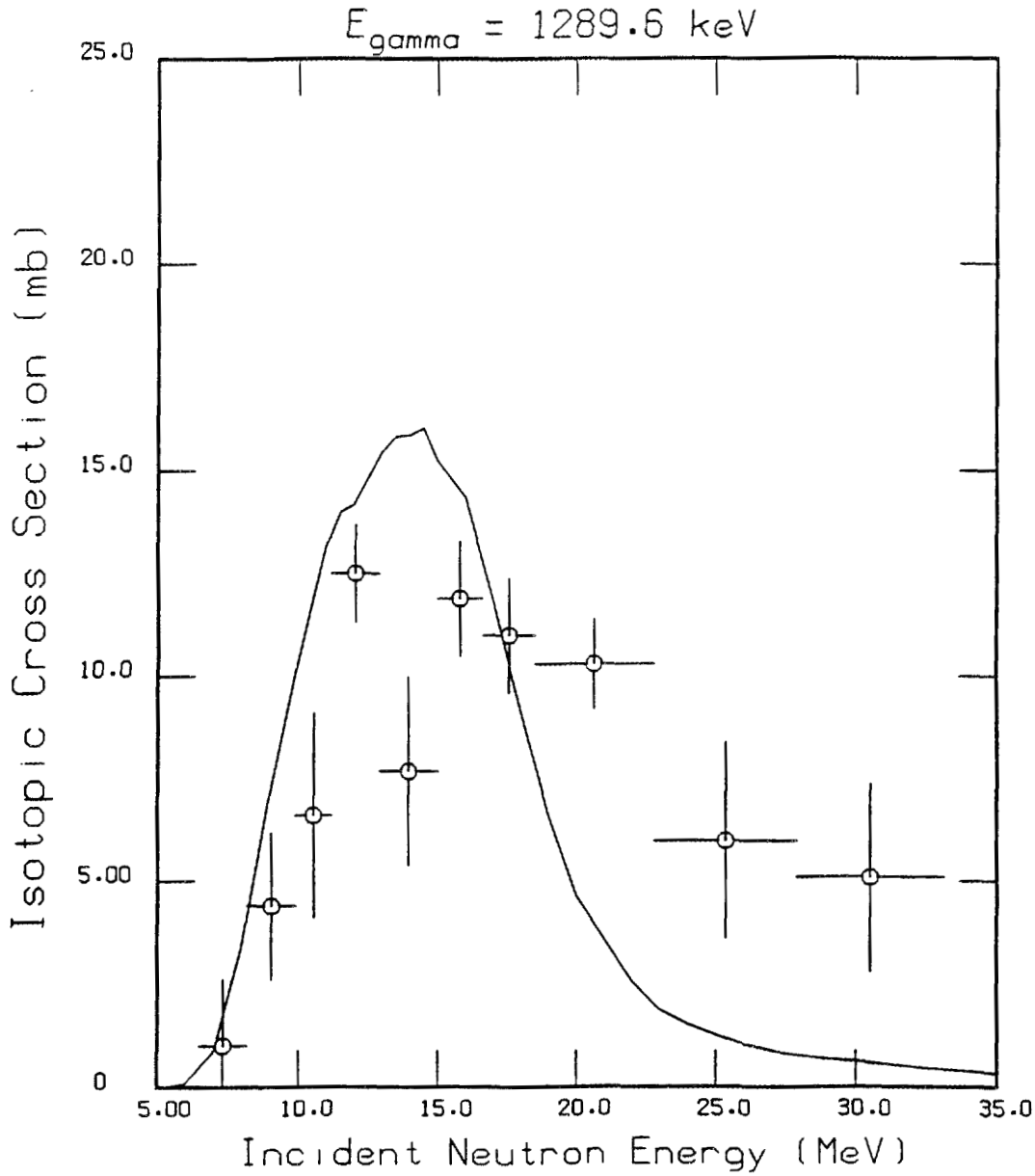

Figure 3. Original calculated excitation function for E_γ = 1289.6 keV[3] compared with the data of Dickens et al.[1]

Some of the changes made for the (n,α) reaction had the additional purpose of improving the ^{56}Fe(n,n')^{56}Fe 846.8 keV gamma ray calculation. Figure 4 shows that the original calculation is slightly high above 15 MeV. These attempts were unsuccessful, bringing no significant changes to the (n,n') calculation. The ^{56}Fe(n,p)^{56}Mn 314.4 keV gamma ray calculation, whose original is shown in Figure 5, was also not affected by these changes.

Since the binary reactions resisted all attempts at satisfactory improvement, the analysis was focused on tertiary and quaternary reactions. Original calculations for the ^{56}Fe(n,nα+αn)^{52}Cr 1434.1 keV gamma ray, the ^{56}Fe(n,2n)^{55}Fe 931.4 keV gamma ray, the ^{56}Fe(n,np+pn)^{55}Mn 858.4 keV gamma ray, and the ^{56}Fe(n,3n)^{54}Fe 1408.1 keV gamma ray (shown in Figures 6, 7, 8, and 9 respectively) warranted improvement.

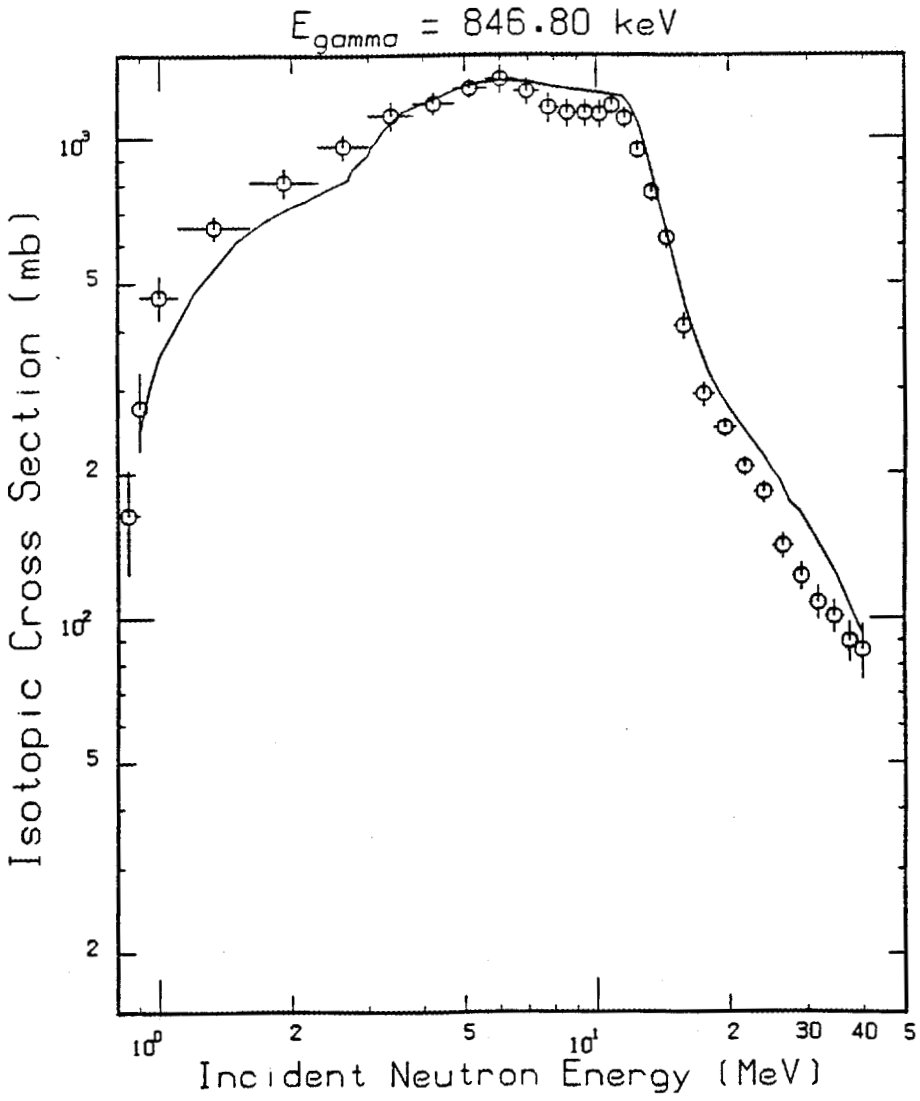

Figure 4. Original calculated excitation function for E_γ = 846.8 keV[3] compared with the data of Dickens et al.[1]

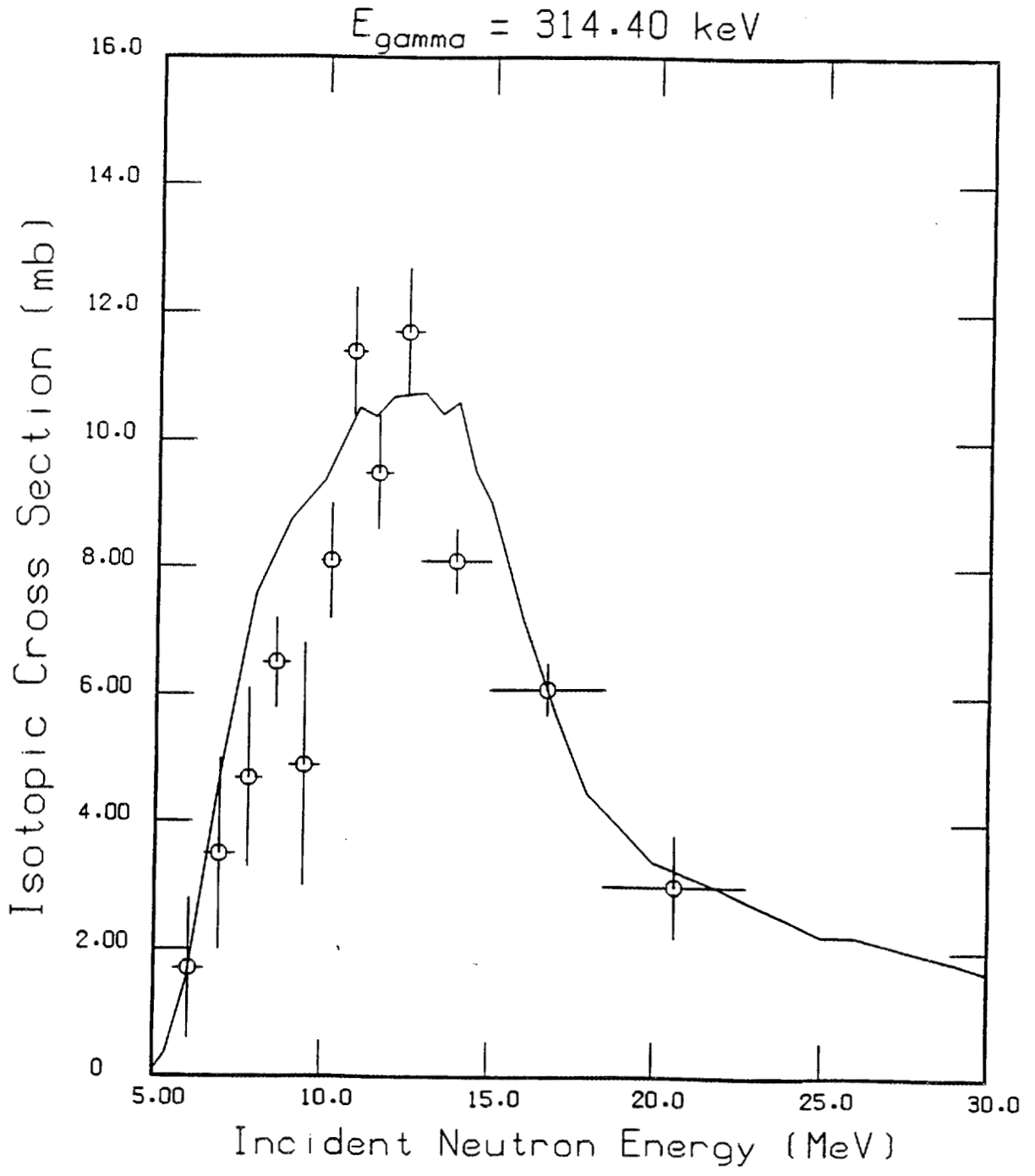

Figure 5. Original calculated excitation function for E_γ = 314.4 keV[3] compared with the data of Dickens et al.[1]

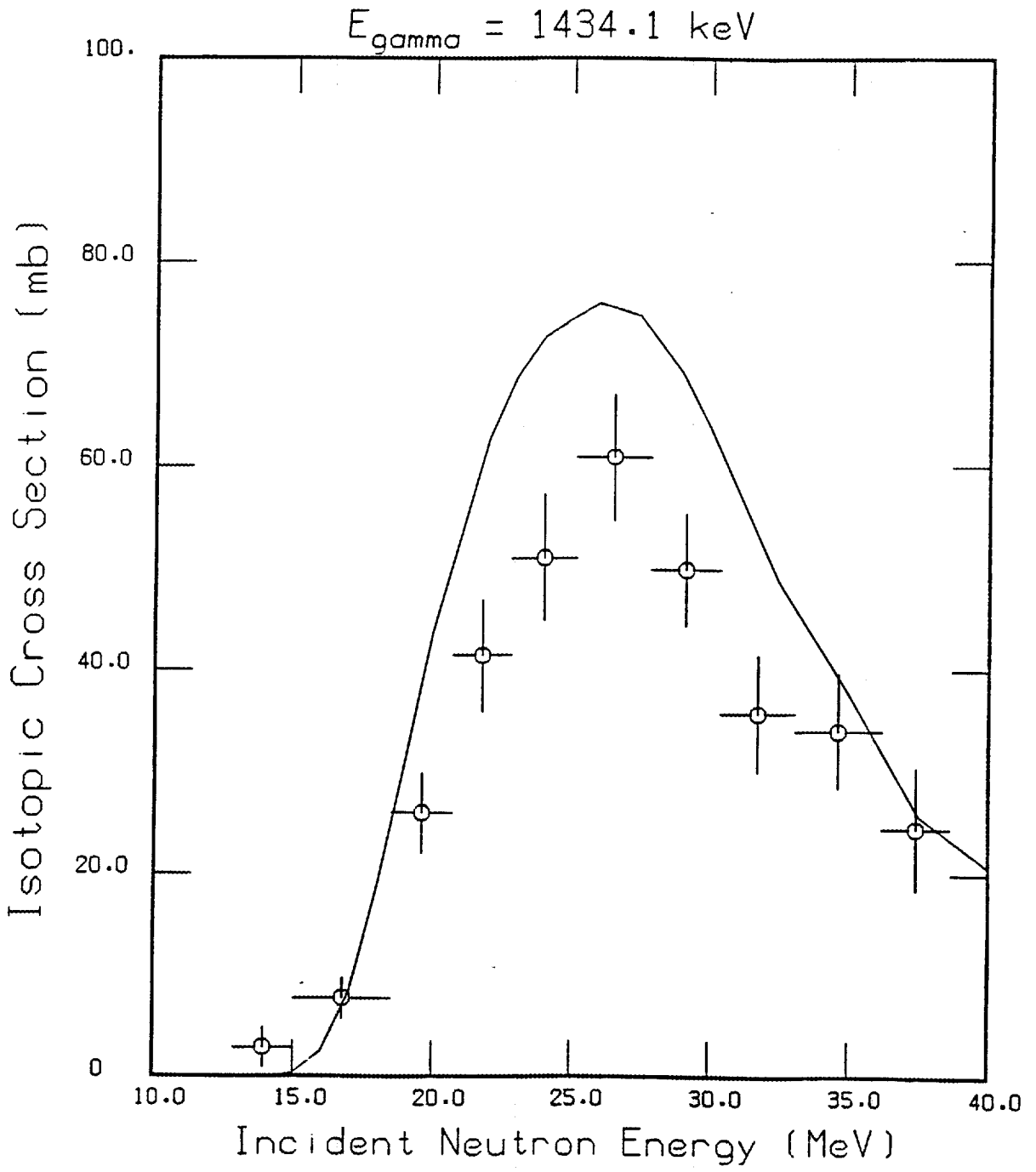

Figure 6. Original calculated excitation function for E_γ = 1434.1 keV[3] compared with the data of Dickens et al.[1]

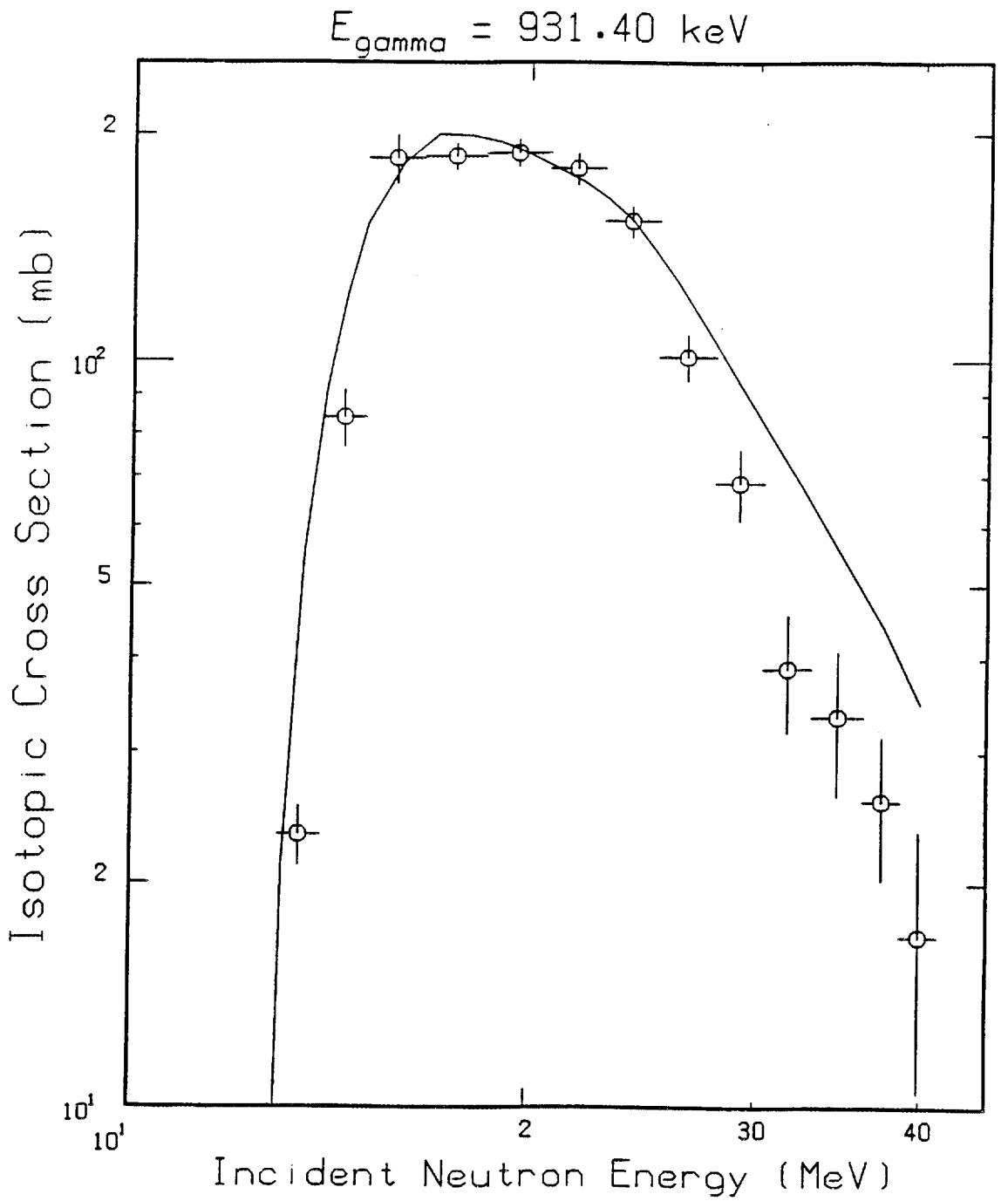

Figure 7. Original calculated excitation function for E_γ = 931.4 keV[3] compared with the data of Dickens et al.[1]

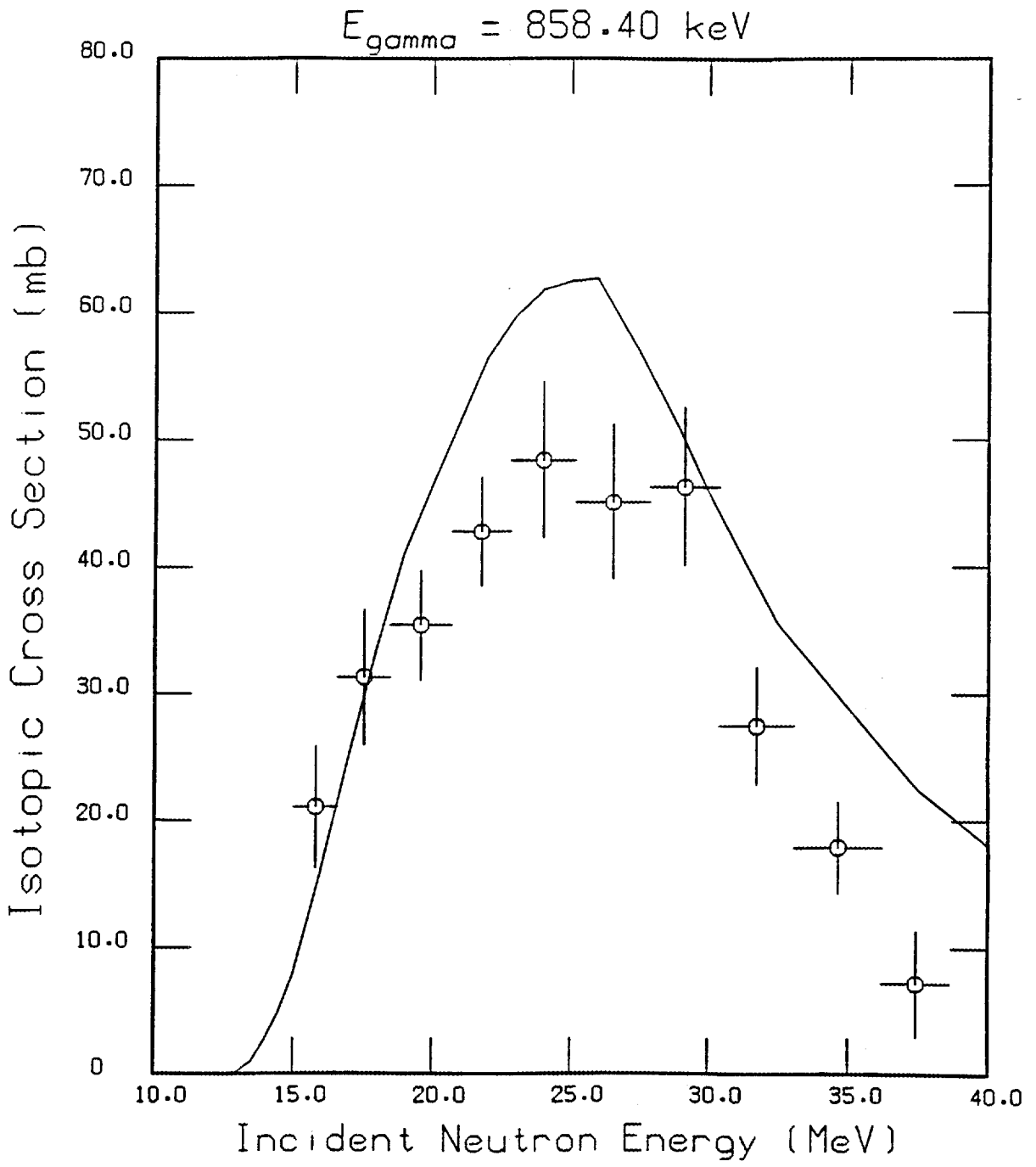

Figure 8. Original calculated excitation function for E_γ = 858.4 keV[3] compared with the data of Dickens et al.[1]

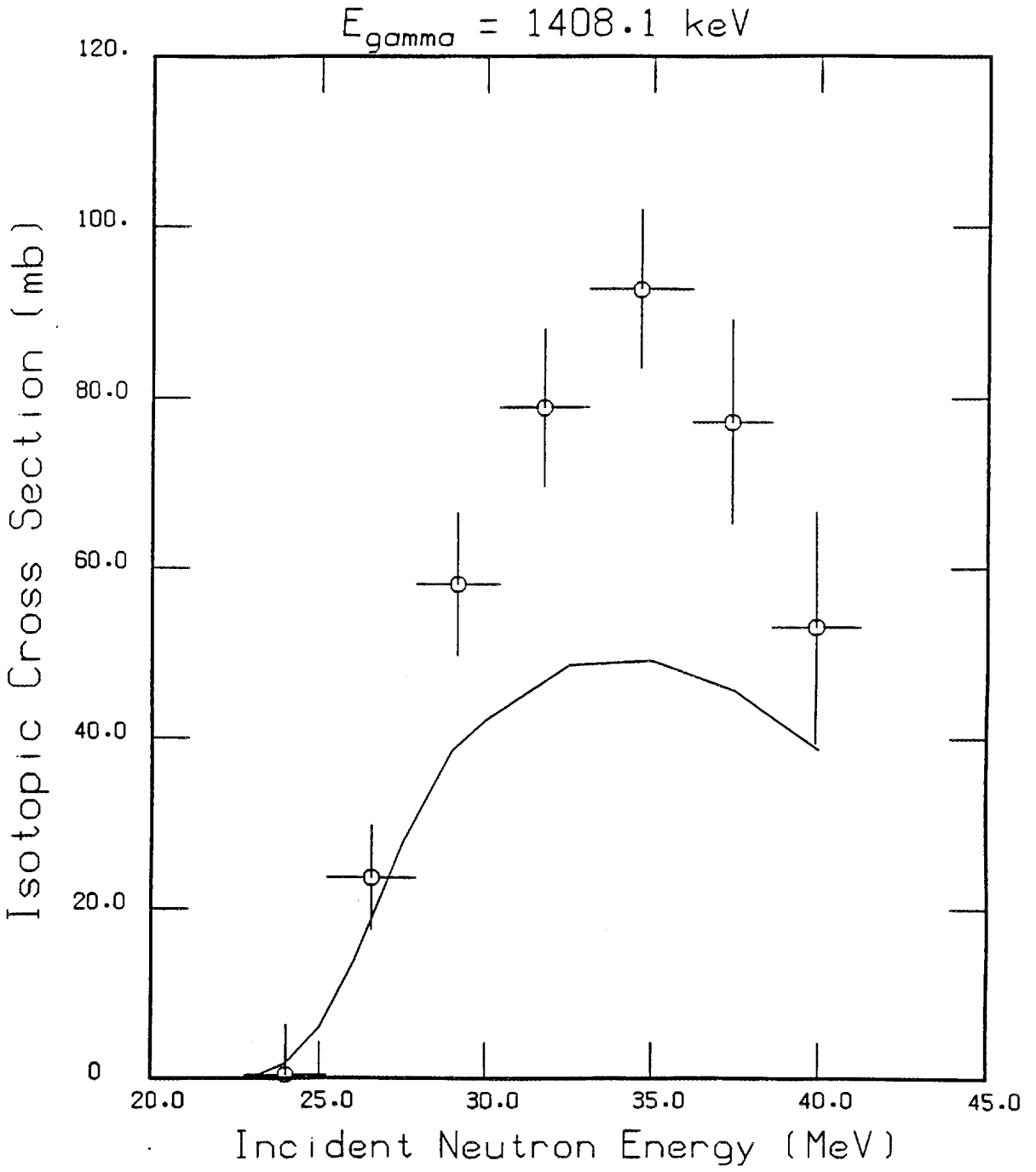

Figure 9. Original calculated excitation function for E_γ = 1408.1 keV[3] compared with the data of Dickens et al.[1]

In the TNG code the level density parameters for a particular reaction will affect the calculations for all its daughter reactions. For instance, if the threshold excitation energy for a particular tertiary reaction is in the level density region of its antecedent binary reaction most of whose yield arises from the discrete levels, then changes to the level density of the binary residual may have a strong effect on results for the tertiary reaction. Work on the tertiary and quaternary reactions began with adjustment to the binary level density. Later, some adjustments to level densities for both the binary reactions and a few tertiary reactions proved useful in fine tuning the calculations for the tertiary and quaternary reactions. It was prerequisite that these improvements would not be at the expense of the binary calculations.

Table 2. Final set of level density parameters for $^{56}Fe(n,x)$

Reaction	E_c(MeV)	E_x(MeV)	E_0(MeV)	T(MeV)	α(MeV^{-1})	c	U(MeV)
(n,n')	4.539	11.544*	-0.448*	1.522*	6.0*	8.26	2.810
(n,p)	0.754	8.724*	-2.618*	1.380*	16.75*	9.401	0.525
(n,α)	2.681	7.898*	-0.732*	1.351*	6.115*	8.144	1.35
(n,2n)	3.120	8.845*	-1.41*	1.369*	6.4*	7.589	1.54
(n,np)	2.570	9.282*	-1.585*	1.452*	6.15*	8.56	1.27
(n,nα)	3.7	9.794	-0.183	1.392	6.154	7.613	2.65
(n,3n)	4.0	10.75	-0.1	1.435	6.4	8.26	2.81
(n,2np)	1.15	7.676	-2.2	1.256	7.233	9.401	0.525
(n,2nα)	2.32	7.673	-0.762	1.288	6.5	9.144	1.35
(n,4n)	2.4	9,859	-1.483	1.509	5.909	7.589	1.54
(n,3np)	2.839	7.92	-1.045	1.289	6.665	8.56	1.27

(* denotes a change from the original set[3])

The final set of optimized level density parameters is given in Table 2. Used along with the optical model parameters of Set C, these gave the best overall results for the (n,nα+αn), (n,2n), (n,np+pn), and (n,3n) reactions. Final calculations for these parameters are shown for the gamma rays considered in Figures 10-16.

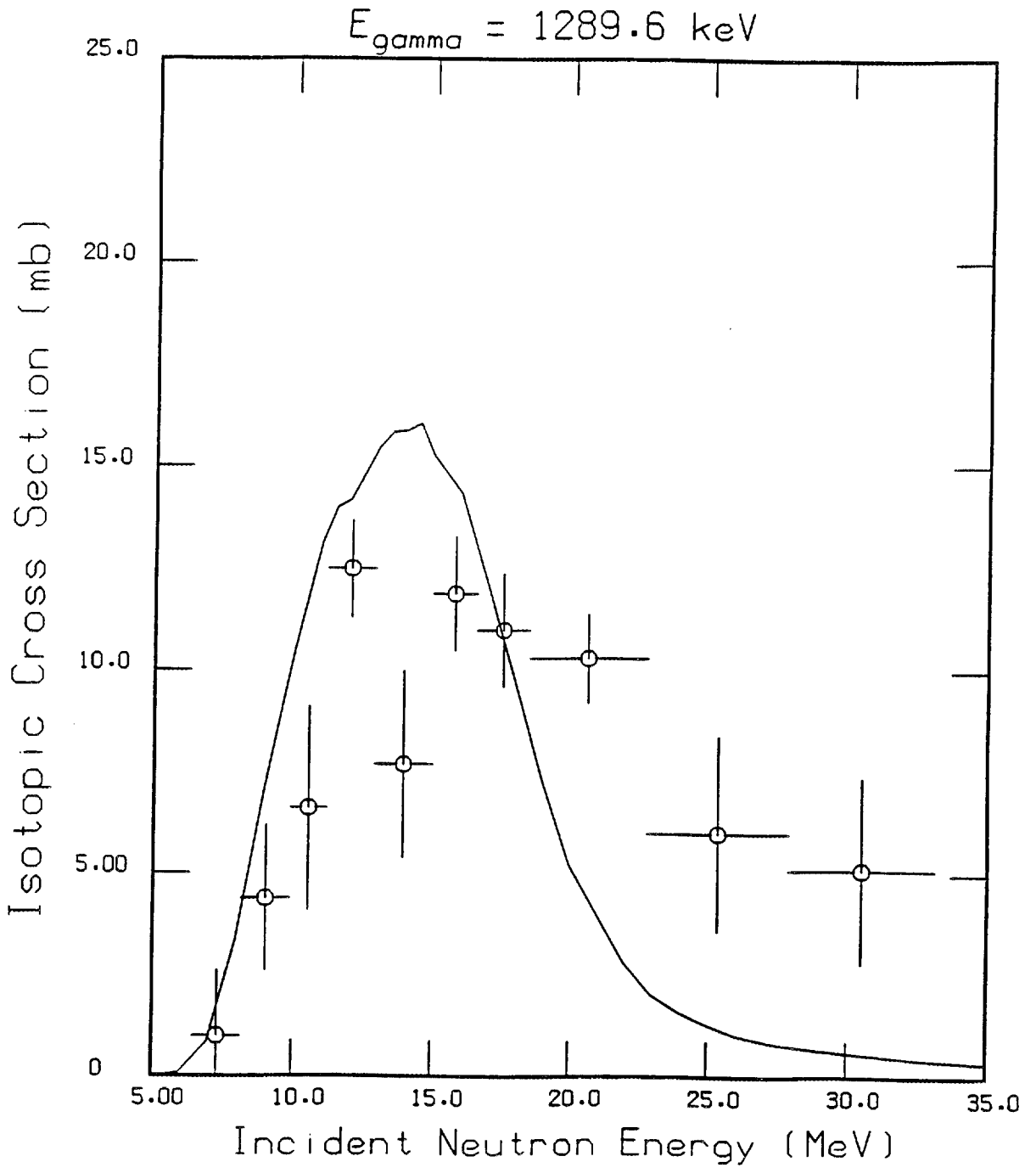

Figure 10. Present calculated excitation function for E_γ = 1289.6 keV compared with the data of Dickens et al.[1]

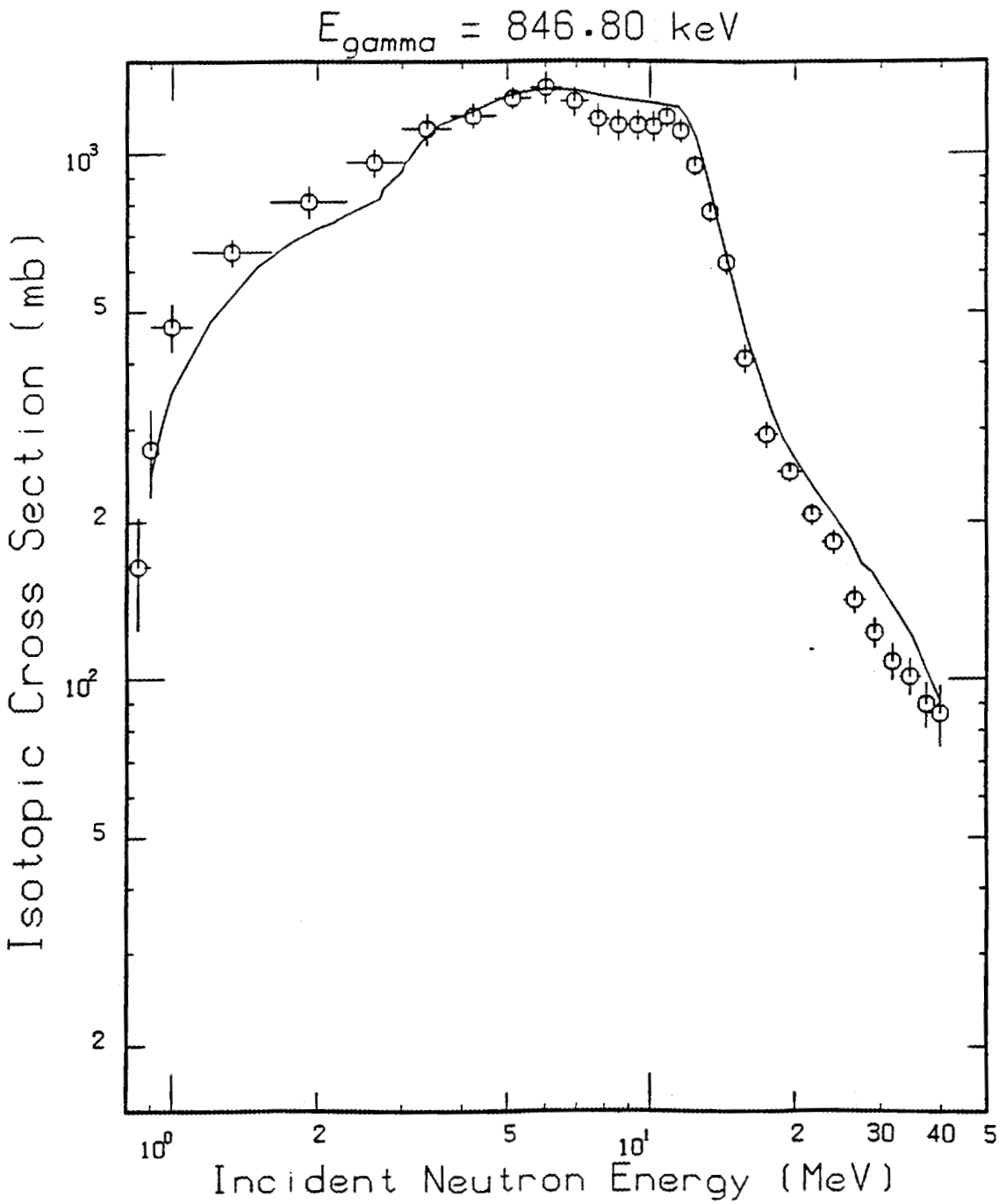

Figure 11. Present calculated excitation function for E_γ = 846.8 keV compared with the data of Dickens et al.[1]

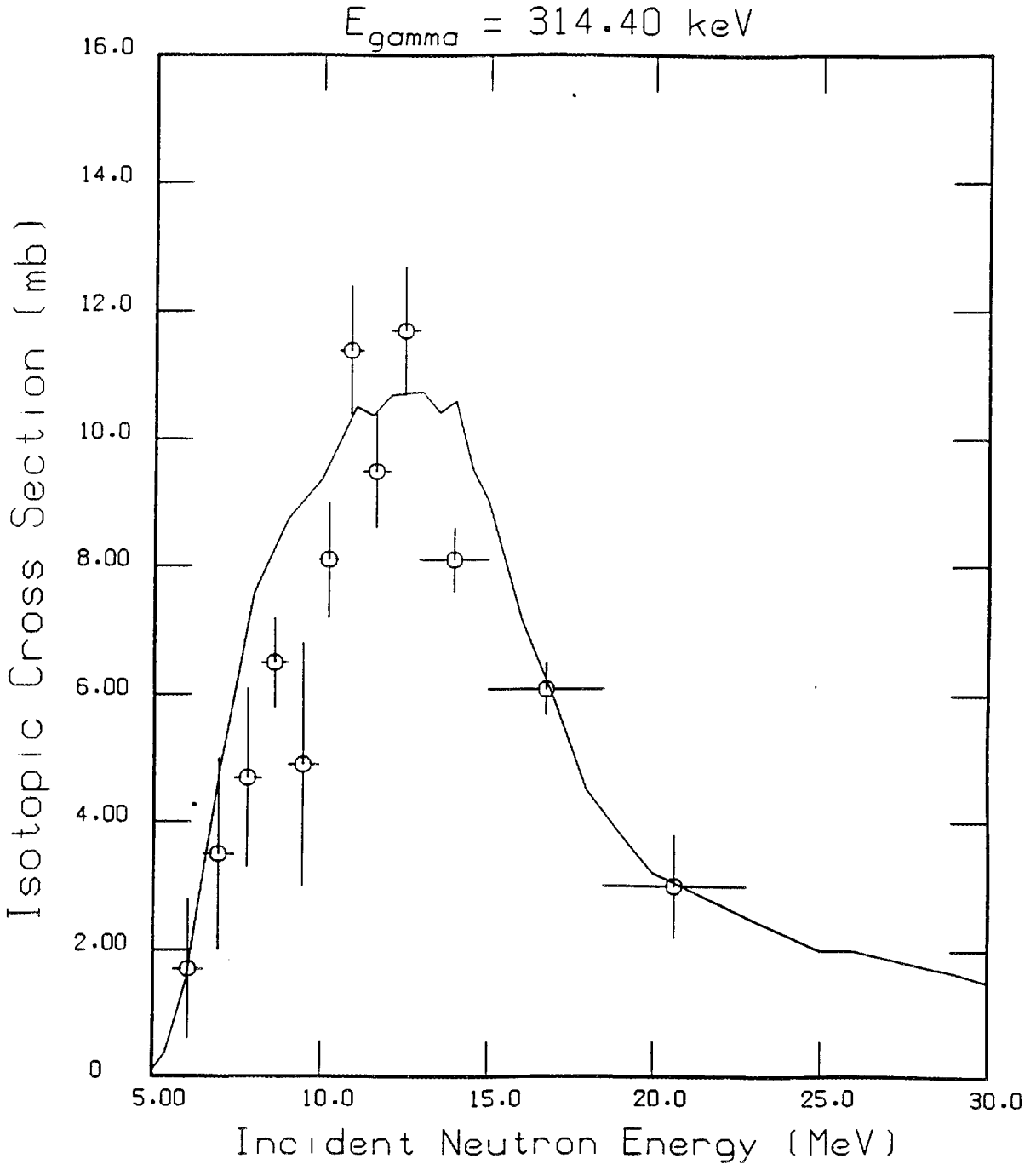

Figure 12. Present calculated excitation function for E_γ = 314.4 keV compared with the data of Dickens et al.[1]

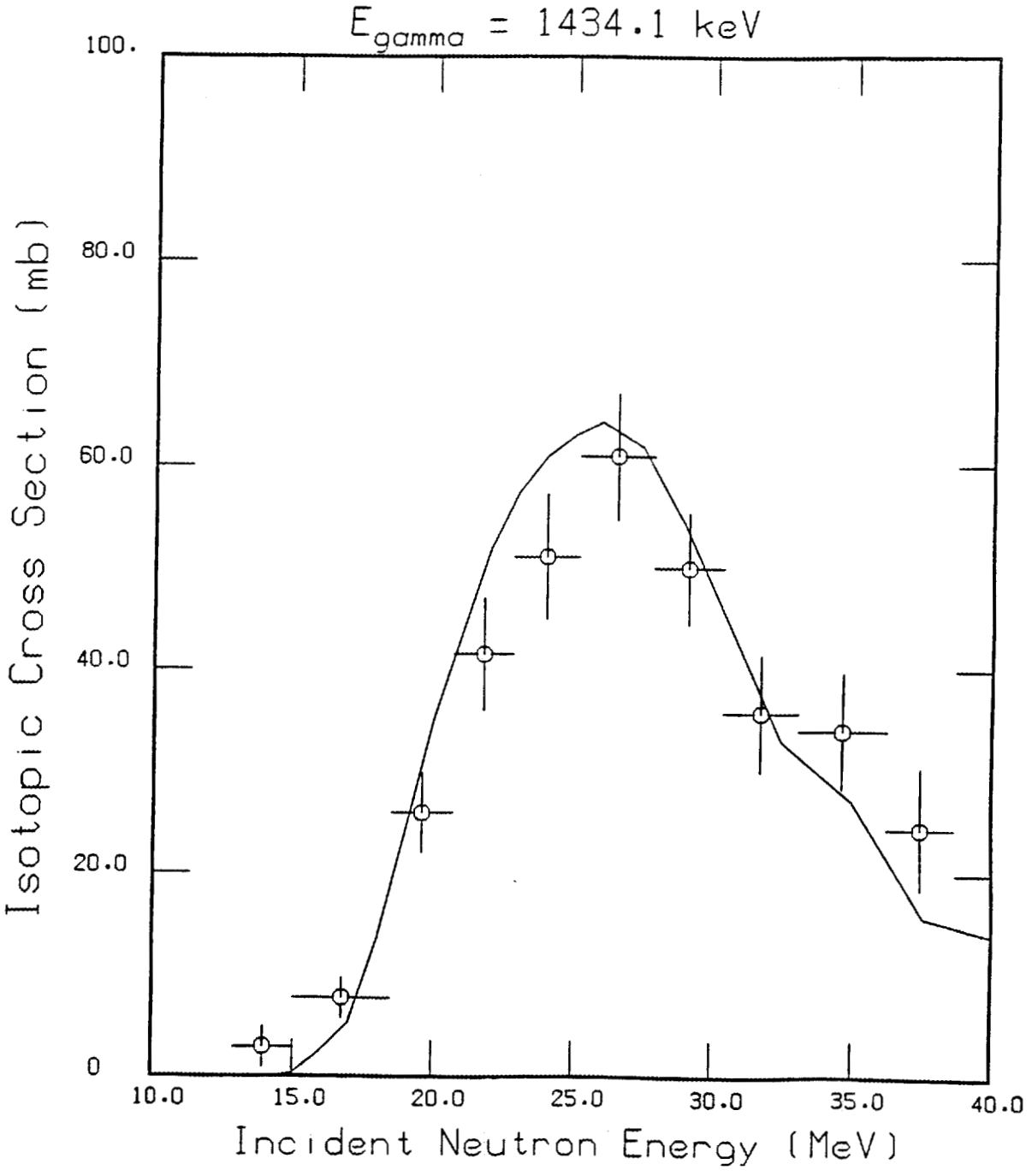

Figure 13. Present calculated excitation function for E_γ = 1434.1 keV compared with the data of Dickens et al.[1]

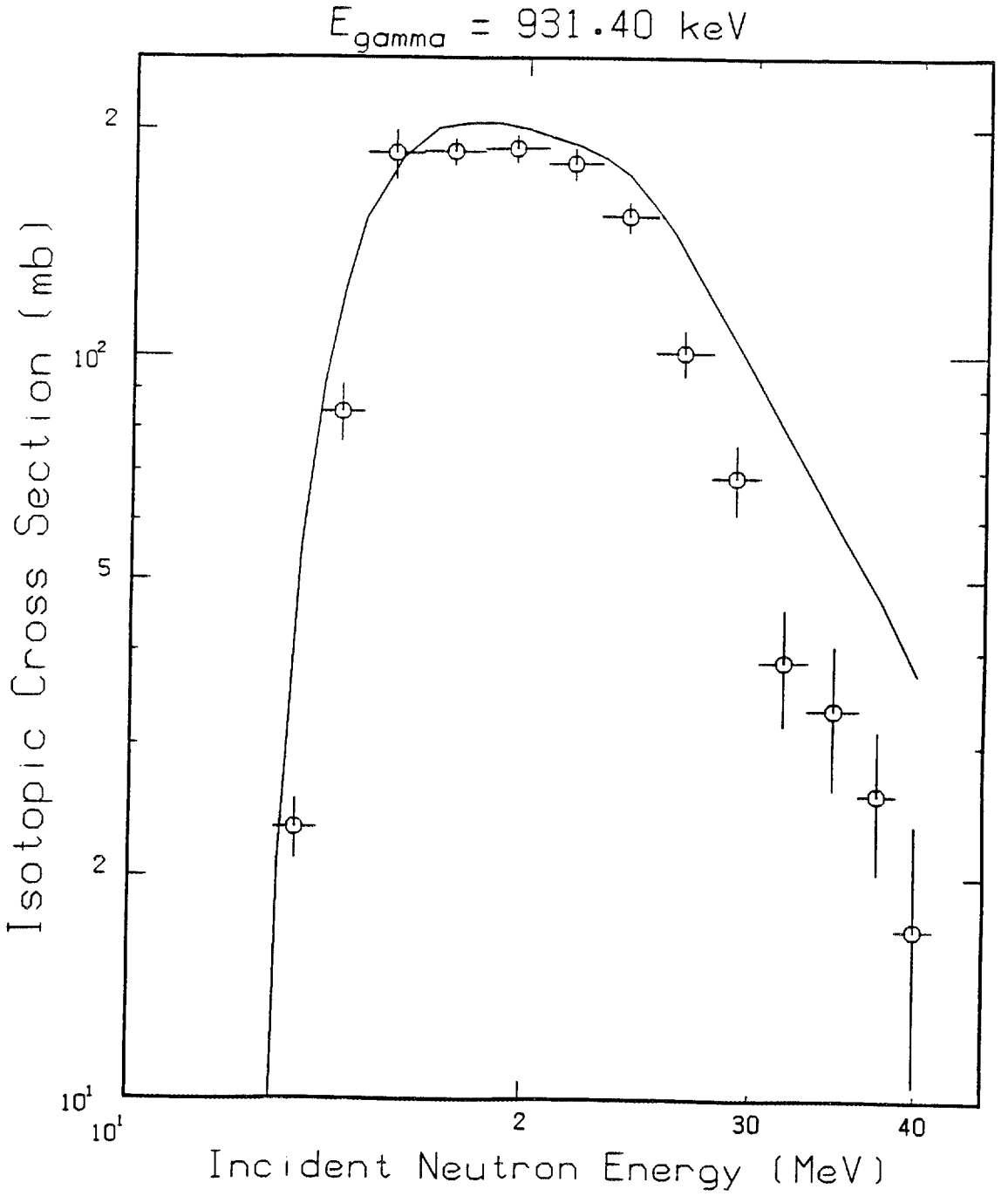

Figure 14. Present calculated excitation function for E_γ= 931.4 keV compared with the data of Dickens et al.[1]

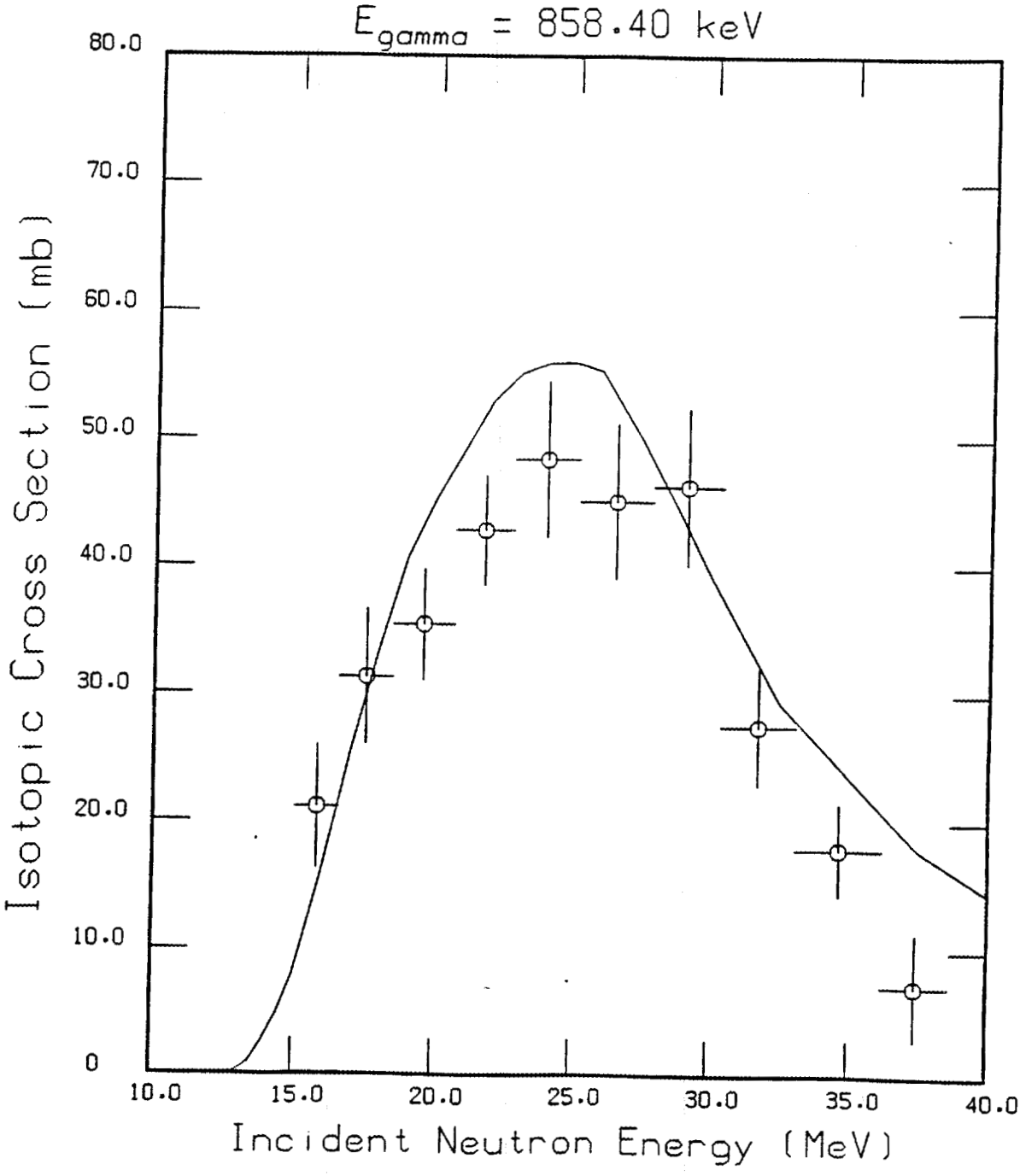

Figure 15. Present calculated excitation function for E_γ = 858.4 keV compared with the data of Dickens et al.[1]

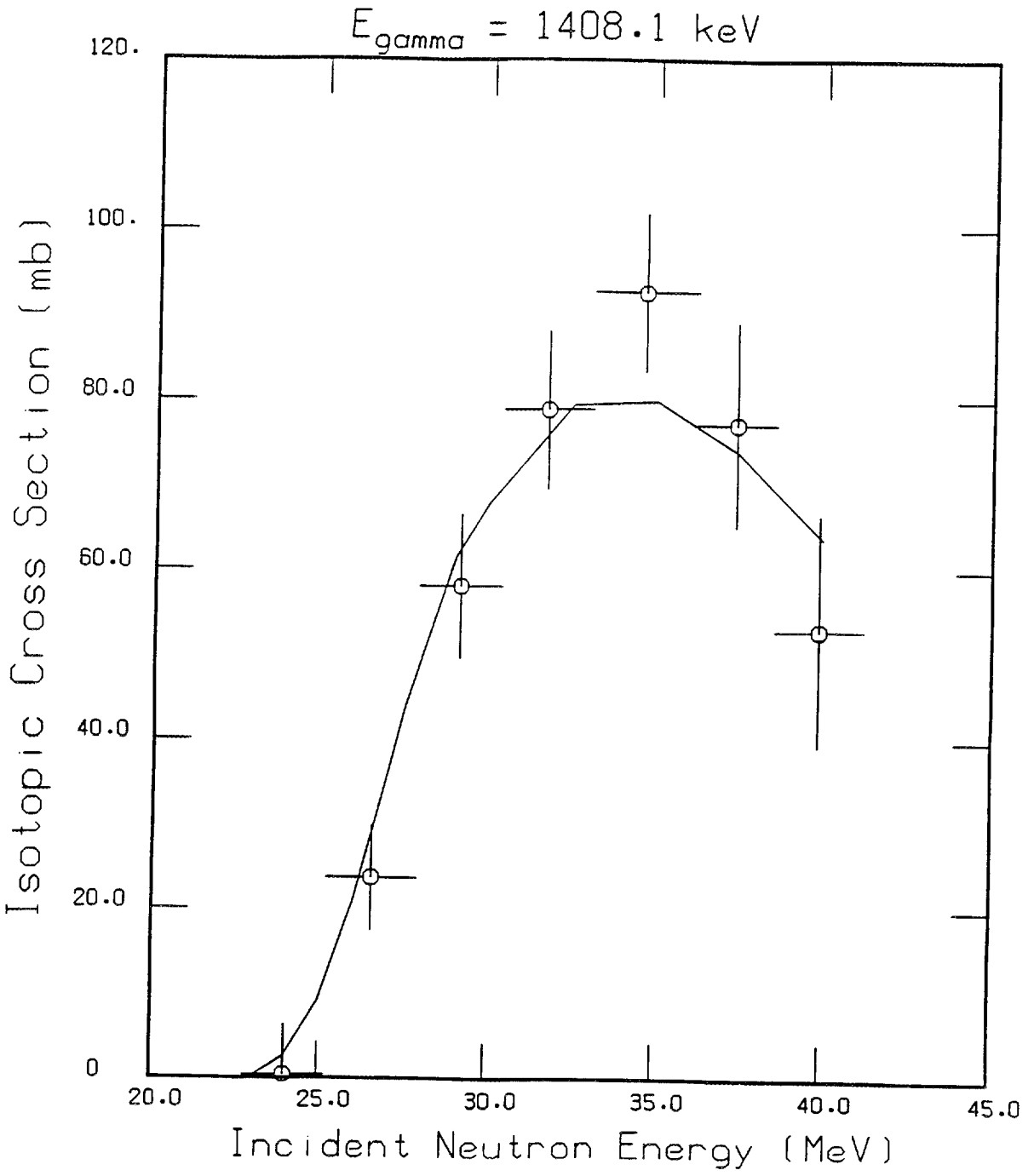

Figure 16. Present calculated excitation function for E_γ = 1408.1 keV compared with the data of Dickens et al.[1]

3. DISCUSSION

Improvement for gamma rays of tertiary and quaternary reactions for ^{56}Fe was affected, mostly through adjustment of the alpha optical model and certain level density parameters in the TNG code. The binary reactions were left unimproved. In this analysis, the level density was varied more extensively than the optical model, and the results indicate the limitations of such an approach. As mentioned above, adjustment to the level density parameter 'a' for a particular reaction will have little effect on the gamma ray calculations for that reaction if a significant portion of the yield for the reaction lies in the discrete level structure rather than the level density region. However, other subsequent and dependent reactions may be strongly affected. Therefore, adjustments to the level density cannot be expected to have significant effect on the binary reactions. This is shown in Figures 3-5 and 10-12, in which the original and final calculations are virtually identical.

There remains a pronounced lack of agreement in the (n,α) reaction at incident neutron energies above 20 MeV (Fig. 10). It is unclear whether this is due to an unseen flaw in the alpha optical model parameters or to a more fundamental characteristic of the TNG code. The code calculates compound and pre-compound reactions, but does not include direct interactions in its algorithm. But in this case a compound interaction, in which an alpha-like object would somehow coalesce from the disorder of the nucleus' interior, seems less and less likely with increasing energy and number of degrees of freedom. The measured yield at these high energies may be due instead to direct interactions, in which the energetic neutron immediately induces an alpha-like object to leave the previously 'cool' nucleus. If so, the disagreement above 20 MeV in Figure 10 would be due to the absence of direct interaction calculations in TNG. Furthermore, the lack of direct interaction calculations would not preclude TNG agreeing at high energies for the $(n,n\alpha+\alpha n)$ reaction; presumably the ejection of a neutron could cool the nucleus sufficiently to make a compound-type ejection of an alpha particle more favorable.

4. CONCLUSION

Adjustment of TNG parameters, mostly involving the level density, proved ineffective in improving TNG agreement above 17 MeV for ^{56}Fe binary reaction gamma-rays. These adjustments were successful in improving agreement for several tertiary and quaternary reactions. Adjustments to the optical model parameters were fairly coarse, involving few changes to the energy dependence, and did not significantly improve agreement with total cross section and total nonelastic cross section data. Future optimization work with TNG might bring more success through more delicate adjustment of the optical model parameters, predicated on detailed comparison with data for specific binary and tertiary reactions. Further work with the optical model might also help in understanding the disagreement above 20 MeV for the $(n,n\alpha+\alpha n)$ reaction.

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