AAEC/E336

AAEC/E336

AUSTRALIAN ATOMIC ENERGY COMMISSION

RESEARCH ESTABLISHMENT

LUCAS HEIGHTS

COMPARISON OF CALCULATIONS MADE WITH THREE TIME-DEPENDENT NEUTRON CODES TDA, MORSE AND POW

by

B. McGREGOR

B. HARRINGTON

December 1974

ISBN 0 642 99659 8

AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS

COMPARISON OF CALCULATIONS MADE WITH THREE TIME-DEPENDENT NEUTRON CODES TDA, MORSE AND POW

by

B. McGREGOR
B. HARRINGTON

ABSTRACT

Three computer codes were compared to determine their usefulness in analysing a pulsed neutron experiment. The codes were a Monte Carlo code (MORSE) a diffusion kinetics code (POW) and a time dependent SN code (TDA).

A series of test problems were devised to progressively model the experiment. All problems assumed a spherical system with an isotropic source. The first problem had its source in the first energy group for the first nanosecond. The second problem had its source distributed in time but not distributed in energy. The third problem had a source distributed in energy and time.

POW and MORSE were shown to be in good agreement, with significant differences occurring only at times when the system did not correspond with the approximations made in POW.

The AAEC version of the TDA code did not handle a time-dependent source.

(Continued)

There was also a tendency for the results beyond 50 ns to be higher than those for the other two codes for the problems having a source constant over one time interval.

National Library of Australia card number and ISBN 0 642 99659 8

The following descriptors have been selected from the INIS Thesaurus to describe the subject content of this report for information retrieval purposes. For further details please refer to IAEA-INIS-12 (INIS: Manual for Indexing) and IAEA-INIS-13 (INIS: Thesaurus) published in Vienna by the International Atomic Energy Agency

COMPARATIVE EVALUATIONS; COMPUTER CALCULATIONS; CROSS SECTIONS; M CODES; MONTE CARLO METHOD; NEUTRON FLUX; NEUTRON SPECTRA; NEUTRONS; P CODES; PULSE TECHNIQUES; T CODES; THORIUM 232; TIME DEPENDENCE

CONTENTS

INTRODUCTION

A series of pulsed neutron experiments with a cube of ^{232}Th has been performed at the AAEC Research Establishment, Lucas Heights (Moo, Rainbow & Ritchie 1973). The preliminary analysis of these experiments has been made with a zero-dimensional code TENDS; however, three other codes are available at Lucas Heights to analyse the experiments with less approximation.

Monte Carlo methods of calculation can theoretically calculate the experiment. However, the statistical accuracy obtainable in reasonable computer time may be inadequate, especially if fluxes averaged over a small volume are required at long (> 100 ns times) after the source. The Monte Carlo method may, however, be the only way to represent the angular asymmetry of the source and the details of the geometry. A general purpose Monte Carlo code MORSE (Straker *et al.* 1970) with combinatorial geometry has been used to study the applicability of Monte Carlo methods to this type of calculation.

One-dimensional discrete ordinate (SN) codes have been used successfully in a wide range of time independent calculations; one such code is ANISN. A time dependent outer loop was added by Dupree *et al.* (1971) to develop the code TDA.

A general purpose kinetics-diffusion code POW (Pollard 1974) developed at Lucas Heights, was available as a possible means of calculating the experiments. The 0-Dimensional version of this code is equivalent to TENDS.

To understand the applicability of these codes to the experimental analysis, three test problems were devised which progressively modelled the experiment. Cubical geometry, detector geometry and source asymmetry were not treated exactly in this study.

In the first problem the source was placed in the top energy group in the time interval 0-1 ns. The source spectrum for the second problem approximated the experiment, and also was constant for 1 ns. The third problem entailed a time and energy dependent source.

The three calculations assumed the following factors :

- a spherically symmetric source;
- spherical geometry;
- cross sections from the ABBN 26-group set; and
- no fission neutrons produced to allow easy calculation with MORSE.

2. DETAILS FOR CALCULATIONS

The range of interest is less than 500 ns after the source is injected. Calculations are normalised by the codes to one source neutron. The energy group structures, source spectra for problems 2 and 3, and response functions approximating those used in the experiment are given in Table 1. Table 2 presents the time mesh used in each code. Other constants are:

- radius of sphere = 23.72 cm;
- atom density of ^{232}Th = 0.028697 x 10^{24} atoms cm^{-3};
- the source is at the centre of the sphere;
- calculations are made of total flux, responses and spectra at 2, 6, 10, 14, 18 and 21.86 cm radii; and
- the source width is 1 ns for problems 1 and 2.

MORSE - A boundary crossing estimator was used at the required radii, and required the use of dummy material numbers to generate the call to BDRYX. No splitting or 'Russian Roulette' was used as every radius and energy group was considered important. Histories were terminated when a neutron leaked or reached the time limit of 500 ns. Approximately 55 000 source neutrons were followed in a four-hour run on an IBM360/50 computer.

The MORSE time bin with 400 ns as centre is 100 ns wide in order to obtain reasonable statistics. The results, averaged from 350 to 450 ns, are higher than the true value at 400 ns. The bias was estimated from the POW results and assumes an exponential decay from 350 to 450 ns. The ratio (R) of the calculated endpoints was 0.4, and the ratio of estimated to true fluxes is

$$(1-R)/(-\ell n\ (R)\sqrt{R}) = 1.04;$$

the 400 ns results were divided by this correction factor.

TDA - The required radii were made the centres of 25 mesh intervals (approx. 1 cm mesh). The analytic first collision source option was used with three sources at 0, 0.5 and 1 ns to approximate a continuous source from 0 to 1 ns. The times selected for code comparisons were made the centre of 79 time steps. The space and time meshes are related in such a way that the uncollided source neutrons are at the centre of successive space intervals when at the centre of successive time steps. The source neutrons travel about 4 cm in one nanosecond. An S6 quadrature was required. The time and space meshes and quadrature order were tested for convergence. The calculation required one hour of computer time. (Note: A factor of $4\pi r^2$ is included in TDA activities output.)

POW - The one-dimensional calculation used 13 space intervals (2 cm mesh) with the required radii and times at the endpoint of the intervals. On average, the source is actually misplaced about 1 cm from the centre. 86 time steps were used with initial widths in the range 0.25 to 7 ns when uncollided source neutrons have left the system. Calculations with a coarser time mesh led to alternative positive and negative values at successive times in the group 1 flux at the centre. However, the average value is approximately correct and results beyond 20 ns are unchanged when time mesh is halved. The calculation required 20 minutes of computer time.

The zero-dimensional calculation used the same time mesh with a buckling of 0.01399 corresponding to a 23.72 cm sphere with an extrapolation distance of 2.84 cm. POW is designed to do 2-D kinetics efficiently and not 0-D calculations as can be seen from the computer time usage of 17 mins.

3. RESULTS AND DISCUSSION

Problem 1 The interpretation of POW results is difficult in the early time phase (0-6 ns) while the uncollided source neutrons are travelling through the system. The first comparisons are made at 9.5 ns where some source effects are still evident. Further comparisons were made at 19, 45, 90, 210 and 400 ns as shown in Figures 1 and 2. The MORSE error bars are ±2 standard deviations.

At early times, the POW calculations are lower than the results for the other two codes at the centre and higher at the edge. Such a result is consistent with the use of a diffusion code for a rapidly changing system. Beyond 45 ns, the MORSE and POW results agree.

The TDA total fluxes are consistently high by about 15 per cent from 45 ns to 500 ns.

All three codes have difficulty in calculating the flux at 2 cm radius. MORSE has poor statistics owing to the small surface area of the spherical shell at this radius. POW exhibits oscillations in the central flux in the source group while TDA has some difficulty in calculating the flux near the centre of the sphere. Fortunately the experiment has its closest detector at about 8 cm from the source, so these deficiencies are not important.

Table 3 shows spectrum information (actually group fluxes) at 2 points, at radii of 6 and 21.86 cm for 9.5, 45 and 210 ns. Information is supplied for the three codes; the MORSE results are given only where the standard deviation is less than 20 per cent. Actual statistics are not given, but they were usually about 6 per cent s.d. at the peak of the group flux. MORSE/TDA and TDA/POW ratios are included.

The most noticeable feature of the various spectra is the grouping of the flux into about four or five energy groups, with a sharp falloff in the groups either side of them. MORSE results are usually available only for these groups. The MORSE/TDA comparisons show that any differences in total flux are similar for all the important contributing groups; there is no great tendency for the TDA results to have a harder or softer spectrum than MORSE.

Some noticeable differences are observed in the TDA/POW comparisons. The group 1 (source group) results from POW at 9.5 ns are spurious, presumably owing to the inability of the diffusion theory to describe the system at early times.

Table 4 gives a comparison between TDA and MORSE of the time integral of the total flux for problems 1 and 2. MORSE and TDA integral results for problem 1 agree at the centre, but the TDA results are higher at other points.

Figure 3 shows the variation with time of the average flux ($\int \phi dV/V$) from four calculations with MORSE, TDA, POW-1D and POW-0D. The MORSE results lie between the TDA and POW-1D results, and are closer to TDA at short times and to POW-1D at long times. The POW-0D results diverge from the POW-1D results up to about 100 ns and then they slowly begin to approach them.

Problem 2 The energy dependence of the source (Table 1) approximates the experimental spectrum. The system is now a larger number of mean free paths thick at source energies, which lead to a greater radial variation and the need for a finer (1 cm) mesh in POW-1D. Three other responses were calculated to approximate ^{237}Np fission, ^{235}U fission and ^{239}Pu fission (Table 1).

Results: Comparison starts at 19 ns. Figure 4 shows the radial variation of the total flux at five times for the three codes. The comparisons are very similar to those experienced in problem 1, but there is somewhat better agreement between the three codes at long times. The comparisons for the ^{235}U and ^{239}Pu responses were very similar to those for the total flux and so they are not recorded. The ^{237}Np fission cross section is a threshold reaction and the response is sensitive to the high energy part of the spectrum. Figure 5 shows a comparison of the three codes for this response at four times. As expected, the rate of decay with time is greater but, except for a low MORSE result at 90 ns, the comparisons are similar to those for the total flux. The comparisons of average flux and time integrated flux were similar to those for problem 1.

Problem 3 A simple approximation to one of the experimental time spectra (a Gaussian distribution centred at 18 ns) was obtained by integrating over five time intervals. Within each time interval the source was assumed constant in time.

Since the source time extends to 36 ns, a fine time mesh is required to about 40 ns. A 1 and 0.5 ns mesh was used in POW and it produced only slight variations. The AAEC version of TDA was unable to handle this calculation. Examination of the code suggested that the option (IFG>1) was probably untested. These findings have been communicated to the code authors.

Interval	Time Interval (ns)	Source in Interval
1	0 - 12.45	0.14675
2	- 16.185	0.2164
3	- 19.92	0.2737
4	- 23.655	0.2164
5	- 36.105	0.14675

Results: Figure 6 shows the comparison of POW and MORSE for the radial variation of the total flux at various times starting at 45 ns. The comparisons are very similar to those for problems 1 and 2. Figure 7 shows the ^{237}Np fission response.

4. CONCLUSIONS

The MORSE results are in good agreement with one or other of the two codes at various times. Since the Monte Carlo method is not subject to calculational errors related to the choice of time mesh, as are the POW and TDA codes, it is assumed that the MORSE results are correct at both early and late times and that the other codes are in error when they disagree with MORSE. Except for the point at 2 cm radius, the statistical accuracy obtained using about 50 000 source neutrons is quite reasonable; it has a standard deviation of about 2 per cent at early times, which increases to about 5 per cent at long times. The ^{237}Np response has a noticeably higher statistical error.

At early times, the TDA results agree with the MORSE, but at later times they are higher by about 20 per cent in problem 1 and 10 per cent in problem 2. The reasons for the disagreement are not understood, though one possible explanation is the use of single precision arithmetic in TDA.

The POW-1D results give a different radial shape at early times from the TDA and MORSE results. This is consistent with the use of a diffusion code in a non-diffusion application. Beyond 45 ns, the POW-1D and MORSE results are in good agreement at all radii.

The POW-OD results are consistently lower than those from POW-1D with a maximum deviation at about 100 ns (see Figure 3). However, beyond 100 ns the rate of decay of the flux is similar to that found with the other codes.

Two of the codes may be useful in calculating the experiment. MORSE should handle the calculation at all times provided the statistical error is acceptable, while it can be seen that POW (Figure 6) can be used from about 100 ns onwards. This time approximates the end of discernible asymmetric source effects in the experiment. POW will be useful in calculating detailed fluxes at long times and, because of its short running time, in looking at the effects of varying parameters of the calculation. TDA will probably not be used partly because of its failure to handle a time dependent source and partly because of the disagreement with the other two codes found in this study.

A significant bonus to the study, apart from the degrees of confidence gained in the codes, was a better understanding of their use. Intercomparison of codes in simple benchmark problems frequently detects errors in production codes or our understanding of production codes.

5. REFERENCES

Dupree, S.A., Sandmeier, H.A., Hansen, G.E., Engle, W.W. Jr. & Mynatt, F.R. (1971) - Time-dependent neutron and photon transport calculations using the method of discrete ordinates. LA-4557.

Moo, S.P., Rainbow, M.T. and Ritchie, A.I.M. (1973) - Time dependent ^{237}Np, ^{235}U and ^{239}Pu fission rates in a thorium assembly during the interval 0 to 200 ns using a pulsed ^{9}Be(d,n) source. Part I - Experiment. AAEC/E254.

Pollard, J.P. (1974) - AUS Module POW - a general purpose, 0, 1 and 2D multigroup neutron diffusion code including feedback-free kinetics. AAEC/E269.

Straker, E.A., Stevens, P.N., Irving, D.C. & Cain, V.R. (1970) - The MORSE Code - a multigroup neutron and gamma-ray Monte Carlo transport code. ORNL-4585.

TABLE 1

GROUP STRUCTURE, SOURCE SPECTRUM AND APPROXIMATE RESPONSE FUNCTIONS

Group	Upper Energy Boundaries	Source Spectrum	Approx. response functions		
			^{237}Np	^{235}U	^{239}Pu
1	1.0 E + 7	0.012	2.15	1.52	2.09
2	6.5 E + 6	0.240	1.60	1.06	1.70
3	4.0 E + 6	0.209	1.72	1.20	1.84
4	2.5 E + 6	0.214	1.67	1.26	1.93
5	1.4 E + 6	0.130	1.49	1.22	1.72
6	8.0 E + 5	0.079	0.657	1.16	1.57
7	4.0 E + 5	0.060	0.065	1.30	1.50
8	2.0 E + 5	0.030	0.0311	1.48	1.50
9	1.0 E + 5	0.016	0.015	1.74	1.51
10	4.65E + 4	0.006	0.0127	2.25	1.64
11	2.15E + 4	0.003	0.017	2.80	1.86
12	1.0 E + 4	0.0	0.03	3.70	2.20
13	4.65E + 3	0.0	0.048	5.43	3.00
	2.15E + 3				

Since the flux in groups 14 to 26 is negligible at all times considered, the energy boundaries and response functions for these groups have not been tabulated.

TABLE 2

TIME MESHES (ns)

MORSE		TDA		POW					
Problems 1, 2 & 3		Problems 1 & 2		Problem 1		Problem 2		Problem 3	
Time Step	Time To	Time Step	Time To	Time Step	Time To	Time Step	Time To	Time Step	Time To
1	10	0.125	0.125	0.25	7	0.25	10	0.5	40
2	20	0.25	7.125	0.5	10	1.0	20	2.0	60
5	30	0.875	8.0	1.0	20	2.0	40	5.0	100
10	60	1.0	10.0	2.0	40	5.0	100	10.0	220
20	100	2.0	20.0	5.0	100	10.0	220	20.0	300
70	170	5.5	42.0	10.0	220	20.0	300	50.0	500
80	250	6.0	72.0	20.0	300	50.0	500		
100	450	7.0	86.0	50.0	500				
50	500	8.0	150.0						
		9.0	195.0						
		10.0	235.0						
		15.0	370.0						
		20.0	410.0						
		30.0	500.0						

TABLE 3

SPECTRA COMPARISON

(9.5 ns)

	6 cm					21.86 cm				
Group	MORSE	TDA	MORSE/ TDA	POW	TDA/POW	MORSE	TDA	MORSE/ TDA	POW	TDA/POW
1	-	6.07 + 2	-	3.67 + 3	0.17	4.2 + 2	4.71 + 2	0.89	1.39 + 3	0.34
2	-	1.21 + 2	-	2.11 + 2	0.57	-	7.28 + 1	-	6.63 + 1	1.10
3	-	6.66 + 2	-	9.14 + 2	0.73	3.52 + 2	2.39 + 2	1.47	2.22 + 2	1.08
4	5.1 + 3	6.20 + 3	0.83	5.93 + 3	1.05	7.65 + 2	7.95 + 2	0.96	1.08 + 3	0.74
5	2.9 + 4	3.15 + 4	0.92	1.92 + 4	1.64	1.01 + 3	1.12 + 3	0.90	2.19 + 3	0.51
6	6.50 + 4	6.24 + 4	1.04	3.12 + 4	2.00	1.12 + 3	1.02 + 3	1.10	2.09 + 3	0.49
7	3.88 + 4	3.49 + 4	1.11	1.86 + 4	1.88	4.58 + 2	4.07 + 2	1.13	7.15 + 2	0.57
8	9.1 + 3	9.68 + 3	0.94	6.15 + 3	1.57	-	1.10 + 2	-	1.80 + 2	0.61
9	-	1.67 + 3	-	1.26 + 3	1.33	-	2.11 + 1	-	3.42 + 1	0.62
10	-	2.98 + 2	-	2.57 + 2	1.16	-	4.40	-	7.06	0.62
11	-	2.68	-	2.48	1.08	-	1.74 - 2	-	3.97 - 2	0.44
12	-	4.3 - 3	-	4.4 - 3	0.98	-	1.36 - 5	-	4.73 - 5	0.29
TOTAL	1.49 + 5	1.48 + 5	1.00	8.73 + 4	1.70	4.37 + 3	4.26 + 3	1.03	7.98 + 3	0.53

TABLE 3 (Continued)

(45 ns)

	6 cm					21.86 cm				
Group	MORSE	TDA	MORSE/ TDA	POW	TDA/POW	MORSE	TDA	MORSE/ TDA	POW	TDA/POW
1	-	2.0 - 3		1.0 - 4			1.67 - 3		-4.0 - 5	-
2	-	2.9 - 3		1.0 - 4	26.0		1.80 - 3		4.0 - 5	45.0
3	-	7.9 - 2		1.7 - 2	4.6		3.93 - 2		5.9 - 3	6.7
4	-	6.22		4.14	1.50		2.61		1.40	1.86
5	-	5.63 + 2		5.18 + 2	1.09	1.19 + 2	1.81 + 2	0.66	1.67 + 2	1.08
6	5.83 + 3	6.09 + 3	0.96	5.09 + 3	1.20	1.49 + 3	1.51 + 3	0.99	1.44 + 3	1.05
7	7.34 + 3	8.14 + 3	0.90	6.29 + 3	1.29	1.22 + 3	1.17 + 3	1.04	1.20 + 3	0.98
8	5.57 + 3	5.09 + 3	1.09	3.43 + 3	1.40	3.52 + 2	3.47 + 2	1.01	4.26 + 2	0.81
9	1.66 + 3	1.73 + 3	0.96	1.14 + 3	1.52	6.79 + 1	6.01 + 1	1.13	8.48 + 1	0.71
10	2.28 + 2	3.65 + 2	0.65	2.30 + 2	1.59		7.69		1.13 + 1	0.68
11	-	2.12 + 1		1.25 + 1	1.70		3.45 - 1		5.47 - 1	0.63
12	-	2.11 - 1		1.23 - 1	1.72		2.61 - 3		4.4 - 3	0.59
TOTAL	2.10 + 4	2.20 + 4	0.95	1.69 + 4	1.30	3.26 + 3	3.28 + 3	0.99	3.33 + 3	0.98

TABLE 3 (Continued)

(210 ns)

	6 cm					21.86 cm				
Group	MORSE	TDA	MORSE/ TDA	POW	TDA/POW	MORSE	TDA	MORSE/ TDA	POW	TDA/POW
1	-	2.0 - 29	-	1.3 - 6	-	-	2.0 - 29	-	9.6 - 7	-
2	-	1.0 - 25	-	9.3 - 10	-	-	8.0 - 26	-	-3.0 - 9	-
3	-	2.0 - 20	-	2.1 - 8	-	-	1.0 - 20	-	4.2 - 9	-
4	-	2.0 - 13	-	-4.0 - 8	-	-	8.0 - 14	-	3.0 - 8	-
5	-	9.0 - 5	-	4.0 - 5	2.2	-	3.0 - 5	-	1.45 - 5	2.0
6	-	4.29	-	4.21	1.02	-	1.20	-	1.26	0.95
7	6.88 + 1	1.04 + 2	0.66	9.46 + 1	1.10	1.75 + 1	2.43 + 1	0.72	2.32 + 1	1.05
8	3.72 + 2	4.05 + 2	0.81	3.49 + 2	1.16	8.62 + 1	8.24 + 1	1.05	7.43 + 1	1.11
9	3.78 + 2	4.55 + 2	0.83	3.77 + 2	1.21	7.60 + 1	8.27 + 1	0.92	7.27 + 1	1.14
10	1.34 + 2	1.48 + 2	0.91	1.18 + 2	1.25	2.05 + 1	2.18 + 1	0.94	1.96 + 1	1.11
11	-	2.97 + 1	-	2.28 + 1	1.30	-	3.66	-	3.44	1.06
12	-	1.49	-	1.06	1.41	-	1.40 - 1	-	1.44 - 1	0.97
TOTAL	9.36 + 2	1.15 + 3	0.81	9.67 + 2	1.19	2.08 + 2	2.16 + 2	0.96	1.95 + 2	1.11

TABLE 4

TIME INTEGRAL OF TOTAL FLUX FROM 0 TO 500 ns

Radius	2	6	10	14	18	21.86
Problem 1						
MORSE	2.998-2	5.791-3	2.647-3	1.413-3	7.553-4	3.517-4
2 s.d.	0.010	0.014	0.014	0.015	0.014	0.014
TDA	2.991-2	5.951-3	2.778-3	1.496-3	7.973-4	3.708-4
MORSE/ TDA	1.002	0.973	0.953	0.945	0.947	0.948
Problem 2						
MORSE	2.97-2	5.16-3	2.23-3	1.15-3	5.97-4	2.75-4
2 s.d.	0.018	0.014	0.014	0.014	0.016	0.014
TDA	2.84-2	5.30-3	2.35-3	1.22-3	6.28-4	2.84-4
MORSE/ TDA	1.04	0.97	0.95	0.94	0.95	0.97

s.d. = standard deviation

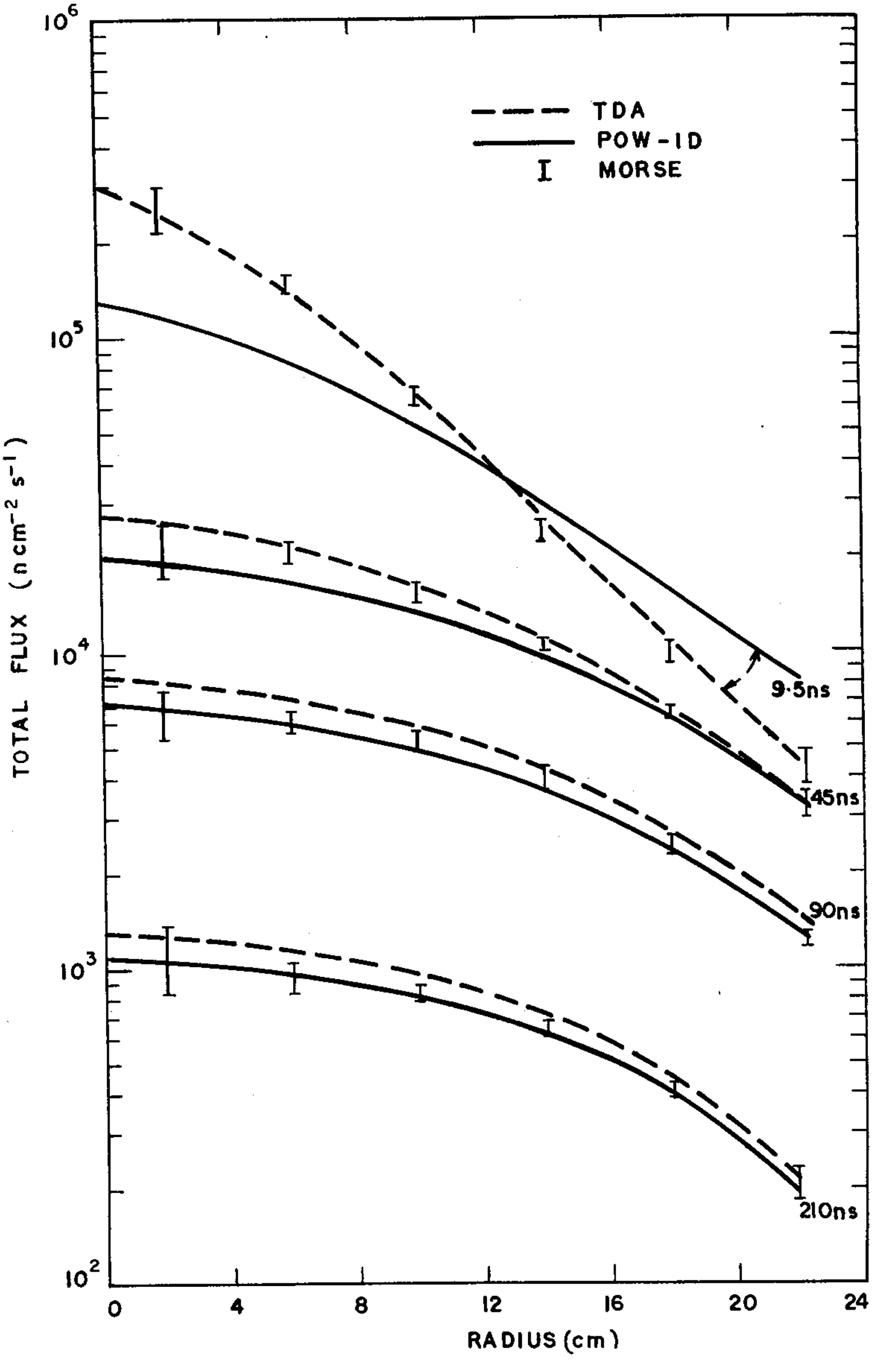

FIGURE 1. RADIAL VARIATION OF TOTAL FLUX IN PROBLEM 1

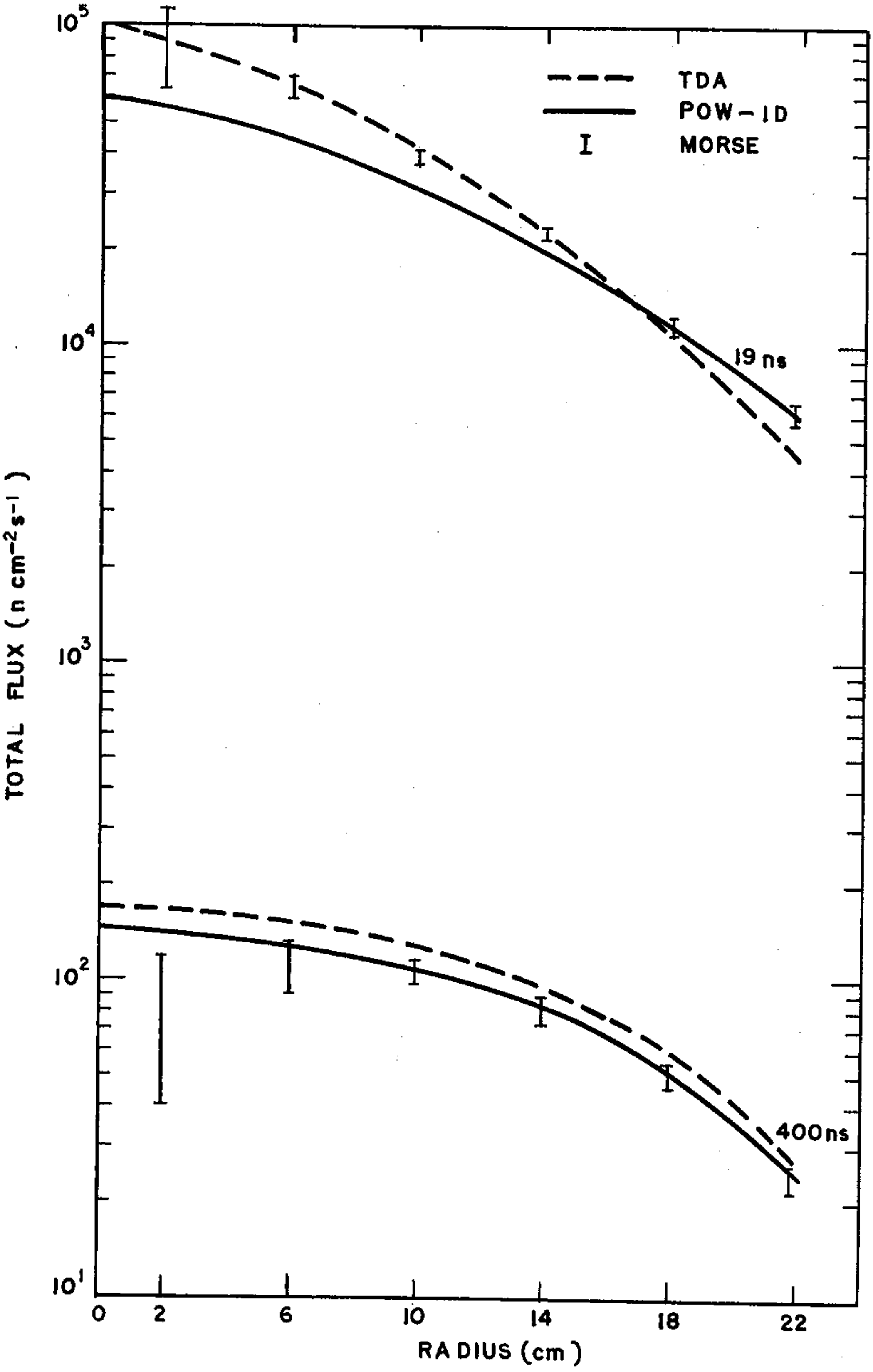

FIGURE 2. RADIAL VARIATION OF TOTAL FLUX

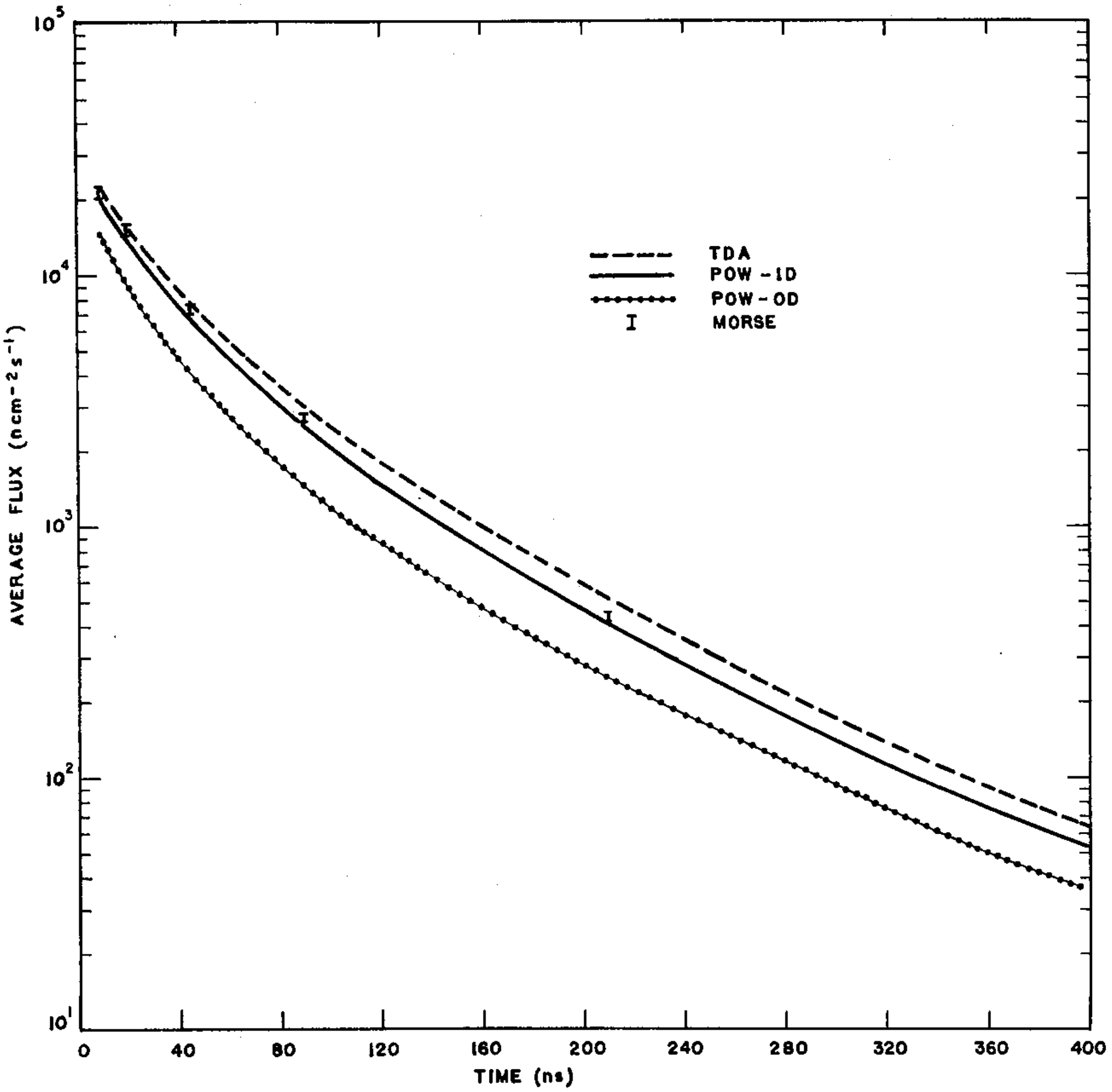

FIGURE 3. AVERAGE TOTAL FLUX IN PROBLEM 1

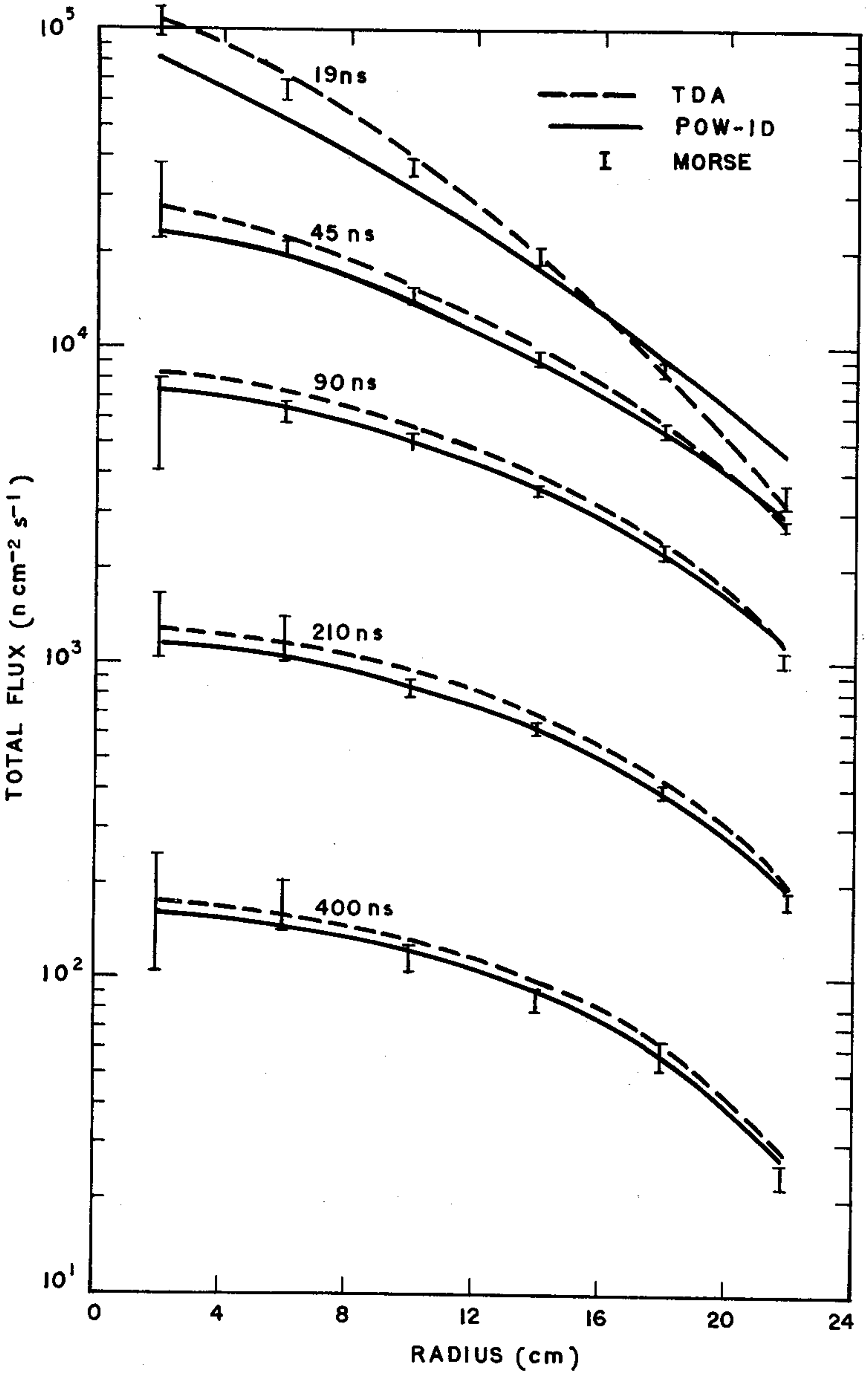

FIGURE 4. RADIAL VARIATION OF TOTAL FLUX IN PROBLEM 2

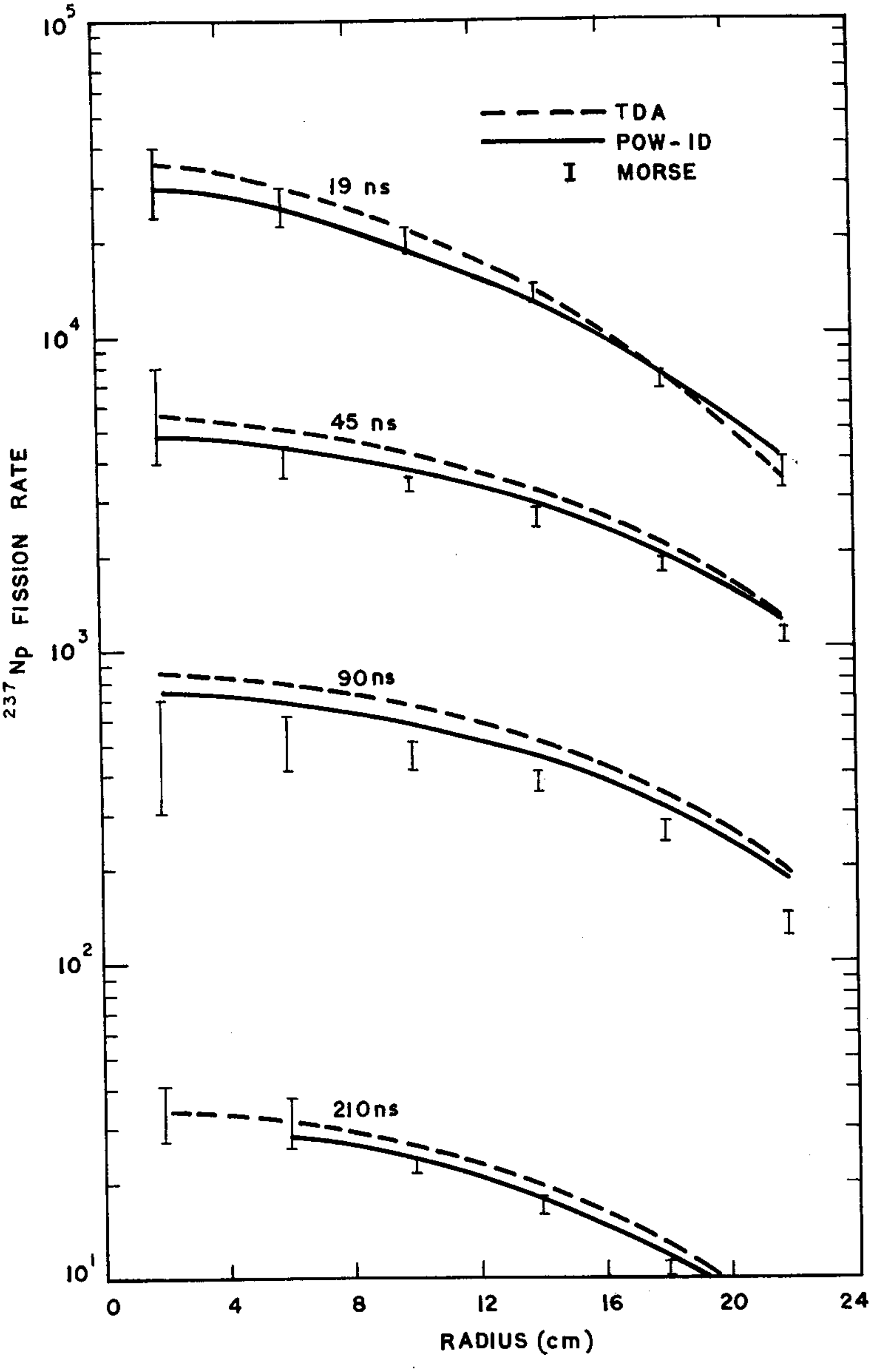

FIGURE 5. RADIAL VARIATION OF ^{237}Np FISSION RATE IN PROBLEM 2

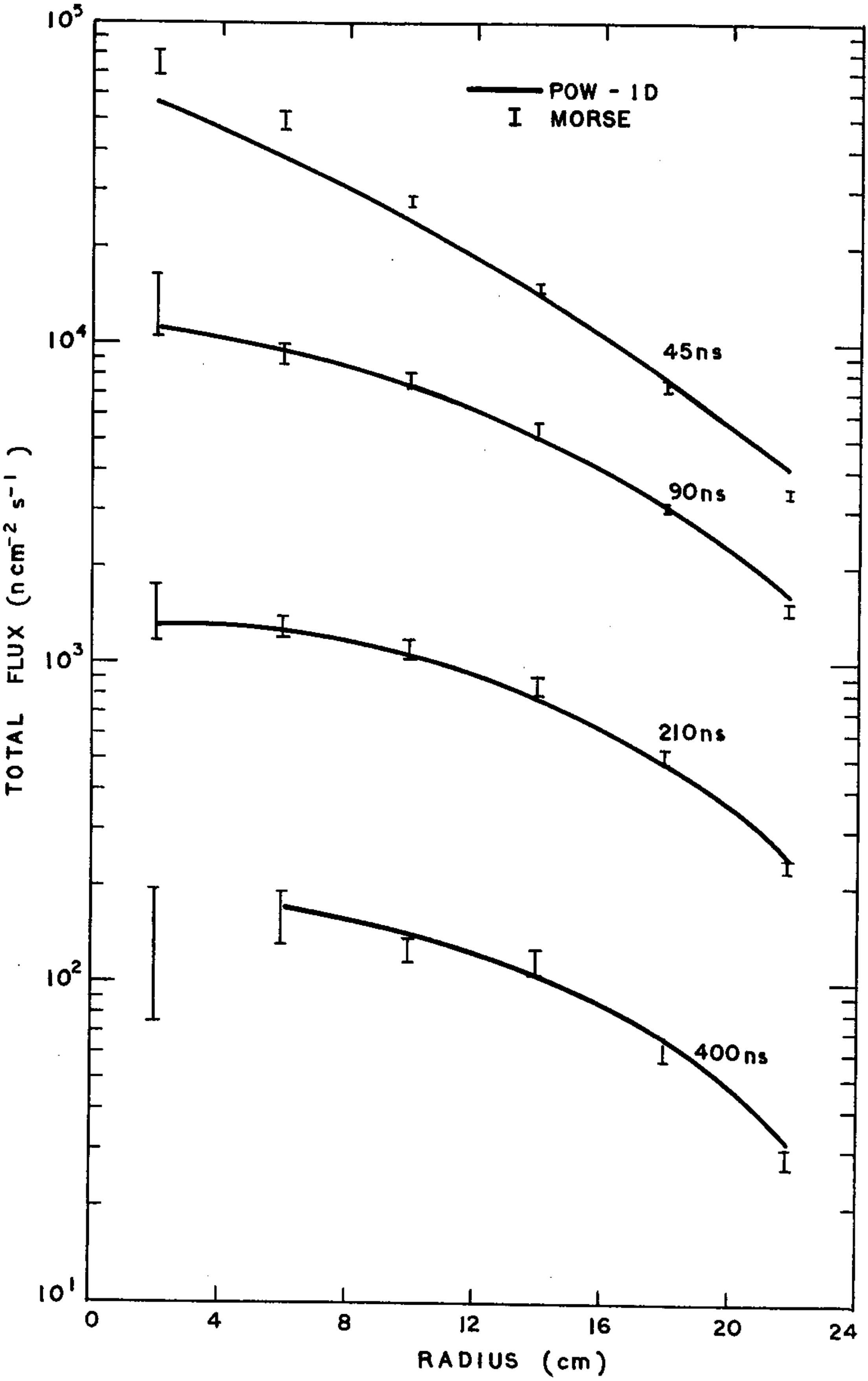

FIGURE 6. RADIAL VARIATION OF TOTAL FLUX IN PROBLEM 3

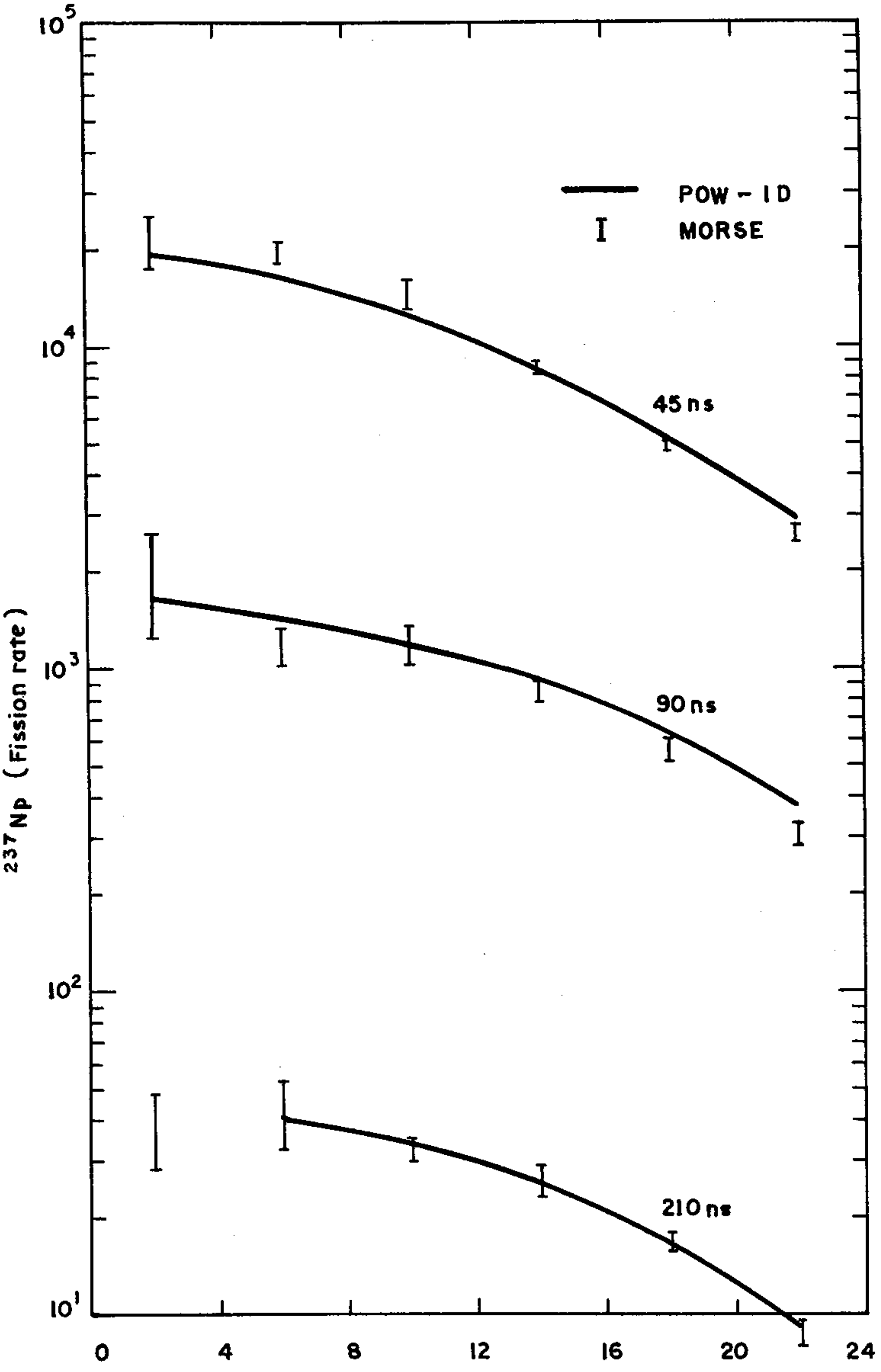

FIGURE 7. RADIAL VARIATION OF ^{237}Np FISSION RATE IN PROBLEM 3