AUSTRALIAN ATOMIC ENERGY COMMISSION

RESEARCH ESTABLISHMENT

LUCAS HEIGHTS

COMPARISON OF CALCULATIONS OF A REFLECTED REACTOR WITH DIFFUSION, SN AND MONTE CARLO CODES

by

B. McGREGOR

January 1975

ISBN 0 642 99673 3

AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS

COMPARISON OF CALCULATIONS OF A REFLECTED REACTOR WITH DIFFUSION, SN AND MONTE CARLO CODES

by

B. McGREGOR

ABSTRACT

A diffusion theory code, POW, was compared with a Monte Carlo transport theory code, KENO, for the calculation of a small C/^{235}U cylindrical core with a graphite reflector. The calculated multiplication factors were in good agreement but differences were noted in region-averaged group fluxes. A one-dimensional spherical geometry was devised to approximate cylindrical geometry. Differences similar to those already observed were noted when the region-averaged fluxes from a diffusion theory (POW) calculation were compared with an SN transport theory (ANAUSN) calculation for the spherical model. Calculations made with SN and Monte Carlo transport codes were in good agreement. It was concluded that observed flux differences were attributable to the POW code, and were not inconsistent with inherent diffusion theory approximations.

National Library of Australia card number and ISBN 0 642 99673 3

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.

CARBON; COMPARATIVE EVALUATIONS; K CODES; MOATA REACTOR; MONTE CARLO METHOD; MULTIGROUP THEORY; NEUTRON DIFFUSION EQUATION; NEUTRON FLUX; NEUTRONS; P CODES; URANIUM 235

CONTENTS

1. INTRODUCTION

As part of a program of checking out the ORNL Monte Carlo criticality code, KENO (Whitesides and Cross 1969), some calculations were performed with KENO on the first assembly mounted on the AAEC Critical Facility, a mockup of the Moata reactor. Comparisons were made with AUS scheme diffusion module POW (Pollard 1974) calculations of the assembly, using the same cross sections. The k calculated by KENO was ~1.5 per cent higher than that found by POW with a standard deviation of ~0.5 per cent. Region-averaged fluxes also disagreed by up to 5 per cent in either direction with standard deviations in KENO of 1 to 2 per cent.

The geometry of the Moata mockup assembly was complicated enough to prevent a judgement being made as to whether the differences could reasonably be attributed to the approximations of diffusion theory or whether one or both codes were in error. However the geometry of the second Critical Facility assembly studied was simpler,consisting of a central region of graphite with ^{235}U inserts surrounded by a graphite reflector region. This assembly, it was hoped, would enable observed differences between diffusion theory and Monte Carlo calculations to be attributed to either diffusion theory approximations or code deficiencies.

2. KENO-POW TWO-DIMENSIONAL COMPARISON

Comparison was made between KENO and a POW calculation with both calculations using the same 8-group cross section sets. The model calculated was a cylindrical fuelled region of radius 25.55 cm and height 80 cm, surrounded by a reflector region of radius 84.63 cm and height 160 cm. The C/^{235}U atomic ratio in the core was approximately 450/1. The KENO calculation followed 50,000 source fission neutrons in ~15 hours on an IBM360/50. The calculated k was 1.007 with a standard deviation of 0.004. The POW calculations used a mesh of ~2.5 cm in the core and ~5 cm in the reflector. The k calculated by POW was 1.003.

For this comparison the agreement in k was acceptable but there were still differences in region-averaged fluxes beyond the expected KENO statistics. Table 1 shows this comparison. Significant differences are evident in Group 1 in both core (POW low) and reflector (POW high). The ratios approach unity and go slightly beyond it as the group energy decreases. FSD is the fractional standard deviation of the KENO calculation.

3. POW-ANAUSN ONE-DIMENSIONAL COMPARISONS

To determine whether differences observed in the two-dimensional comparison were attributable to approximations of diffusion theory, another set of comparisons was made between POW and ANAUSN, an AUS module which performs one-dimensional S_n calculations. The geometry of this problem was spherical with a 35 cm radius core surrounded by an 82.675 cm radius reflector. This model was an attempt to approximate cylindrical geometry.

Equal numbers of mesh intervals were chosen in the core and reflector and three separate comparisons were made with 20, 40 and 80 intervals. For the ANAUSN calculations an S6 quadrature was used, though S4 would have been adequate. Table 2 shows calculated multiplication factors and ratios (POW-ANAUSN) of volume-averaged group fluxes in the core and reflector.

There is a striking similarity between the 40-mesh interval results in Table 2 and POW-KENO comparisons in Table 1, indicating that the one-dimensional spherical model produced similar average effects to those observed in the comparison of calculations of the two-dimensional finite cylinder.

Table 2 shows that as the number of mesh intervals increases, the ratio of fluxes calculated by the diffusion and transport codes moves toward unity but fails to converge to unity. The 80-mesh interval results show that in the core the average flux calculated by diffusion theory is ~3 per cent low at high energies. The ratio of diffusion to transport theory results steadily increases to ~1.01 at thermal energies. The position is reversed in the reflector where the average flux calculated by diffusion theory is high by ~4 per cent at high energies. The ratio steadily decreases till it becomes unity at thermal energies.

The diffusion theory calculation is also more affected by large mesh intervals as seen in Table 3 where coarse mesh results are compared with the corresponding 80-mesh interval results.

Figure 1 shows the radial variation of the 8-group fluxes calculated by POW with 40-mesh intervals.

While Table 2 illustrates the effects of using diffusion and transport theories on the average core and reflector fluxes, the local radial variation will not follow this average behaviour. Near the core-reflector boundary the differences between diffusion and transport theory are known to be marked. Figure 2 shows the radial variation of the ratio of POW to ANAUSN results with 40 mesh intervals for Groups 1, 3, 6 and 8.

At the centre the ratio of group fluxes is between 0.98 and 0.99 for all groups. Discontinuities in the ratio occur near the core-reflector interface in Groups 1 and 8. The ratio of fluxes in Group 1 changes from ~0.94 on the core side, to 1.07 on the reflector side of the interface, while the Group 8 ratio varies from ~1.04 to ~0.97 for corresponding positions. These variations would be compounded if a reaction rate ratio such as the fission rate in ^{238}U divided by the fission rate in ^{235}U were being calculated near the core/reflector interface. The POW result would be 10 per cent less than the ANAUSN result just inside the core.

4. KENO-ANAUSN ONE-DIMENSIONAL COMPARISON

To check that the differences observed in the initial POW-KENO comparisons could be conclusively attributed to a breakdown of the diffusion theory assumptions of POW, a comparison was made between KENO and ANAUSN for the spherical model. If both transport codes are correct and used properly, no differences should be observed other than those arising from statistical errors in the KENO calculation. The KENO calculation followed 30,000 source fission neutrons in six hours of computer time.

The calculated k was 0.9980 with a standard deviation of 0.0055 which compared well with the ANAUSN 80-mesh interval result of 0.9974. The ratios (KENO-ANAUSN) of core and reflector-averaged fluxes are given in Table 4. The agreement between the KENO and ANAUSN results is excellent.

5. CONCLUSIONS

This study shows that for the second assembly ($C/^{235}U$) the effects of using diffusion theory may be significant depending on which experiments are performed and analysed. If experimental information, *e.g.* space-dependent fission rate ratios, is to be compared with calculation, this type of diffusion-transport comparison can be used to obtain correction factors applicable to two-dimensional diffusion calculations. Alternatively two-dimensional transport calculations may be needed. Two-dimensional transport calculations were possibly necessary to treat accurately the first assembly on the Critical Facility.

Modular systems such as AUS, developed at the AAEC, make comparison calculations simpler to set up and perform. Without these it is difficult and tiresome to ensure that the two codes to be compared are performing exactly the same calculation. With the AUS scheme the problem is described to the module POW which prepares cross section and geometry libraries for use by later modules. The only data required for ANAUSN was a title card and a change of the standard SN option from 4 to 6. Of course, this ready comparison of different methods of calculation making possible choice of the optimum method for future similar applications, is one of the potential bonuses of a modular system. Considering the ease of duplicating the same problem for the two codes, there was some difficulty in comparing their output. Figure 2 was prepared from the flux printout from POW (edge flux) and ANAUSN (centre flux). This seemed simpler than reading the flux dump data sets. Improving this situation is made difficult by the need to define general edit facilities for inclusion in the systems which would handle this type of problem.

Some other benefits of this benchmark study were that the three codes KENO, POW and ANAUSN agreed when applied within their inherent approximations; that practice in these codes gives increased confidence and skill in their use; and that the methods and results possibly can be used to analyse experiments performed on the second assembly at the Critical Facility.

6. REFERENCES

Pollard, J.P. (1974) - AUS Module POW - A General Purpose 0,1 and 2D, Multigroup Neutron Diffusion Code Including Feedback - Free Kinetics. AAEC/E269.

Whitesides, G.E. & Cross N.F. (1969) - KENO - A Multigroup Monte Carlo Criticality Program. Computing Technology Center, Oak Ridge, Tenn., USA. CTC-5.

TABLE 1

COMPARISON OF KENO AND POW FLUXES FOR THE C/^{235}U ASSEMBLY

Group	Top Energy	Core-averaged Flux			Reflector-averaged Flux		
		KENO	FSD	POW-KENO	KENO	FSD	POW-KENO
1	10 MeV	1.77-4	0.007	0.964	6.58-6	0.008	1.047
2	302 keV	1.68-4	0.007	0.971	9.37-6	0.007	1.024
3	9.1 keV	1.24-4	0.008	0.973	1.02-5	0.007	1.021
4	275 eV	8.67-5	0.008	0.977	1.10-5	0.007	1.001
5	8.3 eV	5.02-5	0.008	0.987	1.00-5	0.006	1.003
6	0.41 eV	2.74-5	0.007	0.997	1.97-5	0.005	0.995
7	0.092 eV	2.25-5	0.008	1.011	3.51-5	0.006	0.997
8	0.034 eV	1.21-5	0.010	1.008	2.35-5	0.006	0.995

TABLE 2

(POW-ANAUSN) COMPARISON OF k AND FLUXES FOR THREE MESH SIZES

Mesh	20	40	80
k (POW)	1.00025	0.99619	0.99525
k (ANAUSN)	0.99862	0.99759	0.99738
Δk (POW-ANAUSN)	0.00163	-0.00140	-0.00213
Ratio (POW-ANAUSN) of Core-averaged Fluxes			
Group	20	40	80
1	0.951	0.967	0.971
2	0.966	0.978	0.980
3	0.975	0.982	0.984
4	0.983	0.987	0.988
5	0.990	0.991	0.991
6	0.993	0.996	0.997
7	1.024	1.011	1.008
8	1.034	1.017	1.013
Ratio (POW-ANAUSN) of Reflector-averaged Fluxes			
Group	20	40	80
1	1.065	1.047	1.043
2	1.025	1.022	1.021
3	1.010	1.013	1.014
4	1.002	1.009	1.011
5	0.995	1.006	1.009
6	0.979	0.996	1.001
7	0.974	0.994	0.999
8	0.973	0.993	0.998

TABLE 3

(COARSE/FINE) MESH RATIOS

Mesh	20	40
Δk (POW)	0.00500	0.00094
Δk (ANAUSN)	0.00124	0.00021

Core-averaged Fluxes

Mesh	20		40	
Group	POW	ANAUSN	POW	ANAUSN
1	0.980	1.001	0.996	1.000
2	0.987	1.001	0.997	1.000
3	0.992	1.001	0.998	1.000
4	0.996	1.001	0.999	1.000
5	1.000	1.002	1.000	1.000
6	0.997	1.001	0.999	1.000
7	1.017	1.001	1.003	1.000
8	1.022	1.001	1.004	1.000

Reflector-averaged Fluxes

Mesh	20		40	
Group	POW	ANAUSN	POW	ANAUSN
1	1.024	1.003	1.005	1.001
2	1.009	1.004	1.002	1.001
3	1.003	1.006	1.001	1.001
4	0.999	1.009	1.000	1.002
5	0.996	1.010	0.999	1.002
6	0.989	1.011	0.997	1.002
7	0.986	1.011	0.997	1.002
8	0.985	1.011	0.997	1.002

TABLE 4

RATIO (KENO-ANAUSN) OF FLUXES

	Core		Reflector	
Group	Ratio	KENO FSD	Ratio	KENO FSD
1	0.997	0.007	1.004	0.010
2	0.993	0.009	1.001	0.009
3	0.993	0.009	0.997	0.008
4	1.010	0.008	1.009	0.008
5	1.005	0.010	0.994	0.008
6	0.990	0.010	0.995	0.008
7	1.002	0.010	1.000	0.008
8	1.003	0.012	1.001	0.009

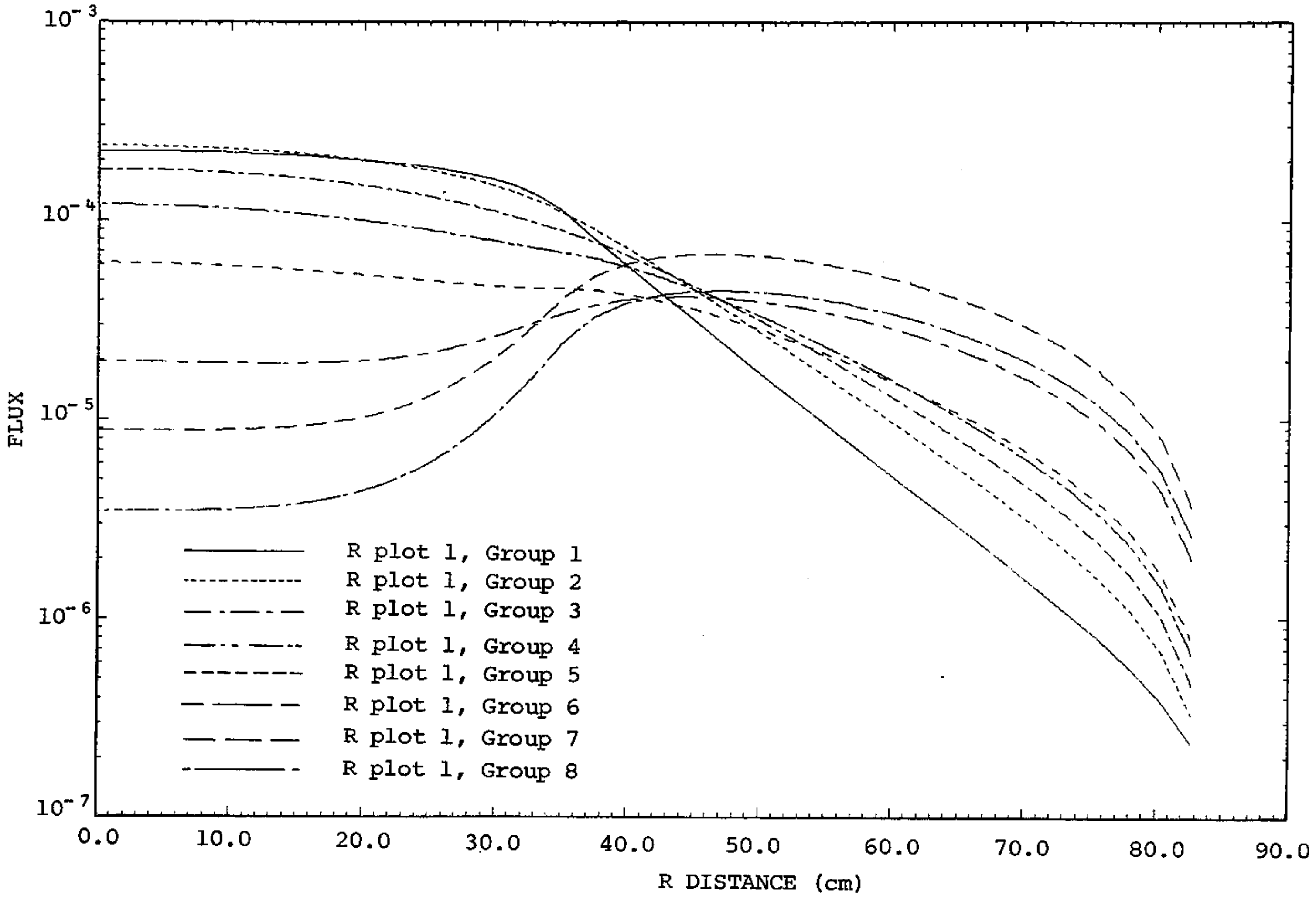

FIGURE 1. RADIAL VARIATION OF FLUXES FROM POW CALCULATION

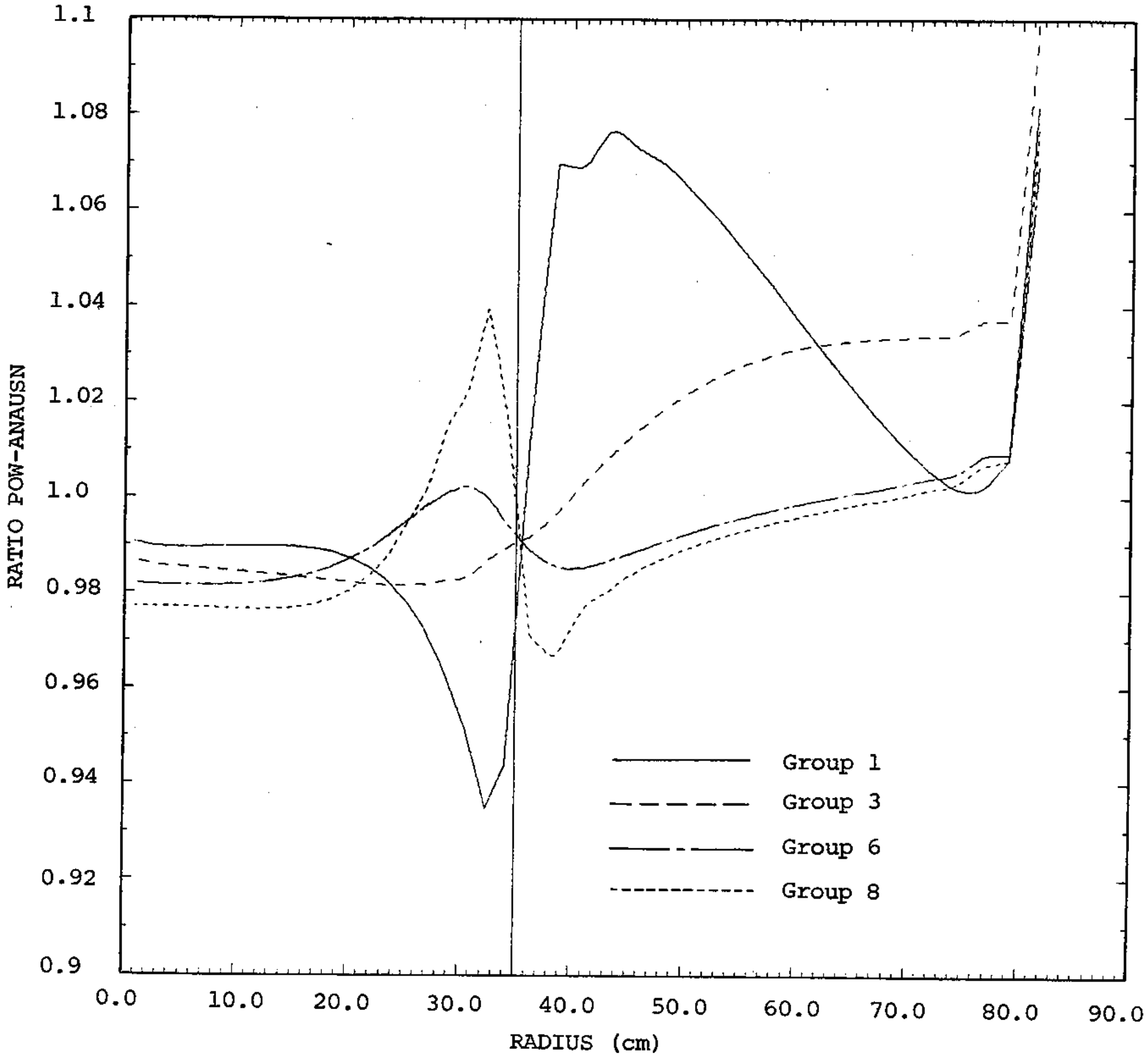

FIGURE 2. RADIAL VARIATION OF THE RATIO OF FLUXES (POW-ANAUSN)