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A COMPARISON OF NEUTRON RESONANCE ABSORPTION IN THERMAL
REACTOR LATTICES IN THE AUS NEUTRONICS CODE
SYSTEM WITH MONTE CARLO CALCULATIONS

by

G.S. ROBINSON

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ABSTRACT

The calculation of resonance shielding by the subgroup method, as incorporated in the MIRANDA module of the AUS neutronics code system, is compared with Monte Carlo calculations for a number of thermal reactor lattices. For the large range of single rod and rod cluster lattices considered, AUS results for resonance absorption were high by up to two per cent.

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NEUTRONS; RESONANCE ABSORPTION; REACTOR LATTICES; FUEL RODS; FUEL ELEMENT CLUSTERS; MODERATORS; WATER; GRAPHITE; M CODES; MATHEMATICAL MODELS; TOTAL CROSS SECTIONS; MONTE CARLO METHOD; HIFAR REACTOR

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1. INTRODUCTION

The AUS neutronics code [Robinson 1975] is a modular system developed for calculations of all types of fission reactor from fast to thermal. The MIRANDA module [Robinson 1977] is used to obtain resonance shielded cross sections by the subgroup method. The subgroup parameters included in a group cross-section library are acquired by fitting them to resonance integrals obtained from numerical solution of the neutron slowing-down equations for mixtures of the resonance nuclide and hydrogen. Subgroup fluxes are calculated by the collision probability method for which the approximate routines of Robinson [1979], based on the work of Bonalumi [1961, 1965], are normally used. A variant of the λ method is used to establish an equivalence between scattering by nuclides of different atomic mass.

The initial validation of the MIRANDA treatment performed by Robinson [1977] was limited to comparisons with the PEARLS code [Chiarella 1971] for homogeneous and simple two-region calculations. PEARLS numerically solves the collision probability formulation of the neutron slowing-down equations with isotropic scattering. The agreement obtained for the cases studied, which included some extreme situations with rod diameters up to 80 mm, was mostly within one per cent. Because the same two-region spatial representation was used in PEARLS and AUS, the comparison provided a validation of the MIRANDA treatment of the energy variable but left some doubt about the spatial representation. There have been only minor modifications to the MIRANDA resonance treatment in the intervening period, hence the comparison is still valid.

This study compares the results using MIRANDA with those obtained with the MCRP Monte Carlo code [Doherty and Robinson 1985]. The major assumption made in MCRP is that scattering is elastic and isotropic in the centre of mass system. The code calculates resonance absorption for neutrons slowing down from an upper energy limit (normally 19.3 keV) with the assumption that the flux is spatially flat and varies as $1/E$ above that limit. The same assumptions have been made in AUS when making the comparison with MCRP. In essence, the AUS calculations are being compared with a method which is exact for the given cross-section data.

2. CROSS SECTIONS AND GROUP STRUCTURE

As part of a recent modification to the cross sections available as an AUS library [Robinson 1984], new point cross-section data sets have been generated for ^{235}U and ^{238}U . These data give the cross section at 124 000 points below 19.3 keV in the structure specified by Chiarella [1971]. The data are used in MCRP and PEARLS, and in generating subgroup parameters for AUS, so they enable direct checks between the three methods. Data for ^{235}U and ^{238}U are available at Lucas Heights at temperatures of 300, 900 and 2100 K as the data sets named GSR.POINTXS.xxxxtttt where xxxx is the nuclide name and tttt is the temperature. The data have been generated from ENDF/B-IV [Garber 1975] using methods outlined by Robinson [1977, 1984]. This comparison has been performed for a temperature of 300 K, except where otherwise stated.

For moderator and can nuclides, constant scattering and zero absorption cross sections have been assumed in the comparison. The scattering cross sections used for H, D, C, O, Al, Zr were 20.2, 3.4, 4.7, 3.8, 1.4 and 6.4 barns, respectively. A slightly incorrect atomic mass for D of 2.02472 was required in the PEARLS code to simplify the treatment of the large collision range for D. This value has been retained throughout the comparisons.

Two group cross-section libraries with different group structures are currently in use with the AUS system. The original 128-group library AUS.ENDFB has groups of 0.25 lethargy width from 19.3 keV to 10.7 eV and groups of 0.1 lethargy width below 9.19 eV. The more recent 200-group library AUS.ENDF200G has groups of 0.125 lethargy width from 19.3 to 1.234 keV, 0.25 lethargy width from 1.234 keV to 3.059 eV, and 0.1 lethargy width below that. The extra groups in the keV range were added to give greater accuracy in fast reactor and fusion blanket studies. The change in the group structure between 10 and 3 eV was made to reduce the splitting of the important ^{238}U , 6.67 eV resonance into many groups.

The present comparison has been made in terms of the AUS.ENDF200G group structure. The difference in total ^{238}U resonance captures due to the change in group structure between 10 and 3 eV is typically zero to half a per cent for single rods but is as large as one per cent for some rod clusters. The AUS.ENDF200G group structure gives the larger result. The difference in total resonance captures is small, and the AUS.ENDF200G structure has been preferred because this gives a greater consistency in the treatment of the 6.67 eV resonance compared with that of other resonances.

A special AUS library covering the energy range 19.3 keV to 1 eV, which is consistent with the MCRP treatment of scattering, has been used in the comparison. Anisotropy of scattering in the laboratory system was represented by a P_1 expansion.

3. OUTLINE OF AUS CALCULATIONS

The three AUS modules used in these calculations were MIRANDA, the one-dimensional discrete ordinate module ANAUSN [Clancy 1982], and the collision probability module ICPP. The resonance subgroup calculation in MIRANDA assumes an asymptotic source for each group and derives shielded cross sections from the calculated resonance integrals.

One of the changes to the original MIRANDA module has been the replacement of the collision probability routines by the routines of Robinson [1979]. Although, for single rod calculations, the results from both sets of routines are practically identical, the new routines provide a treatment of square and hexagonal boundaries to the lattice. The numerical routine of Doherty [1969] for cylindrical cells with a white boundary condition has also been included. This was used for calculations in which a fine spatial mesh was used in the subgroup calculation. The group condensation feature of MIRANDA was not used, because a 'best' AUS result was required for the comparison.

The resonance shielded cross sections from MIRANDA were passed to the transport theory modules in which the multigroup flux distribution for neutrons slowing down from an asymptotic source above 19.3 keV was calculated. The ICPP module includes the same collision probability routines as MIRANDA as well as other numerical routines of Doherty [1969]. All results have been normalised to an asymptotic source of 1 neutron s^{-1} .

4. DETAILED STUDY OF TWO SIMPLE LATTICES

4.1 Introduction

Two of the simple two-region lattices used in the 1977 comparison between AUS and PEARLS have been chosen for a detailed study in which the options that may be used in AUS resonance calculations have been investigated. The method which has become standard in AUS is to use only one mesh interval in each discrete material in the MIRANDA resonance calculation. The effect of a finer spatial mesh is the main consideration here. The comparison with PEARLS has also been repeated for the data used in the present study. The two lattices considered are a 10 mm diameter ^{238}U oxide rod in water and a 20 mm diameter ^{238}U metal rod in graphite.

4.2 Uranium-238 Oxide Rod in Water

The specifications for this lattice are a 10 mm diameter rod, a volume ratio of moderator to fuel of unity, and densities for ^{238}U , O and H_2O of 0.0223, 0.0446 and 0.0335×10^{24} atoms cm^{-3} , respectively. The results for a circular outer boundary are given in table 1.

In all tables comparing resonance reactions per source neutron, the MCRP results are given with percentage standard deviations and other results are given as the percentage difference from MCRP. Table 1 includes a breakdown into a number of energy groups. This detail has been included to show the extent to which the agreement in total resonance absorptions is the result of cancellation of errors and to compare the accuracy for broad resonances at low energy with that for the narrow resonances at high energy.

There is only a 0.9 ± 0.3 per cent difference between a two-region PEARLS calculation and MCRP, which demonstrates that the assumption of a flat source distribution in each of the fuel and moderator is quite reasonable in this tight lattice. The first AUS case makes the same assumptions as PEARLS and shows that the -0.6 per cent difference between AUS and PEARLS in the 1977 comparison has reduced to a -0.1 per cent difference, mainly as a result of the changed group structure.

AUS cases 2 and 3 represent the normal AUS method. For this study a higher order S_n approximation and a larger number (14) of mesh points than usual have been used to ensure a 'best' solution. This policy is adopted throughout the report. It can be seen that the spatial subdivision and P_0 to P_1 effects are very small.

TABLE 1
²³⁸U OXIDE ROD IN H₂O
 MODERATOR/FUEL VOLUME RATIO = 1, CIRCULAR BOUNDARY

Energy Range	MCRP		Percentage Error compared to MCRP					
	Captures	% Error	PEARLS	AUS				
				1	2	3	4	5
19.3-5.5 keV	0.01263	± 0.5	0.2	0.2	0.2	0.3	0.3	0.3
5.5-0.45 keV	0.03856	± 0.3	0.4	0.5	0.6	0.6	0.4	0.4
450-130 eV	0.02365	± 0.7	1.0	1.6	1.6	1.7	-1.1	0.1
130-10.7 eV	0.09966	± 0.4	1.4	0.9	1.1	1.2	-2.8	-1.3
10.7-1 eV	0.08057	± 0.5	0.8	0.7	0.9	1.1	0.7	1.2
Total	0.25507	± 0.3	0.9	0.8	1.0	1.1	-0.9	0.0

- AUS Cases: (1) Two-region MIRANDA and ICPP.
 (2) Two-region MIRANDA, multi-region S₈ P₀ ANAUSN.
 (3) As for (2) but P₁.
 (4) Multi-region MIRANDA and ICPP.
 (5) As for (4) but λ not mesh-dependent.

AUS cases 4 and 5 are for eight-region calculations using the numeric collision probability routines in MIRANDA and ICPP. The approximate method was unsatisfactory for this study as continual mesh refinements caused increasing errors. Very fine mesh intervals (the smallest being 0.0625 mm) were used near the surface of the rod. It was necessary to pass shielded group cross sections which were dependent on mesh interval to ICPP to avoid introducing an error of the same order as the actual effect. Case 4 uses the original MIRANDA method in which the value of λ varies with mesh interval because of the dependence of λ on an effective σ_p for each mesh. This clearly overestimates the effect of spatial subdivision. Case 5 includes a minor modification in which the average value of λ is used for all the fuel. This option appears to be more appropriate to spatial subdivision of a fuel rod.

TABLE 2
²³⁸U OXIDE ROD IN H₂O
 MODERATOR/FUEL VOLUME RATIO = 1, SQUARE BOUNDARY

Energy Range	MCRP		AUS Percentage Error	
	Captures	% Error	1	2
19.3-5.5 keV	0.01262	± 0.6	-0.1	0.1
5.5-0.45 keV	0.03821	± 0.6	0.2	0.4
450-130 eV	0.02317	± 0.9	1.8	2.2
130-10.7 eV	0.09920	± 0.5	-0.7	0.4
10.7-1 eV	0.07922	± 0.5	0.4	1.9
Total	0.25242	± 0.2	0.0	1.0

- AUS Cases: (1) Two-region MIRANDA and ICPP.
 (2) Two-region MIRANDA, multi-region S₈ P₁ ANAUSN.

An investigation of the same lattice with a square boundary condition is given in table 2. Only two AUS cases are given. The first is a two-region calculation using approximate collision probabilities with a square boundary. The second uses the same method in MIRANDA but follows this with an ANAUSN calculation with a circular white boundary. Calculations with numerical collision probabilities in ICPP gave a 0.7 per cent difference between a square boundary and a white circular boundary at the multigroup level compared to the one per cent difference between the two AUS cases given in table 2. The difference between using approximate and numerical probabilities in ICPP was only 0.1 per cent. However, the difference between the two MCRP cases gives a one per cent effect due to the boundary change compared with the difference between the two AUS two-region cases of 1.8 per cent. The discrepancy is well outside the statistics of the MCRP results.

TABLE 3
COMPARISON OF SUBGROUP FLUXES

Case	Boundary	Percentage Diff. from Circ. Subgroup 4	Percentage Error in Flux Compared to Numerical P_{ij}			
			Subgroup 1	Subgroup 2	Subgroup 3	Subgroup 4
UO ₂ /H ₂ O Vol. ratio = 1	circ.	-	-0.02	0.02	-0.10	-0.11
UO ₂ /H ₂ O Vol. ratio = 1	square	-2.85	-0.08	-0.44	-0.54	-0.55
UO ₂ /H ₂ O Vol. ratio = 2	square	-1.64	-0.03	-0.11	-0.15	-0.17
TRX1	hex.	+0.38	-0.02	0.19	0.36	0.38
MIT1	hex.	-0.06	0.00	0.04	0.05	0.05
PWR	square	-2.10	-0.03	-0.04	0.52	0.48

NOTES: Subgroups correspond to ²³⁸U resonance total cross section of 2.4, 40, 640 and 10 240 barns. For the first case, numerical P_{ij} with a white boundary condition overestimates the subgroup fluxes by 0.01, 0.21, 0.68 and 0.62 per cent for groups 1 to 4 compared to a 128-mesh interval, S_{32} calculation.

A further investigation of the discrepancy has been made by a comparison of subgroup fluxes given in table 3. This table gives the errors in subgroup fluxes from the approximate collision probability method relative to numerical probability results for the narrow resonance subgroup equations for a number of lattices. The first two results show a 0.4 per cent difference between the errors for the two boundary conditions at high cross sections. The resulting error in total resonance captures would be considerably smaller. A further source of error comes from using a white boundary condition on circular boundaries in the collision probability calculations. The circular boundary condition in MCRP and ANAUSN assumes an isotropic boundary flux distribution for each polar angle rather than the completely isotropic flux in the collision probability method. The difference is about 0.6 per cent in subgroup flux for large cross sections in this tight lattice. The combination of these two errors is sufficient to account for the discrepancy.

4.3 Uranium-238 Metal Rod in Graphite

The specifications for this lattice are a 20 mm diameter rod, a moderator diameter of 160 mm, and densities for ²³⁸U and C of 0.04749 and 0.0803 x 10²⁴ atoms cm⁻³, respectively. The results obtained are given in table 4. For this lattice there is a greater effect due to spatial subdivision as illustrated by the 3.2 ± 0.4 per cent difference between a two-region PEARLS and an MCRP calculation.

TABLE 4
²³⁸U METAL ROD IN GRAPHITE

Energy Range	MCRP		Percentage Error Compared to MCRP					
	Captures	% Error	PEARLS	1	2	AUS 3	4	5
19.3 - 5.5 keV	0.00882	± 0.8	1.2	2.0	1.1	1.2	1.1	1.1
5.5 - 0.45 keV	0.02218	± 0.8	2.3	3.5	2.0	2.1	1.4	1.6
450 - 130 eV	0.01217	± 1.2	2.5	3.1	1.5	1.6	-2.7	-0.4
130 - 10.7 eV	0.04654	± 0.9	4.9	4.8	1.3	1.8	-3.0	-0.6
10.7 - 1 eV	0.04173	± 0.7	2.5	2.8	-1.9	-1.3	-1.4	-1.1
Total	0.13144	± 0.4	3.2	3.6	0.4	0.8	-1.5	-0.2

- AUS Cases: (1) Two-region MIRANDA and ICPP.
 (2) Two-region MIRANDA, multi-region $S_8 P_0$ ANAUSN.
 (3) As for (2) but P_1 .
 (4) Multi-region MIRANDA, multi-region $S_8 P_1$ ANAUSN.
 (5) As for (4) but λ not mesh-dependent.

The first AUS case is consistent with the PEARLS case and shows that the +0.3 per cent difference between AUS and PEARLS in the 1977 comparison is practically unaltered. The normal AUS cases (2 and 3) performed with 22-interval ANAUSN calculations were in reasonable agreement with MCRP and showed some effect from the use of a P_1 scattering expansion in this lattice. AUS cases 4 and 5 were performed with a 16-region MIRANDA using numerical collision probabilities followed by a 22-region ANAUSN calculation. The use of a region dependent λ in case 4 clearly overestimates the effect of spatial subdivision, while the use of an average λ in case 5 yields obviously better results.

4.4 Discussion

For these two cases, the normal AUS method overestimates resonance captures by about one per cent. If spatial subdivision is to be used in the resonance calculation, the average λ option should be used. However, mesh-dependent cross sections must be passed to the multigroup transport calculation by MIRANDA. As this procedure would make practical calculations rather complicated, and also considerably increase the required computer time, the use of spatial subdivision to effect only a one per cent reduction in resonance captures is not recommended.

The remaining comparisons were performed with, at most, one mesh interval in each discrete region in the MIRANDA resonance calculation. The comparisons have also used square or hexagonal boundary conditions in the MIRANDA subgroup calculations where appropriate, but ANAUSN with a circular white boundary condition was used for the multigroup transport calculation.

5. RESULTS FOR SINGLE ROD LATTICES

5.1 An Additional Uranium-238 Oxide Rod in Water

This lattice is identical to that described in section 4.2 except that the moderator to fuel volume ratio is 2. A circular white boundary has been used. The results are given in table 5. The difference between AUS and MCRP of 0.6 ± 0.5 per cent compares with 1.1 ± 0.3 per cent for the tighter lattice. These two lattices span the normal range of moderator to fuel ratio for 10 mm diameter oxide rods in water. The remaining lattices to be considered are practical cases.

TABLE 5
 ^{238}U OXIDE ROD IN H_2O
 MODERATOR/FUEL VOLUME = 2.

Energy Range	MCRP		AUS
	Captures	% Error	% Error
19.3-5.5 keV	0.00648	± 0.8	0.6
5.5-0.45 keV	0.02084	± 0.8	1.3
450-130 eV	0.01338	± 1.3	1.7
130-10.7 eV	0.05935	± 0.8	0.5
10.7-1 eV	0.05100	± 0.8	0.2
Total	0.15105	± 0.5	0.6

5.2 A Typical PWR

This case represents a typical pressurised water reactor (PWR) lattice with a 3.3 per cent enriched UO_2 rod. The precise specifications for this lattice are 8.19 mm diameter fuel, a can of outside diameter 9.5 mm and thickness 0.57 mm, a square lattice with a pitch of 12.6 mm, a temperature of 900 K and densities for ^{235}U , ^{238}U , O, Zr and H_2O of 0.000755, 0.0222, 0.045924, 0.04325 and $0.02387 (\times 10^{24} \text{ atoms cm}^{-3})$, respectively. The can and void were smeared together in the MIRANDA subgroup calculation.

The results are given in table 6 for captures in ^{238}U and both absorptions and fissions in ^{235}U . The results for ^{238}U are marginally worse than those for the simpler lattices, and results for ^{235}U are reasonable.

The largest error for ^{235}U occurs in the energy range between 10 and 1 eV and is due to an underestimate of the shielding of the 6.4 eV resonance by the 6.67 eV ^{238}U resonance. The resonance overlap treatment in MIRANDA takes no account of resonance position within a group and can only be expected to give reasonable results on average. Any individual resonance may have an associated large error when the overlap effects are large.

TABLE 6
A TYPICAL PRESSURISED WATER REACTOR

Energy Range	²³⁸ U Captures			²³⁵ U Absorptions			²³⁵ U Fissions		
	MCRP		AUS	MCRP		AUS	MCRP		AUS
	Result	% Error	% Error	Result	% Error	% Error	Result	% Error	% Error
19.3-5.5 keV	0.01099	± 0.8	0.1	0.00227	± 0.6	0.0	0.00160	± 0.6	0.0
5.5-0.45 keV	0.03858	± 0.8	0.3	0.01128	± 0.5	0.4	0.00806	± 0.5	0.8
450-130 eV	0.02522	± 0.9	0.6	0.01304	± 0.8	1.5	0.00880	± 0.7	1.6
130-10.7 eV	0.08837	± 0.7	1.7	0.05199	± 0.5	2.0	0.03195	± 0.5	1.5
10.7-1 eV	0.06517	± 0.7	1.9	0.03094	± 0.6	5.1	0.02069	± 0.6	2.5
Total	0.22834	± 0.3	1.3	0.10952	± 0.3	2.6	0.07110	± 0.3	1.7

5.3 The TRX1 Benchmark Lattice

The TRX1 lattice is one of the thermal reactor lattice experiments chosen as a benchmark [NNDC 1974] by the Cross Section Evaluation Working Group (CSEWG). TRX1 is a 1.3 per cent enriched uranium metal rod of 10 mm diameter on a triangular pitch of 18 mm. The rod is clad in Al and has water as a moderator. The benchmark specifications [NNDC 1974] have been used for the comparison. The results given in table 7 are similar to those for the PWR calculation.

TABLE 7
TRX1 — METAL ROD IN H₂O

Energy Range	²³⁸ U Captures			²³⁵ U Absorptions			²³⁵ U Fissions		
	MCRP		AUS	MCRP		AUS	MCRP		AUS
	Result	% Error	% Error	Result	% Error	% Error	Result	% Error	% Error
19.3-5.5 keV	0.01098	± 0.8	0.8	0.000962	± 0.6	0.2	0.000679	± 0.6	0.3
5.5-0.45 keV	0.03006	± 0.6	0.8	0.004821	± 0.5	0.5	0.003448	± 0.6	0.9
450-130 eV	0.01673	± 0.8	2.9	0.005644	± 1.1	2.4	0.003793	± 1.1	2.9
130-10.7 eV	0.06693	± 0.6	2.2	0.023775	± 0.7	1.0	0.014630	± 0.7	0.3
10.7-1 eV	0.05663	± 0.7	1.3	0.015095	± 0.7	4.4	0.010210	± 0.9	1.2
Total	0.18133	± 0.4	1.7	0.050300	± 0.3	2.1	0.032760	± 0.3	0.9

The comparison of subgroup fluxes (table 3) for these cases gives some insight into the slight variations in the AUS errors for the various cases. There is a tendency for the application of the boundary condition for square and hexagonal lattices (which was derived for two-region fuel/moderator lattices) to cause an overestimate of subgroup fluxes for rods with cans compared to those without cans.

5.4 The MITI Benchmark Lattice

MITI is another of the CSEWG benchmarks. The 25.65 mm diameter natural uranium metal rod is clad in Al and moderated by D₂O. The triangular lattice pitch is 114.3 mm. The results given in table 8 are similar to the TRX1 results for ²³⁸U captures and are slightly better for ²³⁵U reactions.

TABLE 8
MITI — METAL ROD IN D₂O

Energy Range	²³⁸ U Captures			²³⁵ U Absorption			²³⁵ U Fissions		
	MCRP		AUS	MCRP		AUS	MCRP		AUS
	Result	% Error	% Error	Result	% Error	% Error	Result	% Error	% Error
19.3-5.5 keV	0.00847	± 0.7	2.4	0.000428	± 0.9	1.9	0.000302	± 0.9	2.0
5.5-0.45 keV	0.02082	± 0.7	2.5	0.002157	± 0.7	1.6	0.001543	± 0.7	1.9
450-130 eV	0.01137	± 1.1	-0.3	0.002623	± 1.3	-0.4	0.001766	± 1.3	-0.1
130-10.7 eV	0.04010	± 1.0	2.4	0.010970	± 1.0	-2.0	0.006680	± 0.9	-1.7
10.7-1 eV	0.03570	± 0.9	0.5	0.006990	± 1.2	5.6	0.004810	± 1.3	1.5
Total	0.11646	± 0.5	1.6	0.023170	± 0.6	0.9	0.015100	± 0.6	0.0

6. RESULTS FOR ROD CLUSTER LATTICES

6.1 Clusters with 7, 19 and 36 Rods

The three cluster lattices considered by Robinson [1979] have been used for comparisons of ^{238}U captures. All the clusters are UO_2 rods clad in Al and moderated by D_2O . The 7-rod and 19-rod clusters are cooled by D_2O and both water and voided coolant have been used for the 36-rod cluster. The specifications of the 1979 work have been followed except that the ^{235}U was replaced by ^{238}U . These specifications included coolant subdivisions and, for the 36-rod cluster, a ring smearing model in which an S_n calculation with smeared cross sections followed the synthetic collision probability calculation. An S_8P_1 calculation was used for the smeared calculation.

TABLE 9
CLUSTERS WITH 7, 19 AND 36 RODS
 ^{238}U CAPTURES BY RING

Ring	7-Rod			19-Rod			36-Rod H_2O			36-Rod Voided		
	MCRP Result	% Error	AUS % Error	MCRP Result	% Error	AUS % Error	MCRP Result	% Error	AUS % Error	MCRP Result	% Error	AUS % Error
1	0.01353	± 1.0	4.6	0.00566	± 1.6	1.3	0.02086	± 1.4	1.2	0.02717	± 1.0	0.6
2	0.10270	± 0.6	-0.3	0.03533	± 0.9	1.5	0.04210	± 0.8	-0.6	0.05309	± 0.8	3.0
3				0.08839	± 0.5	0.7	0.06816	± 0.7	0.8	0.10511	± 0.5	-0.5
Total	0.11622	± 0.5	0.2	0.12938	± 0.5	1.0	0.13112	± 0.4	0.4	0.18537	± 0.3	0.7

The results for ^{238}U resonance captures by ring are given in table 9. They are good for total captures but show some deterioration for the distribution in each ring. As is to be expected, the ring distributions reflect the distributions for subgroup flux depression reported by Robinson [1979]. The change in resonance captures when the water coolant is voided in the 36-rod cluster is particularly well calculated.

6.2 Cluster with 28 Rods

Comparisons of ^{238}U and ^{235}U reactions have been made for a 28-rod natural UO_2 cluster, cooled and moderated by D_2O for which buckling measurements were reported by Serdula [1966]. The specifications of Serdula were followed with the exception that Al was used instead of the Zr cladding. The lattice pitch was 240 mm triangular. In the AUS calculation, artificial coolant boundaries were placed at radii of 19.005, 32.921 and 50.286 mm for the synthetic collision probability routine. The results obtained including a breakdown in energy groups are given in table 10. These results are very similar to the single rod cases.

TABLE 10
CLUSTER WITH 28 RODS

Energy Range	^{238}U Captures			^{235}U Absorptions			^{235}U Fissions		
	MCRP	AUS		MCRP	AUS		MCRP	AUS	
	Result	% Error	% Error	Result	% Error	% Error	Result	% Error	% Error
19.3-5.5 keV	0.01027	± 0.9	0.2	0.000491	± 0.7	0.5	0.000347	± 0.7	0.5
5.5-0.45 keV	0.02755	± 0.8	0.0	0.002386	± 0.9	1.4	0.001706	± 1.0	1.8
450-10.7 eV	0.07347	± 0.6	1.5	0.014240	± 0.5	1.8	0.008880	± 0.5	1.6
10.7-1 eV	0.04508	± 0.7	0.4	0.007310	± 0.8	4.6	0.005010	± 0.8	1.2
Total	0.15638	± 0.4	0.8	0.024420	± 0.4	2.6	0.015940	± 0.4	1.5

7. RESULTS FOR HIFAR ANNULAR GEOMETRY

The AAEC research reactor HIFAR is a DIDO class D_2O moderated reactor. The specifications for the annular fuel geometry have been taken from Harrington [1983] but 20 per cent enriched fuel has been used instead of the standard 80 per cent enrichment. The possible conversion of research reactors to 20 per cent enriched fuel has promoted some interest in resonance captures in this type of annular fuel element. In this

comparison, the densities for ^{235}U , ^{238}U , O and Al were 0.0014943, 0.0059016, 0.019722 and 0.023616×10^{24} atoms cm^{-3} , respectively.

The normal AUS method for HIFAR calculations, in which the resonance subgroup calculation is performed in nine regions with the fuelled section of each of the four fuel tubes represented explicitly, has been followed. The results are given in table 11. The agreement is better than is strictly necessary for a research reactor with some uncertainty in neutron spectrum.

TABLE 11
HIFAR WITH 20 PER CENT ENRICHMENT

Energy Range	^{238}U Captures			^{235}U Absorptions			^{235}U Fissions		
	MCRP		AUS	MCRP		AUS	MCRP		AUS
	Result	% Error	% Error	Result	% Error	% Error	Result	% Error	% Error
19.3-5.5 keV	0.000623	± 1.4	1.1	0.000920	± 1.2	1.2	0.000648	± 1.2	1.5
5.5-0.45 keV	0.003186	± 1.3	0.5	0.004785	± 1.3	0.5	0.003422	± 1.3	0.8
450-10.7 eV	0.024990	± 1.0	1.8	0.032620	± 0.8	1.2	0.020250	± 0.8	1.2
10.7-1 eV	0.019980	± 1.7	3.0	0.018210	± 1.1	1.0	0.011710	± 1.1	1.3
Total	0.048780	± 1.0	2.2	0.056530	± 0.6	1.1	0.036040	± 0.6	1.2

8. CONCLUSIONS

Calculations of resonance absorption using the AUS neutronics code system have been compared with the MCRP Monte Carlo code using cross sections derived from ENDF/B-IV. The comparison has been made for a large range of thermal reactor lattices with uranium fuel in the form of single rods and rod clusters. The calculations were done for resonance reactions in the energy range 19.3 keV to 1 eV for neutrons slowing down by elastic scattering from an asymptotic source above that range.

Using the normal AUS method, in which the resonance subgroup calculation is performed with one mesh interval in each discrete region, the difference between AUS and MCRP ranged from 0.2 ± 0.5 to 1.7 ± 0.4 per cent for ^{238}U captures. The comparison of ^{235}U absorptions was somewhat worse with a range from 0.9 ± 0.6 to 2.6 ± 0.3 per cent. The deterioration was due largely to resonance overlap effects near an energy of 6.5 eV. The agreement for ^{235}U fissions was one per cent better than that for absorptions.

An investigation of the effect of spatial subdivision in the AUS resonance subgroup calculation for two simple lattices showed that a one per cent decrease in resonance captures in ^{238}U was achieved. However, the large increase in the complexity of practical calculations for this small improvement does not warrant the adoption of this method.

9. REFERENCES

- Bonalumi, R.A. [1961] - Neutron first collision probabilities in reactor physics. *Energ. Nucl. (Milan)*, 8:326.
- Bonalumi, R.A. [1965] - Systematic approximations in neutron first collision probabilities. *Energ. Nucl. (Milan)*, 12:1.
- Chiarella, C. [1971] - PEARLS - a code for the solution of the neutron slowing down equations in multiregion lattices of resonance absorbers. AAEC/E213.
- Clancy, B.E. [1982] - ANAUSN - a one-dimensional multigroup SN transport theory module for the AUS reactor neutronics system. AAEC/E539.
- Doherty, G. [1969] - Some methods of calculating first flight collision probabilities in slab and cylindrical lattices. AAEC/TM489.
- Doherty, G., Robinson, G.S. [1985] - MCRP - a Monte Carlo resonance program for neutrons slowing down in single rod and rod cluster lattices. AAEC/E618.
- Garber, D. [1975] - ENDF/B summary documentation. ENDF-201.
- Harrington, B.V. [1983] - Neutronic models for the HIFAR reactor. AAEC/E571.

- NNDC [1974] - Cross Section Evaluation Working Group benchmark specifications. National Nuclear Data Center, Brookhaven. ENDF-202.
- Robinson, G.S. [1975] - AUS - the Australian modular scheme for reactor neutronics computations. AAEC/E369.
- Robinson, G.S. [1977] - AUS module MIRANDA - a data preparation code based on multiregion resonance theory. AAEC/E410.
- Robinson, G.S. [1979] - Approximate first collision probabilities for neutrons in cylindrical and cluster lattices. AAEC/E465.
- Robinson, G.S. [1984] - Extension of the AUS reactor neutronics system for application to fusion blanket neutronics. AAEC/E583.
- Serdula, K.J. [1966] - Lattice measurements with 28-element natural UO₂ fuel assemblies. Part 1 : bucklings for a range of spacings with three coolants. AECL-2606.