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MONTE CARLO CALCULATED MATERIAL BUCKLINGS OF 3 wt% ENRICHED URANIUM-WATER LATTICES WITH URANIUM IN THE WATER MODERATOR

L. L. CARTER

SEPTEMBER, 1965

BATTELLE-NORTHWEST
RICHLAND, WASHINGTON

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MONTE CARLO CALCULATED MATERIAL BUCKLINGS OF 3 wt% ENRICHED URANIUM-WATER LATTICES WITH URANIUM IN THE WATER MODERATOR

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MONTE CARLO CALCULATED MATERIAL BUCKLINGS OF 3 wt% ENRICHED URANIUM-WATER LATTICES WITH URANIUM IN THE WATER MODERATOR

INTRODUCTION

A difficult technical problem of importance in processing reactor fuels involves criticality of uranium rods in uranium solution (problem of uranium dissolution). The material buckling for such a mixture is difficult to evaluate by standard methods. MONTE CARLO techniques were used to evaluate the material bucklings for 3 wt% enriched uranium-water lattices with various uranium concentrations in the moderator. The maximum material buckling that may be obtained under optimum geometry conditions was calculated to occur with uranium absent from the moderator. These results apply to solid rods only since tubular fuel elements were not considered.

SUMMARY AND CONCLUSIONS

Calculational techniques are available that give a relatively satisfactory comparison between experimental and calculated values for clean* solid rod uranium-water lattices. The calculation becomes much more difficult when uranium is present in the water moderator because the resonance integral is difficult to evaluate. The resonance coupling between the fuel rod and the uranium in the moderator forces a considerable modification in the usual techniques used to solve the clean uranium-water lattice problem.

This paper has presented the results of MONTE CARLO calculations on 3 wt% enriched solid rod uranium lattices with uranium present in the water moderator. The major purpose of the calculations was to demonstrate that the maximum material buckling, which may be obtained at this enrichment, occurs with uranium absent from the moderator. The calculations have verified that the maximum material buckling of 3 wt% enriched solid rod uranium-water lattices does occur with uranium absent from the water moderator. The addition of uranium to the water moderator

* The word clean denotes the absence of uranium in the moderating region.

may increase the material buckling of lattices of certain fuel rod diameters and moderator to uranium volume ratios. However, these calculations indicate that the material buckling will never exceed the material buckling of a clean 3 wt% enriched lattice at the optimum fuel rod diameter and moderator to uranium volume ratio.

Error Analysis

A number of small errors exist in MONTE CARLO calculations that are difficult to evaluate. The statistical error, which is present because only a finite number of neutron lifetimes are sampled in any given case, may be evaluated approximately as:[1]

$$\text{Statistical Error} = \frac{C\,\sigma}{\left(n + \frac{1.87}{n} - 3\right)^{1/2}}$$

where:

n = number of samples taken ($\geqq 4$)

C = a constant which for 90% confidence limits is equal to 1.645

σ = standard deviation.

In the LMC calculation, the parameters of the system (k_∞, buckling, etc.,) are written out every x neutron histories. Each group of histories represents a sample in the above equation. The constant C was set equal to 1.645 so that the error limits represent 90% confidence limits. The error limits given in summarizing the MONTE CARLO results are because of these statistical errors only. The magnitude of the total error in the calculation depends upon a number of other things such as:

- Cross sections used.
- Anisotropic elastic scattering data.
- The assumed fission spectrum.
- Determination of the energy loss in inelastic scattering, and the assumption that the angle through which the neutron scatters is isotropic in the center of the mass system.
- Chemical binding in the molecule at thermal energies. The free gas model was used in these calculations.
- Fluctuations in the generated random numbers.

The dominant error other than the statistical error is probably caused by the cross sections used. A list of references for the cross sections utilized is given in Appendix C. Defining the U^{238} resonances satisfactorily was a major problem since the cross sections are determined by a linear interpolation between point values. In these calculations, U^{238} was treated as two separate fictitious isotopes. One isotope defined the U^{238} cross section from 15 MeV to 64.9 eV. The second isotope defined the U^{238} cross section from 64.9 eV to 0 eV. By using this approach, the U^{238} cross section as a function of energy was defined by 200 energy points instead of the usual 100.

The calculated material buckling values for the clean water lattices tend to be somewhat lower than the experimental values. This will probably also hold true for the calculated bucklings with uranium present in the moderator. There is one safety factor which has an effect with uranium in the moderator. These calculations have assumed a pure uranium water mixture so that the poisoning effect from other elements has been neglected. In an actual experimental situation, the moderator would normally contain some nitrogen and other poisons.

DISCUSSION

Theoretical Background

There is presently a significant amount of experimental data available on the material bucklings of slightly enriched uranium water lattices. This data includes a wide enough range of variables (water to uranium volume ratios, uranium rod diameters, and uranium enrichments) so that techniques of calculating nuclear parameters for such lattices may be compared to experimental results quite satisfactorily. Theoretical techniques have been developed and applied to such an extent that there is a reasonably accurate comparison between calculated values and experimental measurements.[2]

A difficult technical problem of importance in processing reactor fuels involves criticality of uranium rods in uranium solution (problem of uranium dissolution). There is generally a considerable simplification in nuclear safety calculations if the maximum material buckling for a given fuel enrichment occurs with uranium absent from the water moderator. Experimental measurements or calculations on uranium water lattices with uranium absent from the water moderator can then be used to determine the nuclear safety parameters of interest.

It would be expected that the maximum material buckling for uranium water lattices would occur with uranium absent from the moderator, providing the uranium enrichment is not too high. The gain in resonance escape probability by lumping the fuel more than compensates for the loss in thermal utilization. However, if the uranium is sufficiently enriched, the maximum material buckling may occur with uranium present in the moderator. The problem then is to determine the material buckling as a function of uranium density in the water moderator, moderator to fuel volume ratios, and fuel rod diameters.

The resonance escape probability of a lattice cell is difficult to evaluate when a resonance material is present in the moderator. The collision density in a solid fuel rod surrounded by uranium solution is given by:

$$\varphi_o(E)\,\Sigma_{to}(E) = \frac{P_c(E)}{\alpha_o}\int_E^{\frac{E}{1-\alpha_o}} \varphi_o(E')\,\Sigma_{so}(E'\to E)\,\frac{dE'}{E'} \tag{1}$$

$$+ \frac{V_o\,P_{1o}(E)}{V_1\,\alpha_1}\int_E^{\frac{E}{1-\alpha_1}} \varphi_1(E')\,\Sigma_{s1}(E'\to E)\,\frac{dE'}{E'}$$

$$+ \frac{V_o\,P_{1o}(E)}{V_1\,\alpha_o}\int_E^{\frac{E}{1-\alpha_o}} \varphi_1(E')\,\Sigma_{som}(E'- E)\,\frac{dE'}{E'}$$

where:

$\varphi_o(E)$ and $\varphi_1(E)$ are the average fluxes in the fuel and moderating regions.
$\Sigma_{so}(E' \to E)$, $\Sigma_{s1}(E' \to E)$, and $\Sigma_{som}(E' \to E)$ are the scattering cross sections in the fuel region, moderator region due to the moderating material, and moderator region due to the fuel in the moderator, respectively.

P_{1o} = Probability that a neutron born at energy E in the moderator has its next collision in the fuel rod.

P_c = Probability that a neutron scattered in the fuel rod down to an energy E has its next collision in the fuel rod.

The term on the right hand side of Equation (1) is the contribution from the absorber in the moderator. If there is no absorber in the moderator, Equation (1) reduced to [3]

$$\varphi_o \Sigma_{to} = \frac{P_c}{\alpha_o} \int_E^{\frac{E}{1-\alpha_o}} \varphi_o \Sigma_{so}(E' \to E) \frac{dE'}{E'} + \frac{(1-P_c)\Sigma_{to}}{V \xi \Sigma_s \quad E} \tag{2}$$

where the source flux in the moderator has been assumed to be an asymptotic flux.

Equation (2) may be solved by using the NR or IA approximation for each resonance. The solution to Equation (2) has been obtained by computer programs in an efficient and relatively accurate manner.[4] However, when there is an absorbing material in the moderator, the right hand term in Equation (1) may not be neglected. Also, the resonance integral of the absorbing atoms in the moderator must be obtained. These factors make the total resonance integral very difficult to obtain by standard numerical integration techniques. Since such a calculation is difficult and there is very little experimental data to verify the results, it was decided to study the problem by means of MONTE CARLO methods.

Description of the Lattice MONTE CARLO Code

The MONTE Carlo calculation traces a large number of neutron lifetimes from birth to absorption in a lattice array. The information that maybe obtained from the calculation includes:

- Flux as a function of energy in the lattice cell.
- The absorptions and fissions that occur in each isotope as a function of energy and region.
- The average neutron lifetime and the average slowing down time
- The neutron age and diffusion length.
- The value of the infinite multiplication factor and the material buckling.

The computer code was written by making a number of changes in the HISMC[5] code (an infinite medium MONTE CARLO computer program) and adding a number of geometry routines. The LMC code was written in the FORTRAN II coding system. This is a three region code consisting of two concentric cylindrical regions surrounded by another concentric region with a hexagonal outer boundary. Neutrons that reach the hexagonal boundary are reflected in such a manner as to simulate an infinite hexagonal lattice.

MONTE CARLO CALCULATED MATERIAL BUCKLINGS COMPARED TO EXPERIMENTAL MEASUREMENTS

Clean Water Lattices*

A number of material buckling measurements have been made at Hanford on 3 wt% enriched uranium water lattices.[6] The buckling values were obtained for various water to uranium volume ratios with four different uranium rod diameters. The uranium rods were positioned in lucite tubes and arranged in a hexagonal lattice array.

A number of calculations were made for these lattices, using the LMC computer code. The material bucklings were calculated from the two group formulation:

$$\frac{(\eta f)_1 (1 - P_1)}{(1 + B^2 \tau)} + \frac{(\eta f)_2 P_1}{(1 + B^2 \tau)(1 + B^2 L^2)} = 1 \qquad (3)$$

where

τ and L are the age and thermal diffusion length, respectively

---

* The word clean denotes the absence of uranium in the moderating region.

B^2 = Material buckling

P_1 = (thermal neutrons absorbed)/(total original neutrons)

$(\eta f)_1$ = (epi-thermal neutrons produced)/(epi-thermal neutrons absorbed)

$(\eta f)_2$ = (thermal neutrons produced)/(thermal neutrons absorbed)

The division energy between the two groups was chosen as 0.60 eV. All the quantities in Equation (3), except the material buckling, were calculated directly using MONTE CARLO techniques (Appendix A). A summary of the calculated and measured values for the 3 wt% enriched uranium-water lattices is given in Table I. The calculated parameters obtained by using the GAMTEC-II computer code [4] are also given in Table I for comparison purposes.

The buckling values calculated by LMC seem to agree quite consistently with the experimental results. Since these calculations cover a wide range of water to uranium volume ratios and fuel rod diameters, the computer code appears reliable for the 3 wt% enriched clean uranium-water lattices.

<u>Uranium-Water Lattices with Uranium Present in the Water Moderator</u>

The results of calculations using the LMC MONTE CARLO computer code on clean uranium-water lattices have been compared to experimental measurements. It would also be desirable to compare calculated results to experimental measurements with uranium present in the moderator. This would further verify the reliability of the calculational method.

There are apparently no experimental results available on 3 wt% enriched uranium-water lattices with uranium present in the water moderator. However, one such experiment has been done on a lattice where the uranium enrichment was 1.007 wt% U^{235}.[7] This experiment was twofold. A buckling measurement was first made with uranium absent from the water moderator. The water moderator was then replaced with uranyl-nitrate solution having a uranium density of 431 g/liter (1.007 wt% U^{235}). The corresponding material

TABLE I

EXPERIMENTAL AND CALCULATED PARAMETERS FOR URANIUM-WATER LATTICES

(3.063 wt% U^{235} Enriched Rods)

Geometry		Calculated Values							Experimental Values
Fuel Rod Diameter, in.	Water/U Volume Ratio	Calculation Method	$(\eta f)_1$	$(\eta f)_2$	P_1	τ^*, cm^2	k_∞	B^2, 10^{-4} cm^{-2}	B^2, 10^{-4} cm^{-2}
0.175	2.24	MONTE CARLO	0.7605	1.7086	0.5586	23.83	1.2901	116.2 ± 10.8	114.77 ± 0.24
0.175	2.24	GAMTEC II	0.8174	1.7276	0.5948	23.53	1.3587	114.3	114.77 ± 0.24
0.175	6.29	MONTE CARLO	0.6726	1.5670	0.7883	23.69	1.3777	143.9 ± 7.3	142.92 ± 0.11
0.175	6.29	GAMTEC II	0.8056	1.5880	0.8068	23.94	1.4369	166.4	142.92 ± 0.11
0.175	9.89	MONTE CARLO	0.7549	1.4499	0.8584	23.89	1.3515	127.3 ± 8.2	123.01 ± 0.36
0.175	9.89	GAMTEC II	0.7996	1.4587	0.8719	24.45	1.3742	136.6	123.01 ± 0.36
0.300	5.00	MONTE CARLO	0.7664	1.5798	0.7584	23.88	1.3333	145.7 ± 7.8	153.52 ± 0.32
0.600	2.06	MONTE CARLO	0.8431	1.6781	0.5980	23.99	1.3424	132.5 ± 7.1	148.34 ± 0.30
0.600	2.06	GAMTEC II	1.0016	1.6875	0.6244	23.56	1.4299	171.5	148.34 ± 0.30
0.600	3.41	MONTE CARLO	0.8834	1.5887	0.7184	23.16	1.3901	150.1 ± 5.6	154.35 ± 0.42
0.600	3.41	GAMTEC II	1.0249	1.5947	1.7390	23.34	1.4460	175.4	154.35 ± 0.42
0.600	5.18	MONTE CARLO	0.9019	1.4564	0.7944	23.59	1.3424	126.7 ± 6.4	129.84 ± 0.38
0.600	5.18	GAMTEC II	1.0436	1.4733	0.8123	23.52	1.3926	149.8	129.84 ± 0.38
0.600	6.84	MONTE CARLO	0.9178	1.3896	0.8343	23.78	1.3114	113.2 ± 5.1	105.76 ± 0.28
0.925	1.89	MONTE CARLO	1.9043	1.6590	0.5842	24.53	1.3452	134.2 ± 9.5	140.68 ± 0.27
0.925	1.89	GAMTEC II	1.0626	1.6186	0.6186	23.63	1.4251	168.5	140.68 ± 0.27
0.925	2.29	MONTE CARLO	0.8806	1.6251	0.6499	24.88	1.3645	139.6 ± 11.0	142.12 ± 0.17
0.925	2.29	GAMTEC II	1.0764	1.6062	0.6665	23.38	1.4295	170.2	142.12 ± 0.17
0.925	3.89	MONTE CARLO	0.9472	1.4497	0.7615	23.33	1.3299	122.9 ± 9.7	121.08 ± 0.52
0.925	3.89	GAMTEC II	1.1133	1.4381	0.7764	23.23	1.3655	141.1	121.08 ± 0.52

* The average age as given by Equation (4) was used in determining the material bucklings

buckling was then obtained for this lattice. A summary of the experimental parameters and the results of this experiment is given in Table II.

It should be noted that the material buckling of the lattice dropped from 3386 x 10^{-6} cm^{-2} to 1394 x 10^{-6} cm^2 with the addition of uranyl-nitrate solution to the moderator. The corresponding experimental values for k_∞ in each case were estimated from the one group critical equation:

$$1 = \frac{k_\infty}{(1 + B^2 \tau)(1 + B^2 L^2)}$$

where

k_∞ = Infinite multiplication factor

B^2 = Measured buckling

τ = Neutron age as calculated by LMC

L = Thermal diffusion length as calculated by LMC.

The difference between these two experimental k_∞ values (0.0496) is the reactivity loss in an infinite system due to replacing the water moderator by uranyl-nitrate solution.

TABLE II

IMPORTANT PARAMETERS AND EXPERIMENTAL RESULTS FOR A URANIUM-WATER LATTICE BOTH WITH AND WITHOUT URANIUM PRESENT IN THE MODERATOR

(1.007 wt% U^{235})

Moderator Solution, g/liter U	Nitric Acid Content of Uranyl-Nitrate, g/liter	Material Buckling, 10^{-6} cm^2	Estimated k_∞
0 (all water)	0	3386	1.0936
431	18.7	1394	1.0440

Uranium Rod Diameter = 0.925 in.

Lattice Spacing = 1.5 in.

$\Delta k_\infty = 0.0496$

The corresponding calculated quantities obtained by using the LMC computer code are given in Table III. The material bucklings as calculated by LMC are substantially lower than the measured bucklings. This general trend can also be seen in Table I for the 3 wt% enriched uranium-water lattices. The difference was not as evident there because the calculated buckling value is a function of $k_\infty - 1$ which is quite large for the 3 wt% enriched lattices. In this 1 wt% enriched lattice, the value of k_∞ is close to unity so that a small difference in k_∞ makes a large difference in the buckling.

TABLE III

MONTE CARLO CALCULATED PARAMETERS
FOR THE EXPERIMENT DESCRIBED IN TABLE II
(1.007 wt% U^{235})

Moderator Solution, g/liter U	τ cm^2	$(\eta f)_1$	$(\eta f)_2$	P_1	k_∞	B^2 $10^{-4} cm^2$
0 (all water)	24.13	0.6790	1.2601	0.6570	1.0608 ± 0.0057	2268
431	27.93	0.5846	1.2905	0.5727	0.9889 ± 0.0081	-

$$\Delta k_\infty = 0.0719 \pm 0.0138$$

The estimated experimental change in k_∞ of 0.0496 is somewhat less than the calculated change of 0.0719, and appears to be a fairly large difference. However, there are many factors that make it very difficult to compare this experimental measurement to the calculation, and two of the most important are:

- The densities of the elements in the moderator are not very accurately known.
- The computer code did not have enough memory storage available to use all the isotopes involved. Therefore, the aluminum region and the moderator region were homogenized into one region. Oxygen was assigned a fictitious macroscopic cross section to account for capture and scattering by aluminum and nitrogen.

$$(\Sigma_x^O)_{\text{fictitious}} = \Sigma_x^O + \Sigma_x^{al} + \Sigma_x^N$$

where

x designates the type of cross section; such as, capture, etc

Σ_x^O = Macroscopic oxygen cross section

Σ_x^{al} = Macroscopic aluminum cross section

Σ_x^N = Macroscopic nitrogen cross section

MONTE CARLO CALCULATED MATERIAL BUCKLINGS OF 3 wt% ENRICHED URANIUM-WATER LATTICES WITH URANIUM IN THE WATER MODERATOR

A large number of calculations are required at a given uranium enrichment to satisfactorily determine the material buckling as a function of fuel rod diameter, water to uranium volume ratios, and uranium concentrations in the moderator. Therefore, these MONTE CARLO calculations were performed at only one enrichment in order to minimize computation time. The 3 wt% enrichment was chosen as a basis for these calculations for two reasons:

- A number of experimental results are available on clean water lattices at this enrichment which provides an opportunity to compare experimental and calculated values when uranium is absent from the water moderator.
- It is assumed that the maximum material buckling at this enrichment will be found to occur with uranium absent from the moderator.

If this is found to be true, then the same may be assumed true for all enrichments less than 3%. A considerable simplification would then result in many nuclear safety calculations involving uranium enrichments of 3% or less.

Three different fuel rod diameters were used in these calculations. At each fuel rod diameter, three water to uranium volume ratios were used.

The median water to uranium ratio was chosen to approximately correspond to the maximum measured material buckling at the given fuel rod diameter with uranium absent from the moderator. At each fuel rod diameter and water to uranium ratio, four different uranium concentrations in the moderator were used; 0 g/liter U, 100 g/liters U, 500 g/liters U, 1000 g/liters U. This requires 36 separate calculations to determine the material buckling as a function of the three variables involved. A few additional calculations were made at other points of interest.

The densities of the elements in the moderator were determined from the assumption that only water (1 g/cc) and uranium (18.9 g/cc) are in the moderator. The poisoning effect of other elements such as nitrogen is neglected. A summary of the densities used is given in Table IV.

TABLE IV

DENSITIES OF THE ELEMENTS IN THE FUEL ROD AND THE MODERATOR

(3.063 wt% Enriched Uranium)

Fuel Rod

Element	Density (g/cc)
U^{235}	0.5789
U^{238}	18.3211
Total	18.9000

Moderator

Uranium Density, g/cc	U^{235} Density, g/cc	U^{235} Density, g/cc	H^1 Density, g/cc	O^{16} Density, g/cc
0.000	0.00000	0.00000	0.1119	0.8881
0.100	0.09637	0.003063	0.1113	0.8834
0.500	0.48469	0.015315	0.1089	0.8646
1.000	0.96936	0.03063	0.1060	0.8411

The radial distribution of fission neutrons is not known at the beginning of each calculation. Since this is an input quantity in the computer code, a guess source spectrum must be used. In these calculations, 1000 neutron histories were traced by using a guess radial spectrum. The new source spectrum obtained from these 1000 histories was used in the subsequent calculation. In most calculations, 3000 neutron histories were traced to determine the reported parameters. An additional 2000 or 3000 histories were traced in certain calculations where the statistical error limits were large, or the radial source spectrum did not converge satisfactorily.

A summary of the calculation results is given in Table V. The material bucklings were determined from the two group model given in Equation (3). At a given fuel rod diameter and moderator to fuel rod volume ratio, the neutron age was found to be relatively independent of the concentration of uranium in the moderator. The material bucklings were determined by using the average age in order to eliminate this statistical variation.

$$\bar{\tau} = \frac{\tau_0 + \tau_{100} + \tau_{500} + \tau_{1000}}{4} \tag{4}$$

where

$\bar{\tau}$ = Average age at a given fuel rod diameter and moderator to fuel rod volume ratio.

$\tau_0, \tau_{100}, \tau_{500}, \tau_{1000}$ = Calculated ages with 0 g/liter, 100 g/liters, 500 g/liters, and 1000 g/liters uranium in moderator.

The material bucklings as a function of moderator to fuel rod volume ratios and uranium concentration in the moderator are plotted in Figures 1, 2, and 3 for each fuel rod diameter. Homogeneous calculations were made for uranium concentrations of 500 and 1000 g/liters so that these curves could be extrapolated toward the homogeneous case (moderator to fuel rod volume ratio approaches infinity).

TABLE V

MONTE CARLO CALCULATED PARAMETERS FOR URANIUM ROD LATTICES MODERATED WITH WATER CONTAINING VARIOUS CONCENTRATIONS OF URANIUM

(3.063 wt% U^{235} Enriched Rods and Solution)

Fuel Rod Diameter, in.	Moderator/U Volume Ratio	Uranium Concentration in Moderator, g/liter	$(\eta f)_1$	$(\eta f)_2$	P_1	τ^*, cm^2	k_∞	B^2, 10^{-4} cm^2
0.175	2.24	0	0.7605	1.7086	0.5586	23.83	1.2901	116.2 ± 10.8
0.175	2.24	100	0.7642	1.7239	0.5488	23.88	1.2909	116.6 ± 4.6
0.175	2.24	500	0.7147	1.7253	0.5180	23.31	1.2382	96.1 ± 8.1
0.175	2.24	1000	0.7312	1.7348	0.5034	23.44	1.2364	95.2 ± 6.5
0.175	6.29	0	0.6726	1.5670	0.7883	23.69	1.3777	143.9 ± 7.3
0.175	6.29	100	0.6716	1.5844	0.7599	24.13	1.3652	140.6 ± 11.6
0.175	6.29	500	0.6640	1.5914	0.7360	22.70	1.3466	134.4 ± 7.5
0.175	6.29	1000	0.6071	1.6378	0.7087	22.78	1.3404	133.2 ± 7.6
0.175	9.89	0	0.7549	1.4499	0.8584	23.89	1.3515	127.3 ± 8.2
0.175	9.89	100	0.6784	1.4764	0.8285	23.97	1.3395	123.6 ± 8.9
0.175	9.89	500	0.6037	1.5272	0.7829	24.15	1.3267	120.9 ± 7.5
0.175	9.89	1000	0.5817	1.5739	0.7530	24.08	1.3288	123.7 ± 4.0
0.300	5.00	0	0.7664	1.5798	0.7584	23.88	1.3833	145.7 ± 7.8
0.600	2.06	0	0.8431	1.6781	0.5980	23.99	1.3424	132.5 ± 7.1
0.600	2.06	100	0.8198	1.6716	0.5916	23.46	1.3237	125.4 ± 11.6
0.600	2.06	500	0.7715	1.7042	0.5457	24.84	1.2805	109.5 ± 13.4
0.600	2.06	1000	0.7958	1.7070	0.5177	24.37	1.2675	104.8 ± 7.8
0.600	3.41	0	0.8834	1.5887	0.7184	23.16	1.3901	150.1 ± 5.6
0.600	3.41	100	0.8286	1.5918	0.6912	24.31	1.3561	137.7 ± 5.4
0.600	3.41	500	0.7712	1.6194	0.6647	23.93	1.3350	130.6 ± 9.1
0.600	3.41	1000	0.7531	1.6603	0.6173	22.57	1.3131	123.6 ± 10.6
0.600	5.18	0	0.9019	1.4564	0.7944	23.59	1.3424	126.7 ± 6.4
0.600	5.18	100	0.8017	1.4903	0.7778	23.21	1.3374	125.7 ± 10.4
0.600	5.18	500	0.7605	1.5284	0.7382	23.09	1.3274	124.3 ± 9.7
0.600	5.18	1000	0.7381	1.5908	0.6958	24.77	1.3314	127.4 ± 6.5
0.600	6.84	0	0.9178	1.3896	0.8343	23.78	1.3114	113.2 ± 5.1
0.600	6.84	1000	0.7017	1.5656	0.7376	23.48	1.3389	128.6 ± 7.7
0.925	1.89	0	0.9043	1.6590	0.5842	24.53	1.3452	134.2 ± 9.5
0.925	1.89	100	0.8674	1.6505	0.5910	24.38	1.3302	128.1 ± 9.2
0.925	1.89	500	0.8413	1.6614	0.5555	23.47	1.2969	116.0 ± 7.3
0.925	1.89	1000	0.8005	1.7058	0.5263	23.50	1.2770	109.0 ± 13.4
0.925	2.29	0	0.8806	1.6251	0.6499	24.88	1.3645	139.6 ± 11.0
0.925	2.29	100	0.8800	1.6340	0.6384	24.01	1.3614	138.6 ± 6.4
0.925	2.29	500	0.8100	1.6422	0.6026	24.02	1.3612	121.0 ± 15.0
0.925	2.29	1000	0.7981	1.6664	0.5657	22.89	1.2893	112.9 ± 12.0
0.925	3.89	0	0.9472	1.4497	0.7615	23.33	1.3299	122.9 ± 9.7
0.925	3.89	100	0.8624	1.4775	0.7324	24.80	1.3129	117.5 ± 6.2
0.925	3.89	500	0.8051	1.5392	0.6938	23.27	1.3144	120.2 ± 3.6
0.925	3.89	1000	0.7610	1.5837	0.6714	22.98	1.3134	121.3 ± 8.7
0.925	6.50	0	0.9489	1.2211	0.8240	24.59	1.1732	60.1 ± 9.6
0.925	6.50	1000	0.7237	1.5421	0.7422	24.05	1.3311	123.2 ± 6.4
Homogeneous	∞	500	0.2877	1.0349	0.9006	24.23	0.9606	-13.6 ± 10.1
Homogeneous	∞	1000	0.4061	1.3346	0.8498	24.82	1.1951	68.7 ± 8.3

* The average age as given by Equation (4) was used in determining the material buckling.

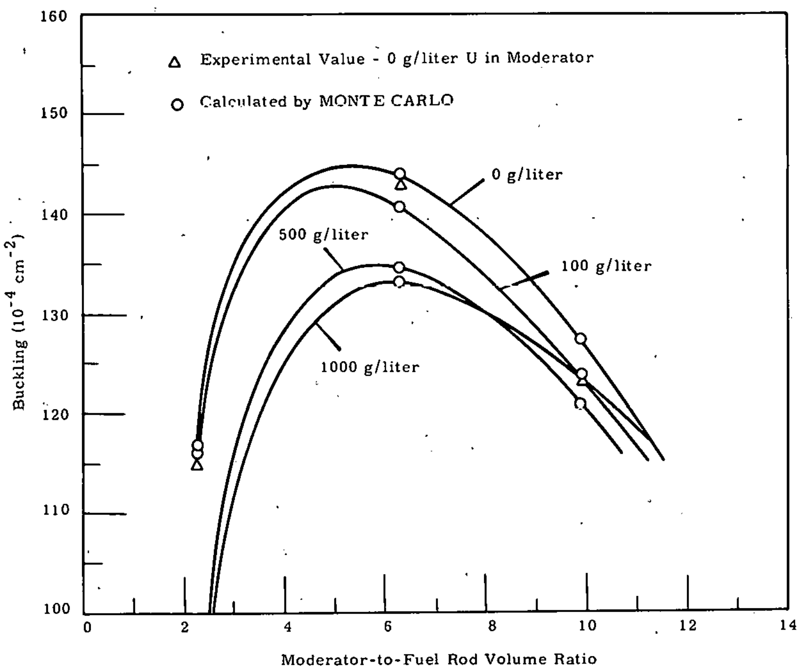


FIGURE 1

Material Bucklings for 3.063 wt% U^{235} Enriched Uranium-Water Lattices with Uranium in the Water Moderator (Fuel Rod Diameter = 0.175 in.)

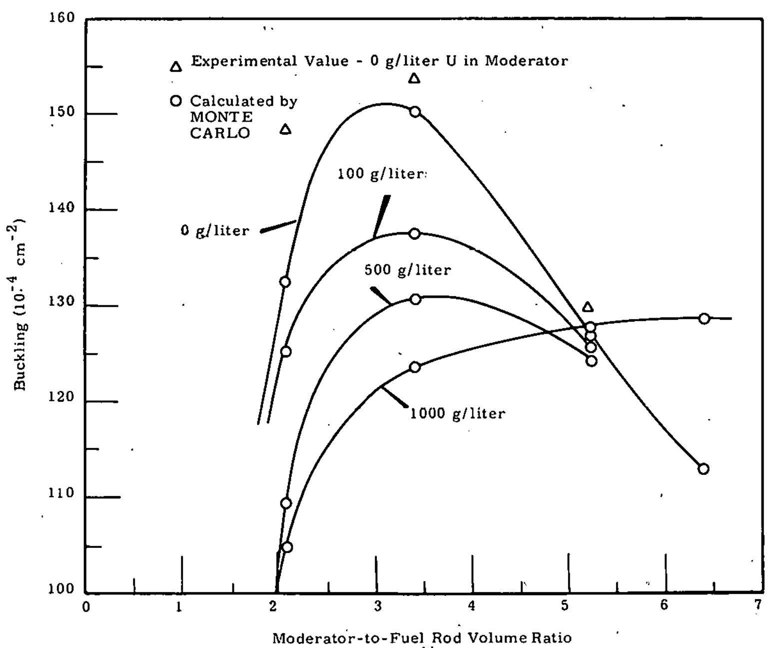


FIGURE 2

Material Bucklings for 3.063 wt% U^{235} Enriched Uranium-Water Lattices with Uranium in the Water Moderator (Fuel Rod Diameter = 0.600 in.)

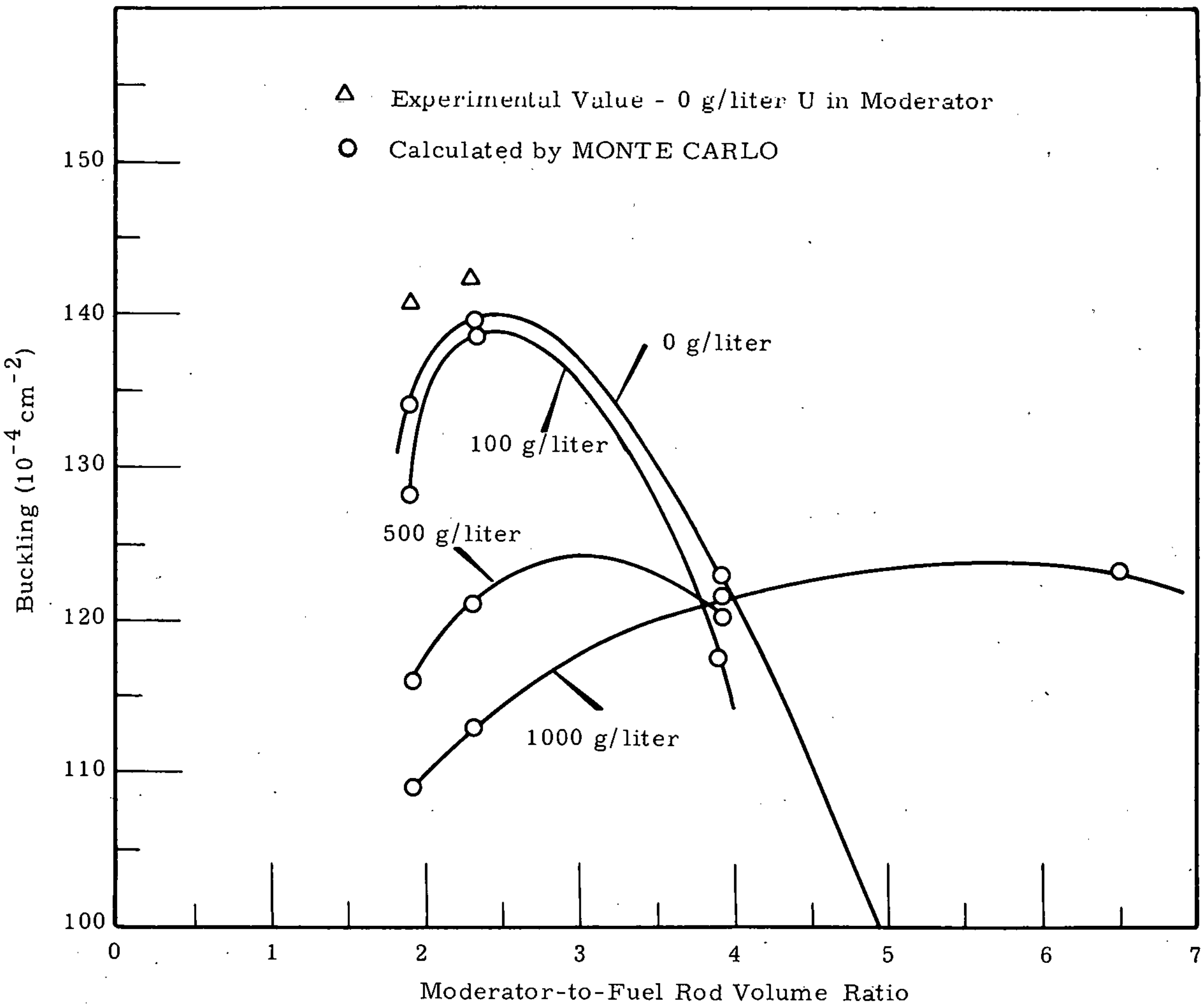


FIGURE 3

Material Bucklings for 3.063 wt% U^{235} Enriched Uranium-Water Lattices with Uranium in the Water Moderator (Fuel Rod Diameter = 0.926 in.)

It should be noted that the material buckling decreases as uranium is added to the moderator in almost all the cases considered. In certain geometries (such as the fuel rod diameter of 0.600 in. and moderator to fuel rod volume ratio of 5.18) the material buckling is approximately constant as a function of uranium concentration in the moderator. In the case mentioned, an additional calculation was made at a larger moderator to uranium volume ratio.

The material buckling for clean 3 wt% enriched uranium-water lattices reaches nearly its maximum value for a fuel rod diameter of 0.600 in. and a water to uranium volume ratio of 3.41. These calculations show a significant decrease in the material buckling as uranium is added to the water moderator at this geometry configuration.

The maximum material bucklings for 3 wt% enriched lattices as a function of uranium concentration in the moderator is plotted in Figure 4. This curve was obtained by finding the maximum values on the curves in Figure 1, 2, and 3. Optimum fuel rod diameters may give slightly higher values, but these fuel rod diameters were chosen in such a way that they should at least span the optimum points. It should also be emphasized that statistical errors exist in the MONTE CARLO calculations which make the reactivity changes (due to small perturbations) difficult to evaluate.

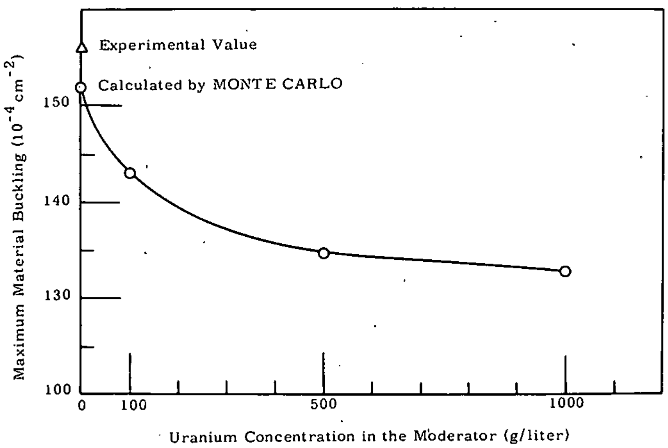


FIGURE 4

Maximum Material Bucklings Obtained with Near Optimum Geometries for Uranium-Water Lattices with Uranium in the Water Moderator (3.063 wt% U^{235} Enriched Rods and Solution)

APPENDIX A

DESCRIPTION OF THE LATTICE MONTE CARLO PROGRAM

Introduction

The HISMC code[5] (an infinite medium Monte Carlo computer program for the 7090 computer) was used as a base for the LMC (Lattice Monte Carlo) code so that programming time could be minimized. This was possible to do because much of the Monte Carlo calculation is geometry independent. The methods used to determine the neutron starting energy, neutron cross sections as a function of energy, type of collision, energy loss in elastic and inelastic collisions, and the absorptions and fissions in each isotope all remain essentially the same as in the original HISMC code. The major change needed was the insertion of a number of geometry routines.

The code was written in FORTRAN II and uses the same two magnetic cross section tapes as the HISMC program For basic information on this computer code, reference should be made to the description of HISMC.[5] The following is a description of the changes and additions made.

Geometry Routines

A portion of an infinite hexagonal lattice array is shown in Figure A-1. The entire Monte Carlo calculation is simulated in a quarter of a lattice cell. The lattice is simulated by reflecting the neutrons at the boundaries with a mirror reflection (Figure A-1). If the usual directional cosines for rectangular geometry are defined as

u = Cosine of the angle between the neutrons direction of flight and a vector parallel to the x axis in the positive x direction

v = Cosine of the angle between the neutrons direction of flight and a vector parallel to the y axis in the positive y direction

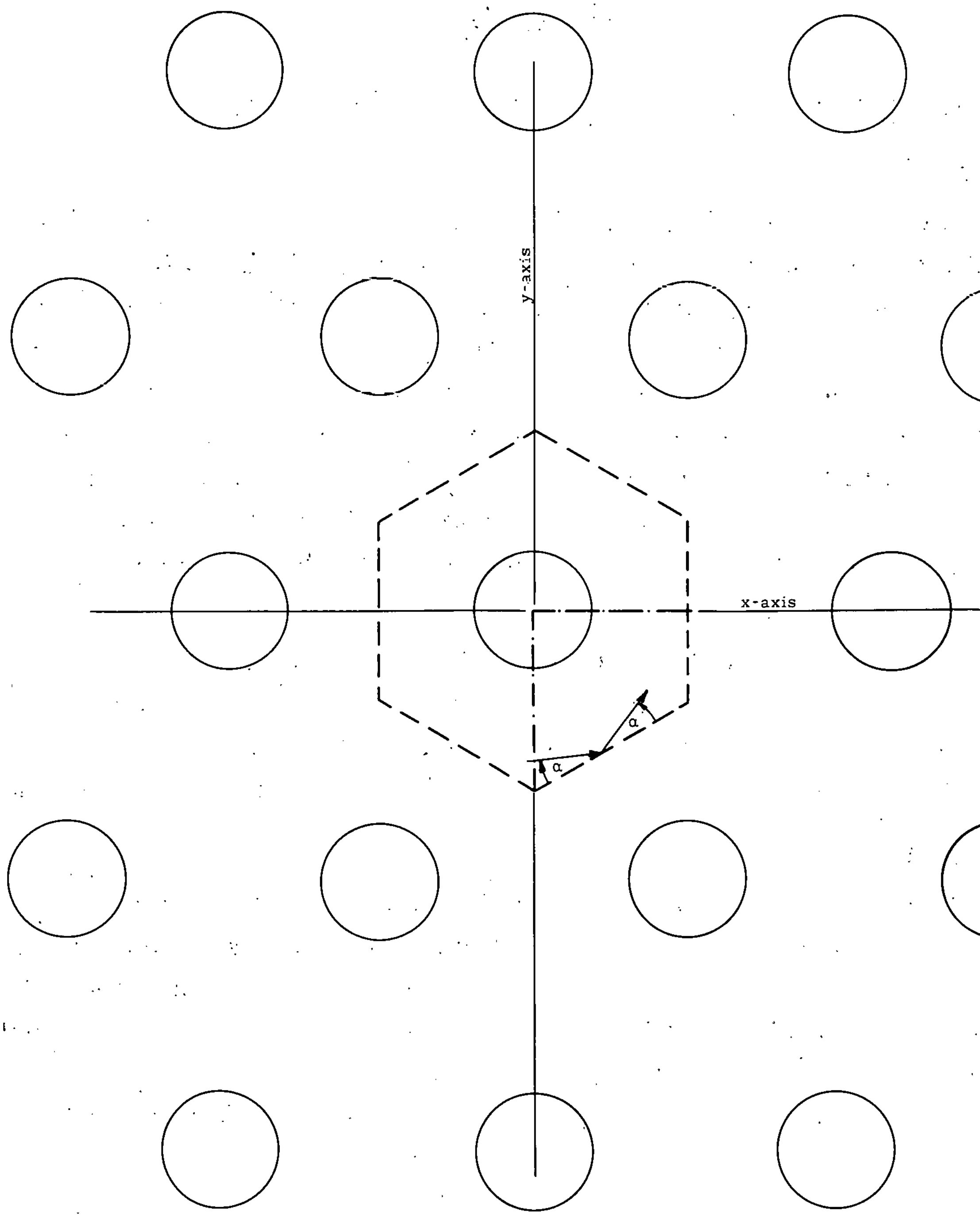


FIGURE A-1

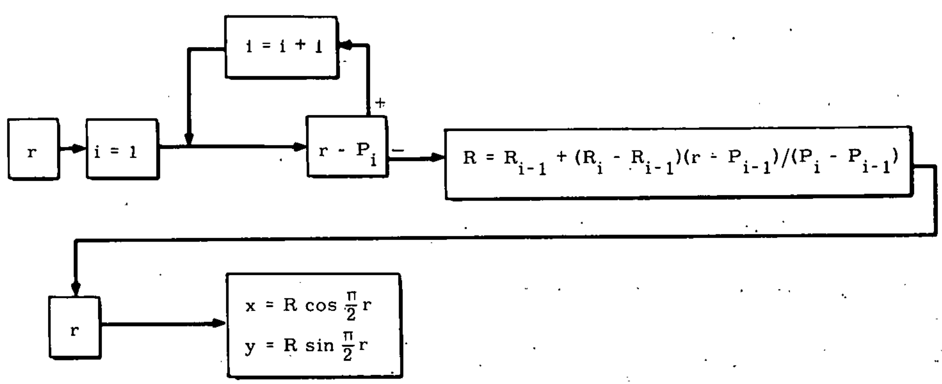
Hexagonal Lattice Array

w = Cosine of the angle between the neutrons direction of flight and a vector parallel to the z axis in the positive z direction,

then, whenever a neutron is reflected at the boundaries x = o or y = o, the only change required in the directional cosines is u = -u' or v = -v', respectively. The same is true at the boundary x = (lattice pitch)/2 so that only one boundary requires a great deal of computation when reflection occurs. This is why a quarter lattice cell was used instead of a full lattice cell or one-sixth of a lattice cell.

Computer storage limitations placed an upper limit of eight on the maximum number of isotopes in any case. The number of regions in the cell is limited to three (fuel, cladding, and moderator in the case of a solid fuel rod).

The initial values of the x and y coordinates that define the starting position of each neutron are determined from two probability tables in the same manner that the starting energy is determined.[5] The first table contains 51 radii values from zero to the maximum radial cell dimension. The second table contains the corresponding probabilities that a neutron will be born with a radii smaller than that in the first table. Figure A-2 illustrates the initial x and y neutron position determination using these tables.



R_i = radii value from table
P_i = corresponding probability from table
r = a random number between zero and one

FIGURE A-2

Initial Neutron Spatial Parameters

The fission source is assumed to emit neutrons isotropically, and the u, v, w direction cosines are chosen from an isotropic distribution as[8]

$$w = 2r_1 - 1$$

$$\varphi = \pi(2r_2 - 1)$$

$$u = \sqrt{1 - w^2} \cos \varphi$$

$$v = \sqrt{1 - w^2} \sin \varphi$$

where r_1 and r_2 are random numbers.

The method of determining the distance the neutron travels before each collision, reflection, or region transfer and the corresponding coordinate transformations is illustrated in Figure A-3.

<u>Second and Fourth Moment Derivation</u>

The neutron age and diffusion length may be obtained in an essentially space independent calculation. The following definitions will be used throughout the discussion:

$\vec{d}_n$ = vector of the n^{th} path length of the neutron

$\vec{R}_n$ = vector from the source point to the n^{th} collision

Θ_n = angle between $\vec{d}_n$ and $\vec{R}_n$

ψ_n = angle between $\vec{d}_{n+1}$ and $\vec{R}_n$

θ_n = angle of scattering at n^{th} collision

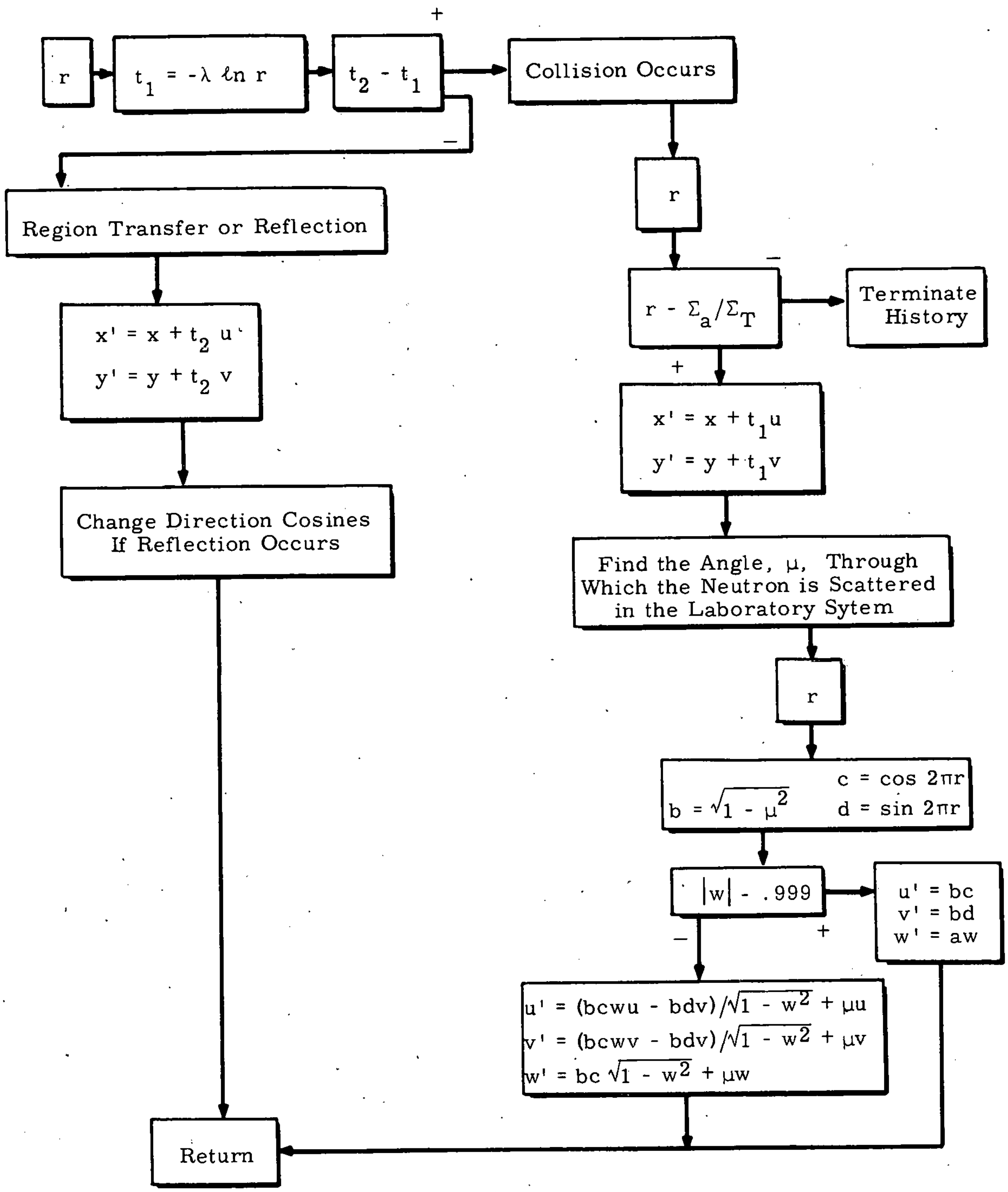
$\langle x \rangle$ = average value of a quantity x.

The following angular relation results are[9]

$$\cos \psi_n = \cos \Theta_n \cos \theta_n + \sin \Theta_n \sin \theta_n \cos \varphi_n \quad . \tag{A-1}$$

If t_{n+1} is the projection of R_{n+1} onto the vector $\vec{d}_{n+1}$

$$t_{n+1} = d_{n+1} + R_n \cos \psi_n = R_{n+1} \cos \Theta_{n+1} \quad . \tag{A-2}$$



t_2 = distance to nearest boundary
λ = neutron mean free path

FIGURE A-3

Collision or Region Transfer Routine

Since neutron scattering is isotropic to the azimuth angle φ_n, the average value of $\cos\varphi_n$ is zero so the average value of $\cos\psi_n$ is from Equation (A-1):

$$\langle \cos\psi_n \rangle = \langle \cos\Theta_n \rangle \mu_n \quad ,$$

then

$$T_{n+1} = \langle t_{n+1} \rangle = R_n \langle \cos\Theta_n \rangle \mu_n + d_{n+1}$$

$$T_{n+1} = \mu_n T_n + d_{n+1} \quad . \tag{A-3}$$

The second moment of the slowing down distribution is defined as the average value of R_n^2. The second moment of a neutron after its n+1 collision can be expressed in terms of $\vec{R}_n$ and $\vec{d}_{n+1}$ as

$$R_{n+1}^2 = (\vec{R}_n + \vec{d}_{n+1}) \cdot (\vec{R}_n + \vec{d}_{n+1})$$

$$= R_n^2 + 2R_n\, d_{n+1} \cos\psi_n + d_{n+1}^2$$

$$\left\langle R_{n+1}^2 \right\rangle = \left\langle R_n^2 \right\rangle + 2T_n\, d_{n+1} + d_{n+1}^2 \quad . \tag{A-4}$$

Equations (A-3) and (A-4) are used to determine the second moment of each neutron. The average second moment due to m neutrons is then given by

$$R^2 = \frac{\sum_{i=1}^{m} \left\langle R^2 \right\rangle_i}{m} \tag{A-5}$$

where $\left\langle R^2 \right\rangle_i$ is equal to the second moment of the i^{th} neutron as determined from Equation (A-4).

The thermal diffusion length calculation is carried out similarly except the contribution to Equation (A-4) is not started until the neutrons energy is reduced below 0.6 eV. Then six times the square of the average thermal diffusion length is computed by Equation (A-5) where the denominator is equal to the number of neutrons that reach thermal energies.

K_∞ and Buckling Calculation

The infinite multiplication factor is determined as the number of neutrons produced in one generation to the number absorbed in the previous generation.

$$K_\infty = \frac{\sum_i \nu_i F_i}{\sum_i A_i} \qquad \text{(A-6)}$$

where

F_i = number of fissions occuring in energy group i

ν_i = average number of neutrons produced per fission in energy group i

A_i = number of absorptions occurring in energy group i

The material buckling for the lattice is calculated from the two-group critical equation:

$$\frac{(\eta f)_1 (1 - P_1)}{1 + B^2 \tau} + \frac{(\eta f)_2 P_1}{(1 + B^2 \tau)(1 + B^2 L^2)} = 1 \qquad \text{(A-7)}$$

where

τ and L^2 = the age and thermal diffusion length squared, respectively

B^2 = material buckling

$$P_1 = \sum_{i=m+1}^{mk} A_i \Big/ \sum_{i=1}^{mk^{**}} A_i$$

$$(\eta f)_1 = \sum_{i=1}^{m^*} \nu_i F_i \Big/ \sum_{i=1}^{m} A_i$$

---

* m = number of epithermal energy groups

** mk = total number of energy groups

$$(\eta f)_2 = \sum_{i=m+1}^{mk} \nu_i F_i \Big/ \sum_{i=m+1}^{mk} A_i \quad .$$

APPENDIX B

INPUT INSTRUCTIONS FOR LMC (LATTICE MONTE CARLO)

The LMC computer code uses the "Generalized FORTRAN Input Routine" commonly known as the Listin Method.[10]

INPUT

Column 1 Format Type	Column 6-10 Location	Description
1	16700	Total number of isotopes in Case ≤ 8. Equal to the number of isotopes in Region 1 plus the number in Region 2 plus the number in Region 3. If the same isotope is used in two regions, it counts as two isotopes.
1	16702	Number of neutron histories.
1	17682	Number of isotopes in inner region (Region 1).
1	17683	Number of isotopes in Region 1 plus Region 2.* If there are only two regions, omit this entry.
1	16709	Equal one if evaporation mode is to be used for inelastic scattering. Equal zero if scattering matrix is to be used.
1	16710	Number of times to start the random number generator before each neutron history. This will change statistics from one run to another.
1	17621	Equal zero for fission spectrum. Equal one for delta energy spectrum. See Location 17622.
0	17622	Energy in eV to start neutrons. If a fission spectrum is used, this entry may be omitted.
0	16459	Physical temperature in °K.
0	17623	Lattice pitch, cm.
0	17625	Outside radius of Region 2. Omit this entry if only two regions are used.

* The outer concentric cylindrical region

0	17626	Outside radius of Region 1.
0	16370 - 16377	ID number of the isotopes being used starting with the center region and going out. If an isotope of a certain ID is in two regions, it must be listed twice.
0	16450 - 16457	Atomic masses of the isotopes.
0	16350 - 16357	Densities of the isotopes in g/cm^3.
0	16560 - 16567	Values of ν (thermal); neutrons produced per fission at thermal energies for each isotope.
0	16711 - 16718	Value of $\frac{d\bar{\nu}}{dE}$ in units of (MeV^{-1}) for each isotope. $\bar{\nu} = \bar{\nu}$ (thermal) $+ \frac{d\bar{\nu}}{dE} E$.
1	17662	First thermal group number for calculating ηf. Suggested value 55.
1	17666	Number of neutron histories to run before each printout of k_∞, B^2, etc.
1	17667	= 0 Cell is divided into 50 subregions for radial source calculation. First n subregions have equal volumes in inner region. Next (49-n) subregions have equal volumes and include the cell volume out to the radius pitch/2. The last subregion is the remaining portion of the cell. n is input in Location 17668. = 1 Cell is divided into 50 subregions except instead of being volume-wise, it is divided on a linear radial basis. = 2 The radii for the source spectrum calculation are read in.
1	17668	Number of neutron source subregions in Region 1. See Location 17667.
1	17669	= 0 No flux as a function of radius printout. = 1 Printout flux as a function of radius only after all neutron histories have been followed. = 2 Printout flux as a function of radius each time k_∞ is calculated, Location 17666.

0	17640 - 17649	Radius values for flux calculation. The first radius value (Location 17640) must not be zero unless the flux calculation is not wanted. The code sets the last radius value (Location 17649) equal to the maximum cell dimension.
9		

The following cards have a format of (7E10.3).

If Location 17667 is equal to two, the values of the 51 radial points are read in. The first value must be zero and the fifty-first value must be the maximum dimension of the lattice cell.

The probability values for the 51 radii points are read in where:

$P_1 = 0.0$

P_n = probability that neutron will be born with radius less than r_n.

The listin program is called again after the number of neutron histories input in Location 16702 have been processed. If Location 16702 is set equal to zero, the cross sections used in the case will be printed out and the calculation terminated. If Location 17602 is sent equal to some number n, n neutron histories will be traced using the radial source spectrum that was generated with the last set of histories. The listin program will be called again after these neutron histories are processed.

Two magnetic tapes are used for cross sections and anisotropic elastic scattering tables. The formats for these tapes are identical to those for the HISMC Monte Carlo code.[5] The anisotropic scattering coefficient tape is loaded on unit A5 and the cross section tape is loaded on unit B6.

APPENDIX C

CROSS SECTION REFERENCE

Isotope	Cross Section Reference	Anisotropic Elastic Scattering Reference	Inelastic Scattering Matrix Reference	Comments
H^1	17	- -	- -	
O^{16}	17	11	- -	
U^{235}	17, 12, 13	14	15	Infinite Dilute Resonance Capture Integral = 170 b Infinite Dilute Resonance Fission Integral = 311 b
U^{238}	16	14	15	Infinite Dilute Resonance Capture Integral = 281 b

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