

TECHNIQUES USED IN THE GEM CODE FOR MONTE CARLO NEUTRONICS CALCULATIONS IN REACTORS AND OTHER SYSTEMS OF COMPLEX GEOMETRY

E. R. Woodcock, T. Murphy,
P. J. Hemmings, and T. C. Longworth
United Kingdom Atomic Energy Authority
Risley, Warrington, Lancs., England
(Paper presented by E. R. Woodcock)

1. Introduction

The Monte Carlo technique has become a practicable method for the solution of many neutronics problems through the development of fast computing machines, which are well suited for the large number of simple repetitive calculations that are required. The method has the attraction that it is, in principle, capable of treating any complexities in geometry and nuclear data without approximation. Such an ideal is not easily achieved. On the one hand, means of feeding in a large amount of geometrical and nuclear data need to be devised. On the other, this must be handled efficiently during the calculation, because a large number of neutron histories must be followed in order to obtain acceptable statistical accuracy.

Nevertheless, a number of codes have been and are being developed to exploit the advantages of the Monte Carlo technique. The GEM Code was designed initially to study criticality-safety problems in chemical plants, and a primary objective was to use nuclear data in as fine a detail as possible. Its geometrical capabilities were extended in 1962 to carry out a survey⁽¹⁾ on behalf of the International Atomic Energy Agency of the factors affecting the nuclear safety of arrays of transport containers carrying fissile materials. Developments since that time have enabled virtually all geometrical restrictions to be removed. The resulting program has proved versatile enough to make neutronic calculations for a complete reactor, incorporating all the significant structural features.

In the description which follows, it is assumed that the reader is familiar with the basic principles of Monte Carlo tracking, such as described, for example, by Parker and Woodcock.⁽²⁾

2. Basic Philosophy

The primary aim of the program is to calculate the overall reactivity of a system of any geometry. A number of possible parameters can be used as a measure of reactivity. Some of these have been discussed at length by Woodcock,⁽³⁾ who concluded that the most useful were the multiplication factor per fission generation, k_{eff} , and the quantity MR, where M is the surface multiplication of an inner portion of the system called the

2.2 Choice of Boundary B

The specification of the boundary B is one of the vital features affecting the efficiency of the GEM technique. In designating this boundary, the three considerations of quick settling, small errors, and sampling importance must be borne in mind. In practice, it is difficult to plan or achieve the ideal precisely. Selection of boundary B can seldom be completely divorced from geometrical detail, although considerable ingenuity may be exercised. Moreover, compromise is necessary, since some of the desirable conditions conflict with each other. A mathematical analysis of optimum conditions has not yet been developed, and the following guidance as to choice of boundary B is based on experience. A poor choice usually reveals itself by creating difficulties in obtaining satisfactory answers.

One good choice, as it will achieve rapid settling, is to make boundary B surround the main bulk of fissile material as closely as possible. But large statistical errors will be encountered unless the core multiplication is small, generally less than 2. This is discussed more fully in Section 4.2 below. For a larger core multiplication it is advisable to choose some surface inside the fissile material. If an air gap exists between the core and reflecting material, the outer surface of the core is a better boundary B than the inside of the reflector, because then all initial neutrons for each stage will enter the core directly, satisfying the importance criteria.

Frequently, and particularly with symmetrical or near symmetrical systems, it is a good plan to include a central plane with mirror reflections as part of boundary B. The neutrons tracked across this plane will settle to an eigendistribution, exhibiting the proper relative importance, except for outer parts of the reflector, which may be oversampled.

Oversampling, such as may occur here or in other cases, in the outer parts of a thick reflector can be avoided by use of a filter. A filter surface is defined so that only a specified proportion of the neutrons reaching it in the outward direction are tracked beyond it and the sample size is restored when neutrons arrive back at the filter.

Careful choice of boundary B and the judicious use of filters enable the tracking to be so arranged that the importance criteria are adequately satisfied.

3. Criticality Parameters - Calculation of k_{eff}

For the usual case in which the boundary B divides the system into a core and reflector, the criticality parameter MR is determined from the neutron counts. To obtain k_{eff} , the direct method is to repeat the calculation with the mean number of neutrons per fission, \bar{v} , divided by k. In this

way M and R are obtained as functions of k and, by interpolation, both $1/M$ and R , being linear in k over a small range, the value of k for which $1/M = R$ can be obtained. This value of k is equal to the required k_{eff} .

Alternatively, a close estimate of k_{eff} can be obtained directly from one calculation in the following way.

Of the S neutrons which enter the core, assume that a fraction l_0 escape and a fraction f_0 cause a fission. Of the ν_0 neutrons which arise on average from each of these fissions, assume that a fraction l_1 escape and a fraction f_1 cause a further (second-generation) fission.

In general, of the ν_{i-1} neutrons arising from an i^{th} generation fission assume that a fraction l_i escape and a fraction f_i cause a further fission. Then the quantities F and M_B may be defined by the following relations:

$$\begin{aligned} F &= S\nu_0f_0 + S\nu_0\nu_1f_0f_1 + S\nu_0\nu_1\nu_2f_0f_1f_2 + \dots; \\ M_BF &= S\nu_0f_0M_{B1} + S\nu_0\nu_1f_0f_1M_{B2} + \dots, \end{aligned} \quad (1)$$

where

$$M_{Bi} = l_i + \nu_i f_i l_{i+1} + \nu_i \nu_{i+1} f_i f_{i+1} l_{i+2} + \dots. \quad (2)$$

Here F is the total number of fission children produced in the sample and M_{Bi} is the total number of neutrons leaving the core as the result of one fission neutron born in the i^{th} generation.

Also, the surface multiplication M can be expressed as

$$M = l_0 + \nu_0 f_0 l_1 + \nu_0 \nu_1 f_0 f_1 l_2 + \dots. \quad (3)$$

Hence, by definition of k_{eff} ,

$$\frac{1}{R} = l_0 + \frac{\nu_0}{k_{\text{eff}}} f_0 l_1 + \frac{\nu_0 \nu_1}{k_{\text{eff}}^2} f_0 f_1 l_2 + \dots. \quad (4)$$

Algebraic manipulation of Eqs. (1) to (4) leads to

$$\frac{S(M - l_0)(M - (1/R))}{M_BF[(1/R) - l_0]} = (k_{\text{eff}} - 1)[1 + (k_{\text{eff}} - 1)\Phi(l_i, f_i \nu_i)], \quad (5)$$

where Φ is a function which is always finite and vanishes if $l_i = 1$, $f_i = f$, for all $i > 0$, and $\nu_i = \nu$ for all i .

MONTE CARLO NEUTRONICS CALCULATIONS

Hence, it follows that the equation

$$k_{\text{eff}} = 1 + \frac{S(M - l_0)[M - (1/R)]}{M_B F[(1/R) - l_0]} \quad (6)$$

gives the true value when k_{eff} is unity or near unity and gives a good approximation elsewhere. Furthermore, this k_{eff} is a perfectly valid measure of reactivity and can for all practical applications be used in place of the more usually defined k_{eff} .

The quantities used in Eq. (6) are all readily derived from counts printed at the end of the calculation, and the k_{eff} given in the print out is obtained from the use of this formula. There is a point about the interpretation of Eq. (6). The fundamental definition of k_{eff} is the multiplication in a cycle that starts and ends in a fission. The k_{eff} from Eq. (6) refers to a cycle that starts and ends in a fission in the core. These represent slightly different definitions for systems which have fissions in the reflector.

4. Statistics

The purpose of the tracking technique used in a Monte Carlo code is to obtain neutron samples representative of the eigendistribution of the steady-state system, and then to estimate some numerical index of reactivity. Due to the probabilistic nature of the processes involved, some statistical error is associated with the reactivity. It is necessary to obtain an estimate of the size of this uncertainty. Furthermore, since the eigendistribution is unknown at the outset, a statistical analysis is needed to ensure that the desired steady-state distribution has been generated and is being sampled.

4.1 Tests for Settling

The GEM procedure for the tracking cycle, whereby the "enter" neutrons for one stage are obtained from the "re-enter" neutrons of the previous stage, has been designed as an efficient way of generating an eigen-distribution. Two difficulties may arise. Firstly, the settling may be so slow that the early stages may not yield samples appropriate to the neutron eigendistribution on boundary B. Secondly, even if settling is rapid, successive stages may not lead to statistically independent estimates.

An analysis of variance has been applied to a number of GEM runs consisting of identical fissile cores in near-identical reflectors, so that the core surface multiplications were known to be the same. This indicated that any differences between the estimated core multiplications were due to chance variation; these runs had settled sufficiently to allow that parameter to be accurately and properly estimated.

Any interdependence from one stage to the next or following stages is likely to produce an oscillation or a gradual drift in the parameter to be estimated as the eigendistribution is reached. Under these circumstances the appropriate statistical test is the mean-square successive-difference test.(4) Alternatively, an analysis of variance may be applied to subsets of a number of stages. No evidence of interdependence has yet been found.

The conclusions drawn from these studies are that neutrons settle rapidly to the eigendistribution and yield proper and independent random samples from this distribution. It follows that the best estimate of a criticality parameter is that obtained by totalling all the various neutron counts over all the stages completed in the particular run.

4.2 Calculation of Statistical Error

The parameter MR measures the return of neutrons to boundary B. The aim of GEM is to estimate its average value. It can be shown that the frequency distribution of the "re-enters" arising from a single "enter" neutron on boundary B will have finite mean and variance. Hence, it follows from the Central Limit Theorem that the mean MR from samples of N neutrons will have a statistical distribution which tends to Normal as N tends to infinity. In such cases the calculation of standard error is straightforward.

The size of sample required to achieve sufficient Normality has been investigated, but no clear answer has emerged. Some typical histograms of MR are shown in Fig. 1 for two cases, one with a core surface multiplication of 1.7 and the other of 3.9. For the former the distribution from 200 neutrons is clearly Normal, and that from 100 neutrons is adequately so. In the second case, samples of 500 neutrons are required before the skewness diminishes. These histograms reveal the expected and generally observed phenomenon that for a given number of neutrons in the sample, the distribution of MR becomes wider and more skew as the core surface multiplication increases.

Goodness of fit, skewness, and kurtosis tests have been applied to a number of such histograms. They indicate that samples of 100 neutrons per stage, which is a convenient number for the computer, are usually adequately normal provided that the core surface multiplication is below 2. Only slight error is introduced here, and this is an overestimate of the true standard error. A confidence interval for MR may be obtained from Normal distribution theory.

MONTE CARLO NEUTRONICS CALCULATIONS

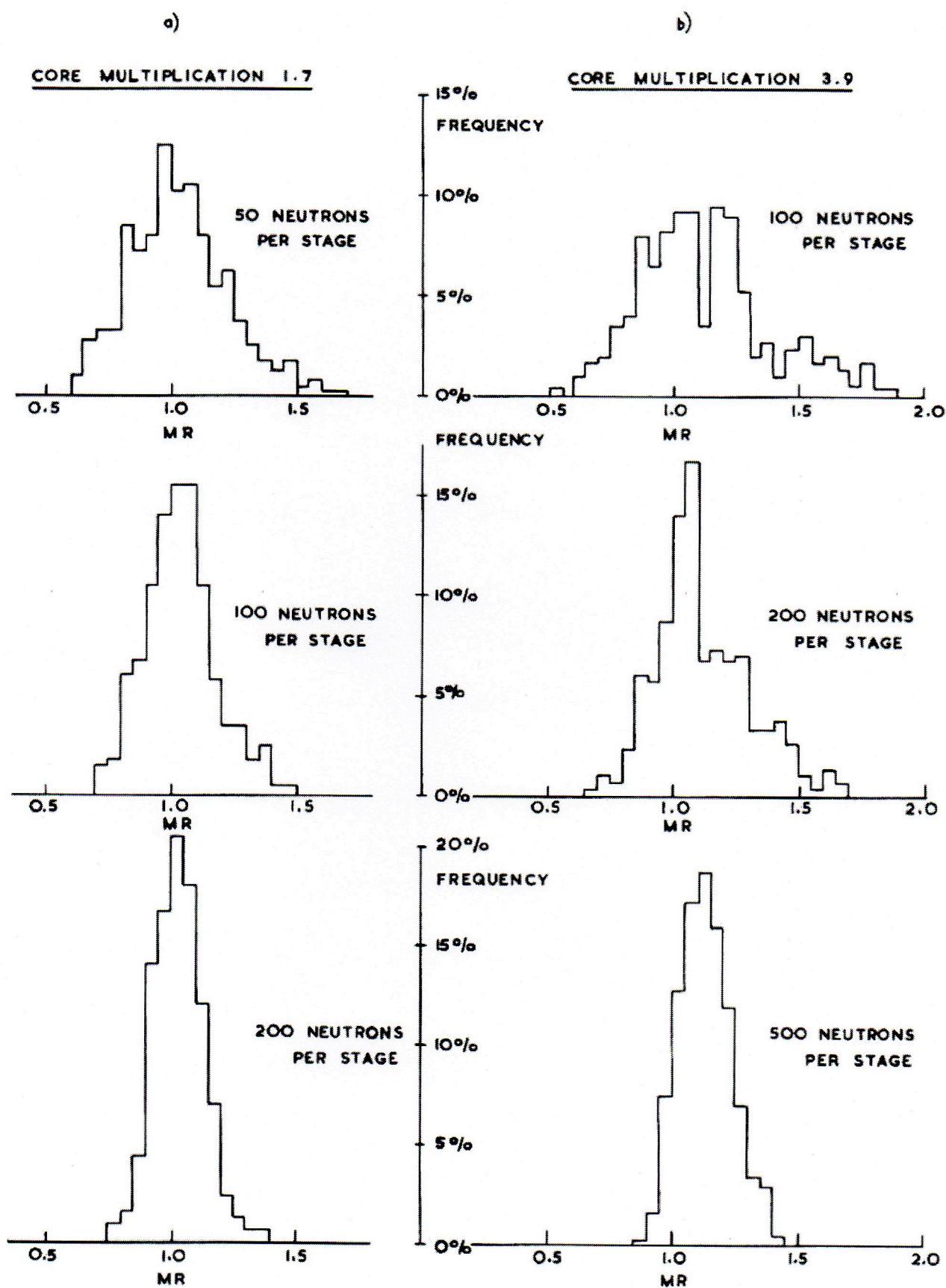


Fig. 1. Frequency Histograms of Distributions of MR

It would appear that a similar argument could be developed for k_{eff} . However, experience has shown that the frequency diagrams of k_{eff} exhibit considerable more skewness than those of MR, making it difficult to calculate the statistical error directly. It is easier, therefore, to consider k_{eff} as a parameter derived from MR. Figure 2 illustrates the relationship

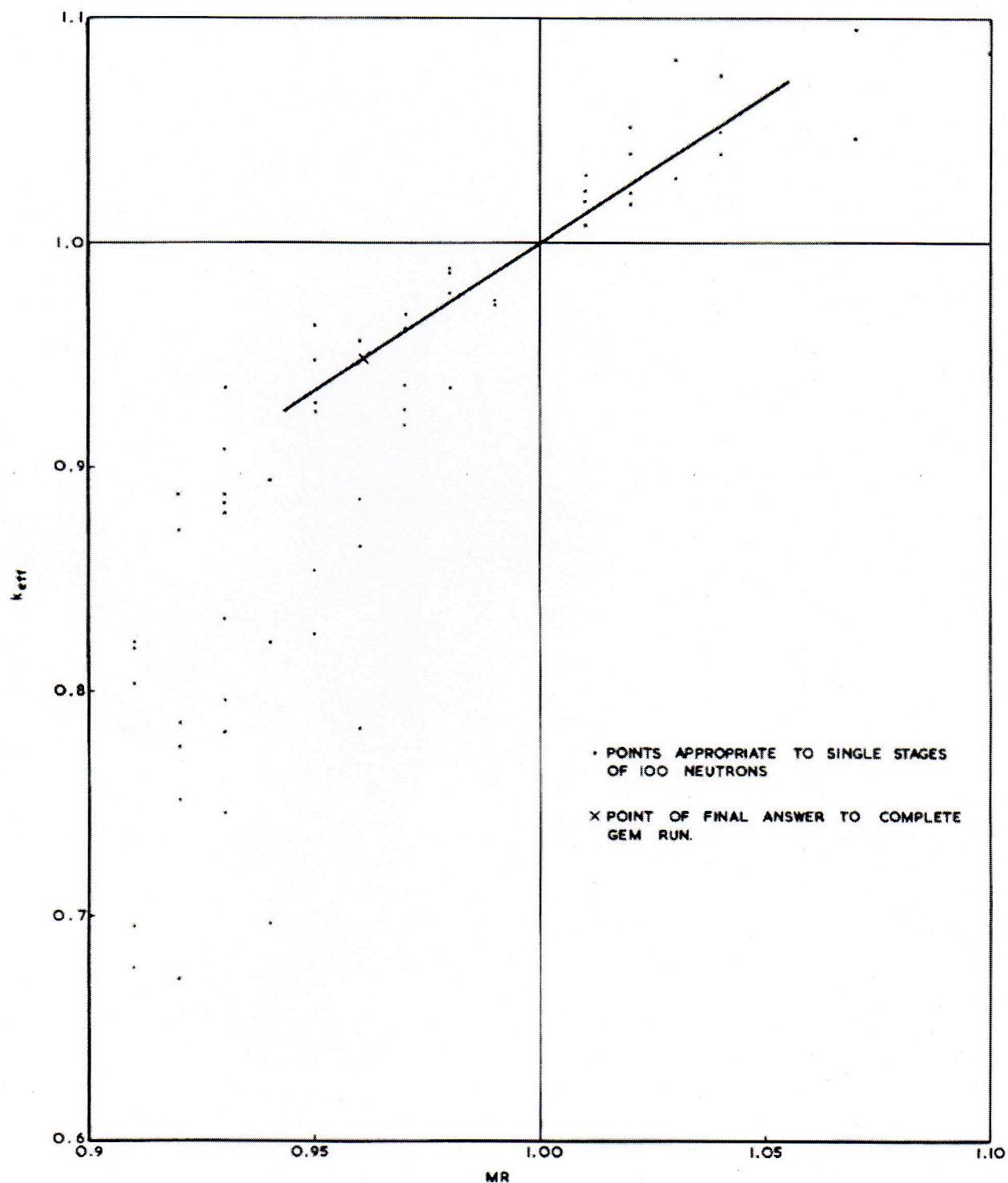


Fig. 2. Plot of k_{eff} against MR for Single Stages of 100 Neutrons

MONTE CARLO NEUTRONICS CALCULATIONS

typically obtained between k_{eff} and MR from single stages of a GEM run. These results were taken from the example discussed in Section 10.4 below. Any curve drawn for this relationship must pass through the point (1,1) and also through the mean point obtained by totalling all the counts. It seems reasonable to approximate to the correct curve by the straight line joining these points. Consequently, the relationship between the standard error of k_{eff} and that of MR may be derived from Eq. (6) as

$$\text{standard error of } k_{\text{eff}} = \frac{S(M - \lambda_0)}{RM_{\text{BF}}[(1/R) - \lambda_0]} \text{ (standard error on MR).} \quad (9)$$

5. Spectra and Flux Distribution

It can readily be deduced that when a steady-state neutron distribution has been achieved, whether in a critical system or in a subcritical system with an imposed neutron source, the flux of neutrons in any energy band in a given region is proportional to the total path length of neutrons in the region in that energy band divided by the volume of the region. In a critical system the factor of proportionality is immaterial, but if a source is present from which a total of N neutrons are started, the flux in neutrons per square centimetre per second will be equal to

$$\frac{\text{Total path length of neutrons in centimeters}}{\text{Volume of region in cubic centimeters}}$$

for a source of N neutrons per second.

Once the flux as a function of neutron energy is obtained, any desired reaction rate can be obtained as the sum over energy of the product of the flux with the macroscopic cross section for that reaction.

Fluxes and reaction rates are calculated in the GEM program in two ways. There is an option to calculate, during the tracking, the total path length in each region* in any specified energy groups. These path lengths are then multiplied by an arbitrary factor for each region, usually the inverse volume, and the results printed out.

Alternatively, the individual path lengths and corresponding neutron energies in specified regions can be read out on tape and subsequently analyzed by a subsidiary program, OPAL, which calculates both spectra and reaction rates. This latter method takes more machine time but will give

*The word "region" is here used in the special sense which is described below in Section 9.

the more accurate reaction rates, as it uses the precise energy of each neutron recorded and interpolates for the cross section at that energy.

6. External Source and Gamma-ray Problems

There is an option in GEM to specify an external source of neutrons which is usually, though not necessarily, specified as neutrons from a given spectrum and angular distribution emitted uniformly from a specified area of a certain surface. In this case the program will make a random choice of the variables to determine the coordinates of the start neutrons.

By use of the external-source option, with photon interaction data and scatter laws, calculations can be made for gamma-ray transmissions. However, since the tracking is basically by direct simulation, this method is suitable only for thin shields. For attenuations exceeding $\sim 10^{-3}$, it is better to use a program specifically designed for this type of calculation, such as UNC-SAM.(5)

7. Tracking Methods

The program is divided into two main parts: TRACK and CRASH. Of these, TRACK deals with the geometry of the system and the general organization, whereas CRASH deals with the nuclear data. In this section the flow pattern of the tracking is outlined. The following two sections give some detail of the manipulation of nuclear and geometrical data.

Each neutron is represented by a set of coordinates, defining position, direction of motion, energy, and history. These require eight 36-bit words to store.

At the start of each stage, the coordinates of a specified number of inward-moving neutrons, usually 100, on boundary B are available in the Birth Store. TRACK selects the first of these neutrons, and calls upon CRASH to calculate the mean free path and then, by a random selection, a path length, assuming the neutron remains in the same material. TRACK then compares this path length with the distance the neutron has to travel to reach the next interface. If the latter is the shorter, TRACK moves the neutron forward to that interface and starts the process again with the material on the other side. If the path length is the shorter, TRACK moves the neutron forward by this distance and calls upon CRASH to determine what happens at this collision point. CRASH will find, by a series of random selections, first the atomic nucleus involved, then the type of interaction and, finally, the directions and lethargies of the emergent neutrons. TRACK will then repeat the process with one of these neutrons, any others being stored at the top of the Birth Store to be picked up later. When, however, a neutron reaches boundary B again, moving inwards, it is placed in the Delay Store, and the next neutron taken from the Birth Store.

The stage ends when all the remaining neutrons are in the Delay Store. To start the next stage the specified number of neutrons are chosen at random from the Delay Store and transferred to the Birth Store. If there are insufficient neutrons in the Delay Store, some of them are chosen twice. During this whole process, counts are kept of all boundary crossings and of all neutron reactions and the various criticality parameters calculated.

8. Nuclear Data Routines - CRASH

The purpose of CRASH is to sample the Nuclear Data when requested by TRACK to provide a path length or to find the numbers, directions, and lethargies of neutrons emerging from a collision. The path length in a given material is derived from the total cross section and the parameters of emergent neutrons from the partial cross sections and collision laws.

8.1 The Total Cross Section

The total cross section of a composite material is obtained from the cross sections and atomic proportions of the constituent nuclides. In CRASH, the cross sections for each nuclide are obtained by interpolation from points given in the UKAEA Nuclear Data File.^(6,7) The energy points tabulated are chosen so that linear interpolation of log (cross section) against lethargy gives acceptably small errors. Each nuclide requires a different set of energy points, and CRASH can use either the complete set or a reduced set with a specified number of points, the reduction being such as to minimize the additional errors introduced.

8.2 The Type of Collision

When a collision has been found, the probability that this occurs with a particular nuclide N is given by the product of the macroscopic cross section for that nuclide with the mean free path in the material, and so random selection enables the nuclide to be identified. The next step is to determine the type of collision.

The probability that the collision is of a given type is just the ratio of partial to total cross section. These partial probabilities are approximated in CRASH by a step function of lethargy, typically with 64 or 80 steps, by a process designed to give a best fit to the original data. The position of the steps will vary from nuclide to nuclide.

Thus, by a random selection the type of collision can be determined. The numbers of collisions of each type with each nuclide are counted and recorded at the end of the print out as an action count.

8.3 The Emergent Neutrons

The final step is to determine the number, directions, and lethargies of all neutrons emerging from a collision. In the case of fission, the mean number of neutrons produced, \bar{v} , is obtained by interpolation and the actual number of emergent neutrons calculated by a random selection. If required, the value of \bar{v} can be multiplied by a specified constant before making the random selection, a facility which is needed if it is desired to calculate k_{eff} by interpolation.

If the collision results in a fission or isotropic scatter, the determination of the emergent direction is straightforward. In the general case of anisotropic scatter it has been found that a cubic equation of the form

$$\mu = a + bZ + cZ^2 + dZ^3 \quad (10)$$

gives an adequate representation, where Z is a random number, and $\cos^{-1} \mu$ is the angle between the directions of the incident and emergent neutrons in centre-of-mass coordinates. The coefficients a , b , c , and d are functions of neutron energy, and can be tabulated at sufficient points to allow linear interpolation.

This method gives a better representation and requires less machine storage than would be needed for tables of equiprobable angles.

In general, the energy of the emergent neutron is dependent on the incident energy and the angle of scatter. When it can be uniquely determined, the appropriate equation is used. In other cases, it is necessary to sample from a probability distribution, which is dependent on the incident and possible emergent energies. A particular case of a probability distribution occurs after a fission, for which the emergent neutron energies are found by sampling from a standard fission spectrum.

8.4 Thermal Neutrons and Multigroup Data

It is necessary to treat thermal neutrons in a different way, since at low energies both the motion of the nuclides and the forces acting between them can have significant effects.

Because of these complications, a multigroup structure has been adopted for neutrons below a specified energy, the group constants depending on the molecules present, rather than the atoms, and on the temperature. The energies of neutrons upscattered out of the groups are estimated by random selection from an exponential distribution.

The multigroup constants have to be determined by a preliminary calculation, e.g., using the PIXSE program.⁽⁸⁾ However, for some applications, a single group of neutrons below 0.1 eV with no upscatter has proved adequate. By extending the multigroup structure to all energies, GEM can use any of the standard sets of constants.

9. Geometrical Specification

The problem in GEM, as in any other field for which a complicated geometrical specification is required, is to devise a method which can readily be applied, which uniquely defines the system, and which can be understood by a computer. In GEM this is achieved by combining a basic specification, by which a system is divided into regions, with a detailed specification which may be used inside any region. The former is built into the program and requires the reading in of certain dimensions and arrangements, whereas the latter calls on special subroutines, called HOLE routines, specifically written for the job.

9.1 Basic Specification

The system is divided into regions by boundaries that form closed nesting surfaces, which may touch or coincide, but may not intersect. The geometry is referred to rectangular Cartesian coordinates in which the boundaries can take the form of spheres, centred at the origin, cylinders with the z-axis as axis or cuboids with edges parallel to the axes. One of these region boundaries is designated as boundary B, dividing the system into core and reflector.

When the boundary B is cuboidal, the core can alternatively be divided into cells, called boxes, by planes parallel to the coordinate plates. These planes need not be equally spaced, but they must pass right through the core, so that boxes do not overlap. Each box has its own origin of coordinates, although no rotation of axes is permitted, and it can be divided into any number of regions by its own individual set of nested surfaces. Boxes with different geometrical or materials content are given different type numbers. The complete core is then specified by listing the type numbers to give the arrangement of boxes, the position of each box being defined by a set of three integral coordinates. If the outer boundary of the reflector is cuboidal, it can be surrounded by a close-fitting specular reflector by specifying an albedo for each face.

For regions which contain only one homogeneous material, this is specified merely by its atomic composition and density. Otherwise, the geometry of an inhomogeneous region is detailed using the stratagem of the HOLE routine.

9.2 HOLE Routines

It is possible to reduce the mean free path in a material to any desired value by adding to the total cross section obtained from those of the constituent nuclides, a cross section for a fictitious reaction in which the neutron experiences no change. Thus, the mean free path for each of the materials in the region can be reduced to the same value and the collision point obtained, using this value, independently of any internal boundaries. The material at the collision is then identified by a routine which tests a series of inequalities. A random test then decides whether this is a real or fictitious collision; in the former case the appropriate collision routine is called and in the latter a new path length is found, and the process proceeds to the next collision point.

In order to check a HOLE routine a program BABS has been written which both checks that the routine links correctly with the main program and gives, to scale, a pictorial cross section of the geometry in any plane perpendicular to the coordinate axes. A typical BABS picture is shown in Fig. 3.

10. Examples

To illustrate the use of GEM a few examples are given.

10.1 A Simple Array of Nesting Uranium Alloy Cups

This example is included to illustrate the basic specification and to show the typical print-out given in Fig. 4. The problem was to find the reactivity of a flooded array of 12 units of two different types placed alternately. Each unit consisted of two uranium alloy cups one inside the other.

Referring to Fig. 4, the core boundary (boundary B) is represented as region 11, which completely surrounds the array. In the reflector, which consists of water, about 15.7 in. thick, a filter has been placed to ensure that only one-third of the neutrons in the outer layers of water are followed. The nesting cylinders shown for each type build up the units, and the arrangement shows how they fit together to form a $2 \times 2 \times 3$ array. The z-direction is treated as the vertical one, and the sequence of numbers under "Arrangement" gives the order in which the types are arranged in each of the three layers, i.e., $\frac{1}{2}^1$ in the lower, $\frac{2}{1}^1$ in the middle, and $\frac{1}{2}^2$ in the upper.

For each stage, the numbers of neutrons entering, leaving, and re-entering boundary B are printed together with the escapes from the system, core multiplication, reflector albedo, and k_{eff} . After each five stages a print is given of the neutron crossings of each boundary, and also a table

MONTE CARLO NEUTRONICS CALCULATIONS

which shows the numbers of neutrons entering each face of the core and the faces from which their descendants leave the core. Finally, a print is given of the total cumulated counts together with the criticality parameters MR and k_{eff} .

X VARIES BETWEEN -1.0000 AND 1.0000(LEFT TO RIGHT) AND
Y VARIES BETWEEN -1.0000 AND 1.0000(BOTTOM TO TOP)

Fig. 3. BABS HOLE Picture

*PR261

FLOODED ARRAY OF NESTING URANIUM ALLOY CUPS

HS/6013

TIME SINCE BEGINNING OF JOB = 21.28 MINS.

TRACK5 VERSION 5MJ 30.10.64

REFLECTED-LATTICE

2 DIFFERENT TYPES OF ELEMENT

ARRAY DATA

NUMBER OF ELEMENTS	2	2	3
PER CENT REFLECTION AT OUTER FACES, +	0	0	0
	0	0	0

ARRANGEMENT

2 1 1 2 1 2 2 1 2 1 1 2

GEOMETRICAL DATA

	REGION NUMBER	GEOMETRY	MATERIAL NUMBER	RADIUS	X	Y	Z
TYPE 1	1	CYLINDER	1	1.44150	+ -		0 -4.18550
	2	CYLINDER	2	1.64800	+ -		0 -4.39200
	3	CYLINDER	1	1.83550	+ -		0 -4.39200
	4	CYLINDER	2	2.05100	+ -		0 -4.60750
	5	CUBOID	1		+ -	2.65120 -2.65120	0.50000 -5.10900
TYPE 2	6	CYLINDER	1	1.63900	+ -		0 -4.17950
	7	CYLINDER	2	1.85050	+ -		0 -4.39100
	8	CYLINDER	1	2.03350	+ -		0 -4.39100
	9	CYLINDER	2	2.25150	+ -		0 -4.60900
	10	CUBOID	1		+ -	2.65120 -2.65120	0.50000 -5.10900
CORE	11	CUBOID	0		+ -	5.30240 -5.30240	1.50000 -15.32700
REFLECTOR	12	CUBOID	1		+ -	11.00000 11.00000	7.00000 -21.00000
	13	FILTER	POWER 3		+ -	21.00000 -21.00000	17.00000 -31.00000
	14	CUBOID	1		+ -		

DIMENSIONS IN INCHES

Fig. 4. Typical GEM Print-Out

MONTE CARLO NEUTRONICS CALCULATIONS

DENSITIES ARE SCALED UP BY 2.5400

THE VERSION OF CRASH IS MASH7 THE UPPER LIMIT OF THE THERMAL GROUP IS 0.1000 EV.

NUCLEAR DATA

MATERIAL	DENSITY	NUCLIDE PROPORTIONS BY ATOMS					
		H238	ONAT	U238	U235	ALNAT	
1	0.9980	2.0000	1.0000	0.	0.	0.	
2	3.1700	0.	0.	0.0700	0.9300	34.8890	

RANDOM NUMBER = 000000000001

STAGE 0 STARTS 64 FISSION NEUTRONS IN REGION 1, CO-ORDINATES (0., 0., 0.) BOX (1, 1, 2)

FINISH AT STAGE 25. 100 NEUTRONS PER STAGE

STAGES

<u>TOTALS</u>												
	ENTER	LEAVE	RE-ENTER	ESCAPE	MULT	REFL	ENTER	LEAVE	RE-ENTER	ESCAPE	MULT	REFL
1 TO 1 100		125	85	0	1.2500	0.6800	100	125	85	0	1.2500	0.6800
KEFF = 0.89934												
2 TO 2 100		175	110	0	1.7500	0.6286	200	300	195	0	1.5000	0.6500
KEFF = 1.02703												
3 TO 3 100		188	106	0	1.8800	0.5638	300	488	301	0	1.6267	0.6168
KEFF = 1.02165												
4 TO 4 100		96	64	0	0.9600	0.6667	400	584	365	0	1.4600	0.6250
KEFF = 0.53846												
5 TO 5 100		114	78	0	1.1400	0.6842	500	698	443	0	1.3960	0.6347
KEFF = 0.80198												
STAGES 1 TO 5												
TO +X	+Y	+Z	-X	-Y	-Z	BOUNDARY	IN	TOTAL	OUT	TOTAL	OUT/IN	TOTAL
FROM												
+X 55	48	2	0	0	2	1	1	293	293	280	0.9556	0.9556
+Y 70	16	74	8	9	6	12	2	314	314	360	1.1465	1.1465
+Z 21	9	11	16	13	8	3	3	368	368	412	1.1196	1.1196
-X 184	6	14	9	162	27	9	4	404	404	544	1.3465	1.3465
-Y 147	19	12	9	37	131	8	5	982	982	1067	1.0866	1.0866
-Z 23	1	1	0	1	1	13	6	327	327	312	0.9541	0.9541
							7	377	377	442	1.1724	1.1724
TOTAL 500	99+	114+	42+	222+	175+	46 = 698	8	428	428	493	1.1519	1.1519
							9	451	451	619	1.3725	1.3725
							10	997	997	1110	1.1133	1.1133
							11	443	443	698	1.5756	1.5756
							12	21	21	42	2.0000	2.0000
							13	7	7	14	2.0000	2.0000
							14	0	0	0	0	0

(ETC. TO STAGE 25)

REQUESTED NUMBER OF STAGES HAVE BEEN DONE

Fig. 4. (Contd.)

CUMULATED COUNTS		STAGES 1 to 25						
FROM	TO	+X	+Y	+Z	-X	-Y	-Z	
+X	479	469	40	23	22	51	22	
+Y	472	52	429	31	42	23	31	
+Z	204	28	24	178	31	20	3	
-X	681	37	77	37	630	83	47	
-Y	481	51	19	22	77	422	27	
-Z	183	31	46	8	39	33	148	
TOTAL 2500		668+	635+	299+	841+	632+	278 - 3353	
BOUNDARY NUMBER	(1) INS	(2) OUTS	(3) INS	(2)/(1)	(3)/(2)			
1	1092	1046		0.95788				
2	1227	1425		1.16137				
3	1442	1634		1.13315				
4	1594	2214		1.38896				
5	4169	4558		1.09331				
6	1295	1241		0.95830				
7	1442	1686		1.16921				
8	1681	1919		1.14158				
9	1769	2438		1.37818				
10	4054	4518		1.11445				
*** 11 ***	2500	3353	2233	1.34120	0.66597	UNFISSIONED INS ± 1393, OUTS ± 1803,		
12		215	120		0.55814			
13		72	40		0.55556			
14		0	0		0			
CORE. REFLECTOR.	MULTIPLICATION, REFLECTION TRANSMISSION	M	- 1.3412					
		R	- 0.6660					
		T	- 0					
		M*R	- 0.8932					
ACTION COUNT	STAGES 1 TO 25							
MATERIAL 1.	NUCLIDE	ABSORB	ELASTIC	(N,N*)	(N,2N)	(N,3N)	FISSION	FISSION CHILDREN
	H DASH	37	46261	—	—	—	—	—
	ONAT	0	6354	0	—	—	—	—
	THERMAL	1568	45457				0	0
	NEUTRON GAIN -	-1605						
MATERIAL 2.	NUCLIDE	ABSORB	ELASTIC	(N,N*)	(N,2N)	(N,3N)	FISSION	FISSION CHILDREN
	U238	2	13	2	0	0	0	0
	U235	65	159	10	0	0	136	334
	ALNAT	6	1618	47	---	---	---	---
	THERMAL	175	121				1000	2451
	NEUTRON GAIN -	1401						

SUM OF FISSIONS FOR ALL NEUTRONS LEAVING CORE = 5588

LIMIT OF 128 FISSIONS PER NEUTRON PER STAGE EXCEEDED 0 TIMES
KEFF = 0.94300TIME SINCE BEGINNING OF JOB = 35.98 MINS
TIME TAKEN FOR THIS CASE = 14.70 MINS

Fig. 4. (Contd.)

10.2 A Lattice of Rods in Water

The second example is a calculation made, as a check on the nuclear data, to reproduce an experimental measurement of critical size of a lattice of $\text{PuO}_2\text{-UO}_2$ rods in light water reported from Hanford.⁽⁹⁾ The rods, of 0.372-in. diameter and 48.5 in. long, were loaded at a spacing of 0.80 in. in a hexagonal lattice and completely reflected by water.

For this calculation the core was taken as a single cylindrical region and the hexagonal lattice geometry incorporated by means of a HOLE routine. In the HOLE routine for a hexagonal lattice it is convenient to make the transformation

$$\begin{aligned} X &= N + \frac{2x}{\phi\sqrt{3}}; \\ Y &= N - \frac{x}{\phi\sqrt{3}} + \frac{y}{\phi}; \\ Z &= N - \frac{x}{\phi\sqrt{3}} - \frac{y}{\phi}, \end{aligned}$$

where ϕ is the lattice pitch and N is an integer large enough to ensure that X , Y , and Z remain positive. All values of X , Y , and Z such that $X + Y + Z = 3N$ then represent points in the x , y plane, and the lattice points are given by integral values of these coordinates.

By making use of this latter property the nearest lattice point to X , Y , Z can readily be found, and a test can then be applied to ascertain whether or not the point is inside the rod centred at that position.

A BABS picture from this HOLE routine is given as Fig. 3, in which 1 represents water, 2 fuel, and 3 cladding.

A time of 87 min was taken on the IBM-7090 for this problem, during which 44 stages were completed and the k_{eff} was calculated to be 1.011, with a standard error of 0.01.

10.3 An Experimental Graphite Moderated Reactor

The Dragon reactor, as described at the third Geneva Conference,⁽¹⁰⁾ has a core built up of hexagonal elements,* each containing 7 fuel rods embedded in graphite, and the reflector is of graphite.

For the purpose of calculation, the complete core was broken into elements of the shape shown in Fig. 5. For convenience the shape of the coolant channels was altered slightly, but, apart from this, these elements fit together to make a core identical with the Dragon core.

*See Fig. 5 of Ref. 10.

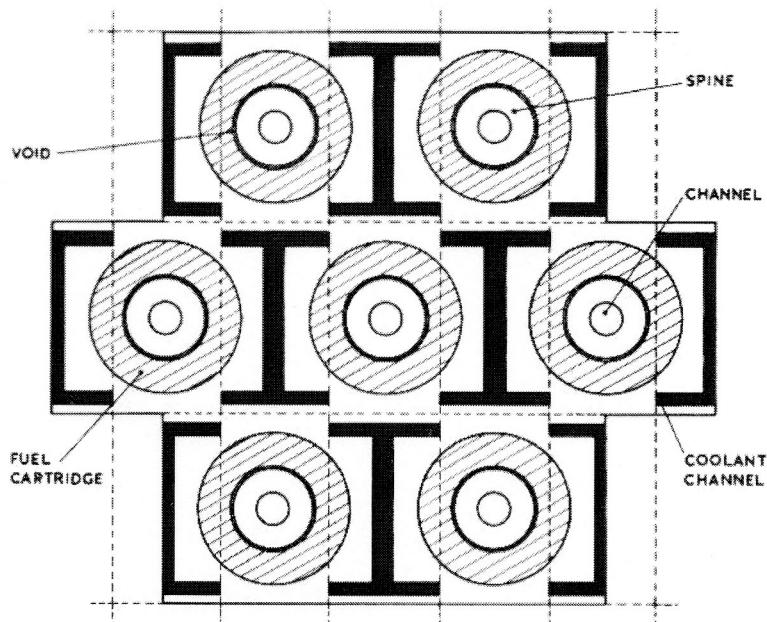


Fig. 5. Fuel Element (See 10.3)

Each element was divided into boxes by the dashed lines shown in the figure. In each box a simple HOLE routine was needed to allow for the fueled region, but the rest of the geometry could be built up of the basic shapes. The boundary B was chosen to be cuboidal, with one face bisecting the reactor horizontally, one lying along the top of the core, and the other four enclosing the core as closely as possible. Outside was a reflector, being 100% specular on the bisecting plane and the correct thickness of graphite elsewhere. Thus the core for calculations was a lattice of size $37 \times 21 \times 1$.

For one particular loading calculated, 50 stages were run in 38 min and a k_{eff} of 1.115 obtained, with standard error 0.01.

10.4 A Thermal Power Reactor

A calculation, for which the statistical analysis of the results is discussed in Section 4.2 above, was for a gas-cooled graphite-moderated power reactor. The core of this reactor consisted of cylindrical fuel elements, control rods, experimental channels, etc., arranged on a hexagonal lattice. Each element consisted of a number of fuel pins. The elements, except for a few treated separately, were spaced widely enough for the core to be built up of cuboidal boxes, alternate ones containing fuel elements and the others graphite moderators. A HOLE routine was required to describe the geometry of the elements. Again, boundary B was chosen to include a horizontally bisecting plane, and the core consisted of a lattice of $41 \times 23 \times 4$ boxes. A typical calculation of this series took 120 min for 100 stages and gave a k_{eff} of 0.948, with a standard error of 0.01.

MONTE CARLO NEUTRONICS CALCULATIONS

References

1. Breton, D., H. C. Paxton, and E. R. Woodcock, Critical Arrays of Transport Packages, International Atomic Energy Agency, Technical Report in Course of Publication.
2. Parker, J. B. and E. R. Woodcock, Monte Carlo Criticality Calculations, Progress in Nuclear Energy, Series IV, Vol 4, p. 435, Pergamon Press, Oxford (1961).
3. Woodcock, E. R., "Fundamentals of Criticality Control" in Criticality Control in Chemical and Metallurgical Plant, OECD European Nuclear Energy Agency, Paris (1961).
4. Hald, A., Statistical Theory with Engineering Applications, John Wiley & Sons, Inc., London, New York (1952), p. 357.
5. Eisenman, B. and F. F. Nokache, UNC-SAM: A Fortran Monte Carlo System for the Evaluation of Neutron or Gamma-ray Transport in Three-dimensional Geometry, United Nuclear Corporation Report UNC-5093 (Aug 1964).
6. Barrington, E. P., A. L. Pope, and J. S. Storey, The Data in the Winfrith Nuclear Data Library: July 1963, UKAEA Report AEEW-R351 (1964), available H. M. Stationery Office.
7. Parker, K., The Aldermaston Nuclear Data Library as at May 1963, UKAEA Report AWRE 0-70/63 (1963).
8. MacDougall, J. D., PIXSE, UKAEA Report AEEW-M318 (1963); available H. M. Stationery Office.
9. Schmid, L. C. et al., Critical Masses and Bucklings of PuO₂-UO₂-H₂O Systems, Trans. Amer. Nucl. Soc. 7 (No. 2) 216 (1964).
0. Shepperd, L. R. et al., Review of Research and Development Work for The Dragon Project, Third United Nations International Conference on the Peaceful Uses of Atomic Energy, p. 122 (1964).

Discussion of Paper Presented by Mr. Woodcock

MR. MILLER (Argonne National Laboratory): I understand this code represents the cross sections quite accurately. You have the energy of the resonance cross sections and, in some regions, very high cross sections.

Then you make the cross section in other regions equal to this, introducing a large number of interactions for a neutron crossing a region which has, physically, a small cross section. Can you give me some idea of the effect this has on increasing computing time?

MR. WOODCOCK: There are two cases. If one material has a high cross section over an extended range of energy, such as in the case of a control rod, it is better to separate that material into a separate region. But in the case of a resonance--a comparatively narrow area of very large cross section--the chance that a neutron is actually of the right energy for that resonance to need a large number of small steps is comparatively small. In fact, I think the best thing to say about this is that we have done quite a number of calculations with U²³⁸ and other materials, and there has been no indication that the time of computation has been increased unduly because of this effect.

MR. IRVING (Oak Ridge National Laboratory): How do you handle the angular distributions and the inelastic scattering in the program?

MR. WOODCOCK: I doubt whether I can say very much in a few words. We take the AWRE data file which contains tabulated values, giving an angular distribution. We have, up to the present, tended to take the value from this tabulated list by interpolation. We are now in the process of changing these tabulated values back into some formula which gives the angular scatter as a function of a random number. This sort of formula takes up less space in the machine and also has the advantage that one can interpolate over energy more easily. For inelastic scatter energy loss we apply a standard formula.

MR. WADE (AERE, Harwell): Can you tell me what treatment of thermal-neutron scattering you use?

MR. WOODCOCK: In the current system neutrons below a certain energy, which we specify, are treated in multigroup fashion. The multigroups are obtained from calculations at Harwell. We are planning to extend this by dividing the energy range into three regions.

We will treat the higher-energy region, in which there is a negligible probability of an upscatter, as in our present general treatment. In the low-energy region a multigroup representation will be used. In an intermediate region we can use a simple formula for a distribution of neutrons from an inelastic scatter. We are looking into the possibility of incorporating that type of scheme.

MR. CHURCH (Savannah River Laboratory): I missed your justification for replacing the actual cross section of a region by the cross section of the surrounding medium.

MONTE CARLO NEUTRONICS CALCULATION

MR. WOODCOCK: In a Monte Carlo calculation if one gets a neutron passing through regions, one has to calculate each boundary crossing point before he can find a collision point. This calculation takes quite a lot of machine time. By doing this trick with cross sections we ensure that a mean free path in each of these regions is the same, so we can find the collision point without having to find the point at which the boundaries have been crossed. Having found a point in this system, the arithmetic to find out which material that point is in is a much simpler and quicker problem. It also has the advantage that these HOLE routines for this different geometry can be written as separate subroutines which can be plugged in. We are gradually building a library of those.

MR. BRICKSTOCK (AWRE, Aldermaston): What are your criteria for determining when k has settled down to an equilibrium value, bearing in mind the statistical deviations for the k values you determine?

MR. WOODCOCK: First of all, we use MR as the fundamental parameter. We first want to find when MR has settled down to its correct value and then deduce the k from it. This is the standard type of statistical test. One can compare the value coming out of successive samples and compare these with the mean values.

MR. BRICKSTOCK: Suppose you have an MR value that is varying slowly; you must relate the rate of change of this to the statistical deviation. At what stage do you say that it is not changing?

MR. WOODCOCK: This doesn't happen. We don't get a monotonic change in MR.