MONTE CARLO METHODS FOR SHIELD DESIGN CALCULATIONS

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ABSTRACT

A suite of Monte Carlo codes is being developed for use on a routine basis in commercial reactor shield design. The methods adopted for this purpose include the modular construction of codes, simplified geometries, automatic variance reduction techniques, continuous energy treatment of cross section data, and albedo methods for streaming. Descriptions are given of the implementation of these methods and of their use in practical calculations.

1 INTRODUCTION

The objectives of the work on Monte Carlo at Winfrith have been to develop methods which can be used by engineers for commercial reactor shield design. The central problem in practical shielding calculations is the determination of radiation attenuation in systems with complicated geometries. Whilst Monte Carlo is the obvious choice of method for treating problems with strong geometric effects, it is not well suited to deep penetration calculations. Two general lines of approach have been adopted to overcome these difficulties: semi-analytic techniques exploiting the well-tried removal and albedo approximations are used for the treatment of streaming phenomena in ducts and voids; and adjoint diffusion theory solutions furnish approximate importance functions for acceleration in bulk penetration problems.

This marriage of the conventional methods which have long been established for shield design with Monte Carlo in "hybrid" calculations has proved to be the deciding factor which has led to the extensive use of Monte Carlo as a shield design tool in the United Kingdom. Thus Dutton, for example, used line-of-sight formulae to calculate neutron sources from AGR fuel clusters for the Monte Carlo treatment of the PCRV penetration-head region [1]. Similarly, Avery and Pugh used two-dimensional Monte Carlo to investigate streaming phenomena in the refuelling machine of the Magnox station at Trawsfynydd [2]. Avery and Warman have employed an albedo-Monte Carlo method in calculating the streaming of neutrons and gamma-rays along air gaps and passageways between the vessel and primary shield of a PWR [3]. The use of diffusion theory in adjoint mode to provide approximate importance functions for accelerating Monte Carlo calculations has been demonstrated by Bendall and McCracken [4].

This paper describes how the methods of coding, data handling and variance reduction have evolved as a result of this emphasis on design applications. The calculational scheme is under continual development to meet the changing needs of reactor programmes; the current status of codes is reviewed, and some indication is given of future trends.

2 GENERAL DESCRIPTION OF THE METHODS

The capabilities outlined above are being provided for shield designers in the form of codes of modular construction [5]. There are two levels of approximation in the basic suite of modules, the Monte Carlo options being supplemented by the fast and approximate methods based on line-of-sight, kernel albedo, and diffusion theory in the various forms used for shielding applications (eg the COMPRASH removal-diffusion method [6] and the Adjusted Diffusion Coefficients (ADC) Method [7]). Apart from their role in the hybrid Monte Carlo calculations these approximate methods furnish a powerful range of tools in their own right for rapid survey calculations and for repetitive runs in shield optimisation studies. The codes and methods developed at Winfrith are complementary to the generalised geometry code MONK which is the subject of another paper at this Conference [8]. This code is used primarily for criticality applications, but it can be utilised for shielding studies where the geometric capabilities are essential for an adequate representation of the problem.

There are a number of special features required for Monte Carlo methods used for shield design. The code system must be flexible so that it is easy to introduce new capabilities as different problems arise. Speed of execution and economical storage requirements are important, and these may even have to be pursued at the expense of some accuracy. It is also essential to reduce as far as possible the degree to which the efficiency and accuracy of the codes depend on the expertise of the users or on preliminary trial runs. Key features which have been developed specifically to meet these requirements include:

(i) modular construction of codes;

(ii) simplified geometries or specially written geometry modules;

(iii) automatic variance reduction facilities;

(iv) a continuous energy treatment of data so that the user is not left with the choice of basic material parameters which affect the accuracy of the calculation;

(v) albedo methods for the solution of streaming problems.

It will be convenient to discuss the shielding code scheme under these five headings. At present, it comprises a series of modules from which a variety of Monte Carlo codes can be assembled. These can be used on a stand-alone basis. Alternatively, they can be coupled to diffusion modules, run in the adjoint mode, for the automatic generation of importance functions in bulk penetration calculations, or to kernel-albedo modules for semi-analytic solutions of streaming problems, in a range of one-, two- and three-dimensional geometries.

3 THE WRS MODULAR CODE SYSTEM

3.1 Relation to other schemes

While the modular approach to programming is now common [illegible] the particular forms which it takes are very varied, reflecting the [illegible] requirements of their users. Basically, the term "modular" implies [illegible] the following approaches:

(i) the assembly of programmes from units or "modules" with the linkages achieved via the fast store;

(ii) the performance of a calculation by means of several separate computer runs with automated data transfers via backing store.

The Winfrith Radiation Physics and Shielding Group (WRS) System [ ] falls into the first category. Programmes assembled from WRS modules are Fortran programmes running under the normal operating system but using standardised coding techniques and standard routines for house-keeping. The aim is to improve the ease and flexibility with which codes can be constructed, especially for the complex series of steps frequently required in a shield design calculation. It is because these calculations include iterative processes, of which the Monte Carlo tracking cycle may be classed as one, that the WRS system concentrates on the construction of single codes rather than automated linkages between separate computer runs as in the second of the basic approaches mentioned above. However, for calculations which can be run efficiently as separate jobs this second approach can be made very powerful through the use of a highly organised data base with special data management routines as, for example, in the COSMOS system [10] which has been developed at Winfrith. The two approaches are complementary since the basic unit in the COSMOS scheme is a code, and this code may be one assembled from WRS modules. Thus, if the shield designers using WRS codes require extensive data banking facilities or automated links with core calculations then these are available through COSMOS.

3.2 Description of the WRS system

A WRS module consists of one or more subroutines. A programme is assembled from one or more modules together with a linking module (a Fortran main programme possibly supplemented by subroutines) which controls the logical flow of the calculation. The ease and flexibility of code construction is achieved through two main features. The first is the convention that a module must be capable of accepting its initial data either from cards or from a general location in core store or on backing store. A similar rule applies to the output, with the line printer replacing the card reader. This provides considerable flexibility since the same module can be used, for example, either on a stand-alone basis (with just a very simple linking module) or as part of a programme in which some or all of its initial data is calculated by other modules. The second feature is the method for the dynamic storage of data in core and on backing store. The data in core resides in a single array in a common [illegible] ". The first partition is a list [illegible] groups in [illegible]. [illegible] required, [illegible] groups [illegible]. [illegible] keep of the [illegible] programmer, who needs only to know [illegible].

[illegible] Use in Monte Carlo programming

The WRS system is [illegible] described in Section [illegible]. [illegible] value in the assembly of [illegible] of source sampling, tracking, collision [illegible], scoring. Experience was [illegible] the system [illegible] for writing the prototype XY geometry [illegible] McBOX [illegible] which was [illegible] primarily as a test-bed for variance reduction [illegible] (see Section [illegible]). Modular programming necessarily [illegible] but these can be minimised in a well designed [illegible]. The [illegible] which must be considered are speed of execution, storage requirements, and programming complexity.

(i) The problem of execution speed is especially critical in Monte Carlo codes, in which modules are entered many thousands of times and any fixed overheads are multiplied correspondingly. Care was taken in the writing of McBOX to avoid these overheads during the generation of particle histories so that the efficiency of the code is not significantly impaired by its modular nature.

(ii) There are two factors which lead to an increase in the storage requirements of WRS programmes. The first is the presence of the system routines which occupy 25 K bytes, and the second is the presence of the full input and output options in every module. However, the latter are often written as separate subroutines so that space can be saved through the use of an overlay. In addition, the dynamic storage system ensures that very economical use can be made of the data storage area by keeping the storage compacted and by removing data when it is no longer required.

(iii) It is a feature of all but the simplest modular systems that the initial task of programming becomes protracted and more complex. This is acknowledged to be true of the WRS system, though by no means to an unacceptable degree.

Experience with the use of the system has confirmed the view that the extra initial coding effort is repaid ultimately during the assembly of large programmes. The ability to use modules on a stand-alone basis has been found useful during the testing stages, which are often especially lengthy and difficult in the case of Monte Carlo codes. The system also provides a very convenient way of linking Monte Carlo with the approximate methods for the types of hybrid calculation described in the Introduction.

4 GEOMETRY

In planning the geometric capabilities of Monte Carlo codes for shield design there are two possible approaches:

(i) to provide a very general three-dimensional capability;

(ii) to rely mainly on the use of simple (but including three-dimensional) geometries, and to write special geometry routines for specific applications when necessary. (The term "simple geometry" is used here to signify that the material boundaries are surfaces of the form α = constant, where α represents any of the co-ordinates.)

The second of these methods has been adopted in the interests of computing speed and on the basis of past experience which has shown that many practical shielding configurations can be adequately represented by means of simple geometries and that the input data for such representations can be quickly set up.

Thus the modules now written allow the tracking of particles in XYZ and RZ geometries (and therefore also in X, XY or cylindrical geometries), and these can accommodate a wide range of practical design problems. However, in the fast reactor and HTR fields there is a need to represent internal shields and core/breeder configurations in triangular-prismatic geometry with provision for the introduction of cylindrical regions representing fuel channels, control rods or, in the case of a sodium-cooled fast reactor, materials testing rigs containing cylindrical specimens. The McRIG code [12] has accordingly been written for this purpose, initially in two-dimensional geometry in which the horizontal reactor plan consists of a mesh of equilateral triangles on which are superimposed circles which may be nested. Within each triangle the technique of Woodcock tracking [13] is used, in which the collision points are determined using the mean free path corresponding to the highest cross section of any material in the triangle. At each point the ratio of the true cross section to this maximum cross section is calculated, and using this ratio as a probability a choice is made between a real reaction and a pseudo-reaction in which no change of energy or direction occurs. This method has the advantage that it is not necessary to calculate distances to region boundaries within the triangle but only to test whether a co-ordinate is inside or outside a region. There is a danger that this saving of effort will be offset by the generation of large numbers of pseudo-collisions if there are materials present with widely different cross sections. However, this has not proved to be a problem in the application of McRIG to gamma-ray heating in fast reactor cores. This is probably due in part to the particular geometric configurations, and also to the fact that the energies at which widely different cross sections occur are unimportant.

While this approach provides geometry capabilities adequate for a large range of problems it is essential to have a more general code for those which are not amenable to a simplified representation and which are not sufficiently common to warrant specially written geometry modules. Reference has already been made to the general Monte Carlo code MONK developed at Risley. An example of this type of problem occurred in the design of the Prototype Fast Reactor when the general geometry code GEM [14] (the forerunner of MONK) was used in calculations for the fuel storage rotor which involved both neutron multiplication and deep penetration [15]. In the field of HTR shield design and in some detailed studies of gamma-ray heating in fast reactors (such as a partially inserted control rod) there is an increasing demand for three-dimensional calculations in triangular-prismatic geometry to be carried out on a routine basis. It is accordingly proposed to incorporate the Z co-ordinate into McRIB to simplify the task of specifying the geometry in such problems which are at present tackled using MONK.

5 VARIANCE REDUCTION METHODS FOR PENETRATION CALCULATIONS

5.1 The use of a calculated importance function

For use in shield design applications acceleration techniques employing splitting and Russian roulette have the advantages of being relatively simple to apply, of being sufficiently powerful for deep penetration problems, and of being useful in a wide range of applications. The method was implemented in a simple form in the RZ geometry programme McNID [16], in which splitting and roulette are applied at spatial surfaces with a fixed splitting power of two. This approach has the disadvantages that no allowance is made for the energy dependence of the importance function and that considerable initial experimentation is often required to find the best position for the splitting surfaces. A considerably improved method was used by Bendall in the prototype one-dimensional code McBEND [4] in which splitting and Russian roulette may occur at collision points and at points distributed uniformly along a particle track. At each point the degree of splitting is determined by reference to an importance function which may depend on position, energy, and direction. It was demonstrated that the use of an approximate importance function obtained from an adjoint removal-diffusion calculation was very effective in accelerating the calculation of a specific pay-off.

The extension of this method to higher dimensions was not immediately possible owing to the lack of a sufficiently fast two-dimensional removal-diffusion programme. This obstacle has now been removed by the development of a method of adjusted diffusion coefficients (ADC) [7] which eliminates the lengthy calculation of first collision sources, and also by the introduction of improved methods for the solution of the diffusion equations [17]. It is now proposed to investigate the further extension to three dimensions by using the diffusion programme SNAP [18] in adjoint mode to calculate importance functions.

5.2 A self-adjusting acceleration method

A method has been established for circumventing the difficulty of calculating importance functions in the rather different, but not uncommon, class of problem in which uniform accuracy is required over a wide range of energies and positions. This is frequently the case, for example, in a gamma-ray heating calculation in a reactor core, and it was the type of output needed from the one-dimensional reference calculations to which diffusion solutions were fitted in the production of adjusted coefficients for the ADC method mentioned above. The technique, which has been tested in the prototype XY geometry code McBOX, is to arrange for the programme continually to adjust importance values on the basis of the histories so far generated, with the aim of assisting the penetration of particles to all parts of phase space in roughly equal numbers. The source module of McBOX samples from a distribution $S'(x,y,E)$, and if the true source function is $S(x,y,E)$ it assigns a weight $T = S(x,y,E)/S'(x,y,E)$ to the particle. For the purposes of the splitting and Russian roulette process the phase space of points (x,y,E) is divided into a number of regions, each of which has an importance value denoted by I. It is convenient to regard $W = 1/I$ as the "region weight". Particles have a tracking weight U which is initially 1 and which is separate from the source weight T so that the total weight used in flux estimation is the product of T and U. Splitting or roulette may occur when a particle enters a new region by crossing a spatial boundary, by suffering an energy loss which transfers it to another region, or when it is first generated as a source particle. The expected number of particles produced is equal to U/W, the ratio of the old particle weight to the weight of the new region. The actual number of particles is selected by random sampling from the integers on either side of this ratio, and the weights of the particles (if any) are divided by this integer. This method ensures that the expected values of the particle weights are equal to the region weights themselves, but the weights within any region are of course distributed somewhat because only integral numbers of particles can be produced by splitting and roulette.

The quantity which the programme calculates for use as a region weight is the "current" entering the region. This is a quantity which would be observed with a true source $S'(x,y,E)$ and no splitting. When splitting is in operation the current from a given number of source particles is estimated by $(\Sigma U)/V$ where V is the region volume and the summation is taken over all particles entering the region. Thus, when the weight adjustments have settled down we have

$$W = (\Sigma U)/V$$

and since the particle weights have a mean value W this implies that the number of particles entering any region is proportional to its volume. This is the quantitative interpretation which has been given to the requirement for particles to be distributed evenly throughout phase space. While this criterion probably gives an approximation to the optimum conditions for most problems of this type, it cannot of course always guarantee equal variances in all regions. For example, the errors still usually increase with distance from the source since the tracks tend to be more highly correlated at larger distances. It is also not always possible to apply the splitting method without modification. It has been found necessary, for example, to limit the number of particles produced by splitting to a maximum of 10 in order to avoid inefficiency in problems in which there is the possibility of transfers between regions of very widely differing weights.

Subject to these qualifications the method has proved to be useful, especially in easing the task of the user in this type of problem. It is, of course, essential for efficiency that the weights should be substantially determined within some reasonable fraction of the total running time. This has been achieved in the applications so far tested in which, for example, the weights had settled down to reasonable values within four minutes of a 30 minute run for neutron penetration through 80 cm of iron.

6 THE HANDLING OF DATA FOR PENETRATION CALCULATIONS

6.1 Neutron data

The choice of a scheme fcr handling interaction data must be made in the face of conflicting demands.

(i) The methods and data must be simple enough to ensure speed of execution and economy of storage.

(ii) The treatment must be sufficiently detailed to give the required accuracy in a wide range of problems.

The scheme which is used in the Monte Carlo shielding codes at Winfrith is the DICE system [19] which consists of two parts:

(i) a programme MOULD which processes data from the UK Nuclear Data Library into a form suitable for use during Monte Carlo tracking and writes it onto a tape;

(ii) a suite of routines which are loaded with the Monte Carlo programme and are called to calculate mean free paths and to determine the outcome of interactions.

In this system energy is treated as a continuous variable but the cross sections (both total and partial) are assumed to be constant in each of a number of groups. These groups, which must be the same for all elements, can be chosen when the data tape is generated by the MOULD programme, which calculates the cross sections by averaging the UKNDL values over each group. Angular distributions are also converted by MOULD into a more convenient form which consists of equiprobable ranges within each of which the probability is assumed to be constant. 32 equiprobable ranges have normally been used. Energy distributions for scattered neutrons are taken from the UKNDL without alteration except that continuous probability distributions are again expressed in terms of equiprobable ranges (64 in number).

As a compromise between the conflicting requirements noted above, the cross sections have normally been represented in 300 DICE groups covering the range 0.025 eV to 15 MeV with equal lethargy intervals. This group size is sufficiently narrow not to require the group averaging process to take account of broad variations in the shape of the flux spectrum. On the other hand, the groups are too wide to follow cross section changes in the vicinity of narrow resonances, and it is therefore necessary to consider the effect of using average values in such regions and to examine the averaging process used. The programme MOULD calculates the group averaged microscopic cross sections for each element using as its weighting factor the reciprocal of the total cross section for the element. Thus, for a pure element the weighting factor approximates to the asymptotic infinite medium flux shape $(E \xi \Sigma_t)^{-1}$, since the energy E and the mean logarithmic energy decrement ξ are almost constant over such a narrow group. In this case the error will therefore depend on how far the spectrum differs from this asymptotic shape. In the case of a mixture of elements an error is introduced since the averaging is done before the macroscopic cross section is calculated and it does not therefore take account of the environment of the element.

6.2 Tests of neutron data

These effects are currently being examined, principally in the context of benchmark experiments [20] performed in the ASPIS shielding facility at Winfrith in which the source is a conventional fission plate. The standard scheme with 300 DICE groups has been used in calculations for an experiment in which spectra were measured in a thick iron shield. As can be seen in Figure 1, the calculated fluxes below a few hundred KeV are higher than the spectrum obtained from proton-recoil counter measurements by up to a factor two. In order to find out whether these differences can be attributed to the cross section representation in this region of narrow resonances and minima some tests have been made in which very much finer DICE groups were used. For these tests the MOULD programme was rerun to process the same basic data into about 1000 groups above 10 KeV. Figure 2 shows in a small but typical energy range how the standard group scheme fails to follow the cross section variation, and that while even the 1000 group scheme is not completely adequate it is sufficient to provide a test of the effect of a finer representation. A one-dimensional case with a plane fission source was used and the flux at up to 70 cm from the source was calculated in fairly broad groups (similar to those used in the ASPIS calculation). The McBOX programme was run for long enough (15 minutes CPU on an IBM 370/165) to give standard deviations of about 10% for the group fluxes. No statistically significant differences were found between the results obtained with the standard scheme and the fine group scheme. With the broad group scoring it was not possible to observe the differences of fine structure which were undoubtedly present, but the result shows that a finer cross section representation does not significantly alter the general flux level. It is concluded that the observed differences from the measured spectra are not due to the cross section representation, and that in problems similar to this the normal DICE group scheme is adequate for predicting at least those response functions which do not show a rapid variation with energy.

6.3 Data sensitivity calculations

Tests of this kind involving the comparison of independent Monte Carlo runs are often difficult because the differences are masked by statistical errors. The problem arises also in calculating the sensitivity of results to small changes in the basic data itself. A way of overcoming this difficulty is to use the same set of histories for both cases and to take account of data changes by means of weighting factors [21]. Consideration is being given to the use of this method for the data sensitivity calculations which are required in shield design problems with complicated geometries in order to identify the major sources of error and to make error estimates. For the method to be useful it is necessary to be able to look at the effects of a large number of different data changes, and this is best done by writing details of the basic set of histories onto a magnetic tape which can then be processed as many times as necessary.

6.4 Gamma-ray data

Data handling is very much simpler for gamma-ray tracking than it is in the case of neutrons. The GAMBLE system [22] was written as a gamma-ray counterpart of the DICE system, and was designed so as to be interchangeable with it. It has been found necessary to consider only three reactions: Compton scattering, pair production (in which the photons are assumed to be produced at the collision point), and photoelectric absorption. The justification for omitting Bremsstrahlung effects is based on the work of Dutton [23] who showed their contribution to be negligible in reactor shield design calculations, when the principal sources are usually below 6 MeV. The GAMBLE system uses a version of the routine HEITLER [24] to derive cross sections for any element from data in the UK Data Library. During programme execution the cross sections are stored point-wise, and linear interpolation is employed.

7 THE ALBEDO METHOD FOR STREAMING CALCULATIONS

The efficiency of reactor shielding is always reduced to some extent by the presence of essential passages and void-spaces containing gases or other low density materials. The coolant passages through the shield of a gas-cooled reactor provide an obvious example, but the problem is not confined to this system since access spaces and structural clearance gaps must also be present in the shields of water-cooled reactors and of sodium-cooled fast reactors. In the scheme described in Section 2 the codes provided for streaming calculations in the survey option are based on the kernel-albedo method. This technique is, however, restricted to the simpler geometries and it is therefore necessary to provide a Monte Carlo option for the correct treatment of more complicated systems. For this purpose, methods have been developed by Miller [25] and have been evaluated by means of a code, RANCYN, for cylindrical ducts and a more general geometry code RANSORD.

7.1 The form of the albedo

The general form of the albedo (representing the probability of reflection of radiation from a surface) may be expressed as

$$\beta(\underline{r}_o \to \underline{r}, E_o \to E, \underline{\Omega}_o \to \underline{\Omega})$$

where $\underline{r}_o$, E_o and $\underline{\Omega}_o$ are the position, energy and direction of the incident radiation and $\underline{r}$, E and $\underline{\Omega}$ are the corresponding quantities for the emergent radiation. For both neutron and gamma-ray data the following general simplifications have been made:

(i) Reflected particles are assumed to emerge at the point of incidence, ie $\underline{r} = \underline{r}_o$.

(ii) The angular distribution of the emergent radiation is assumed to be independent of both the energy and the direction of the incident radiation.

(iii) The energy distribution of the emergent radiation is assumed to be independent of the direction of the incident radiation.

The remaining functional dependences are then expressed in the following particular forms:

(i) Energy is represented group-wise.

(ii) The angular terms depend on a power of the cosine.

Thus, the albedo for a given wall material may be written as

$$\beta(g_o \rightarrow g)\ A(n)\mu_o^{-n(g_o)}\ B(n)\mu^{1-m(g)}$$

where g represents a group number and μ is the cosine of the angle to the surface normal. For neutrons the β term has been obtained from diffusion calculations while the values of A and n or B and m have been derived by fitting the expressions to the results of Monte Carlo calculations. For gamma-rays the functions have been derived from published compilations of differential albedos.

This degree of simplification has been used not only to ensure rapid sampling from the reflected distribution but, more importantly, to reduce the task of calculating albedo data for the wide range of wall materials encountered in practical problems. In future developments it is anticipated that the azimuthal dependence can be introduced into the albedo used with the Monte Carlo method without an appreciable loss of speed or an unacceptable amount of work to calculate the additional data. However, it would not be possible for all the simplifications to be removed, nor does this appear to be necessary on the evidence of the successful applications of the simplified albedo. Two examples of such applications are illustrated in Figures 3 to 6. Figure 3 shows the one-, two-, and three-legged 3 ft. square concrete-walled ducts studied extensively at ORNL [26]. The source from the Tower Shielding Reactor is a collimated neutron beam incident at 45° on a side wall. In Figure 4 the results of RUMORD calculations are compared with measurements of the thermal flux due to incident thermal neutrons. Figure 5 illustrates a three-legged duct of rectangular cross section assembled into the thermal column of the GLEEP reactor at Harwell. A Monte Carlo calculation for this duct was performed with the cylindrical geometry RANCH code by representing the duct cross section by a circular cross section of the same area. The predictions of the response of a BF_3 chamber are compared with the measurements and with the predictions of the thermal-albedo code MULTISORD in Figure 6.

7.2 Variance reduction techniques

In most streaming problems some form of acceleration is required if the Monte Carlo method is to be of practical use, and various techniques have been examined.

(i) The first methods investigated involved biassed sampling from the angular distribution for reflected radiation. Three types of biassing were examined:

(a) The azimuthal angle was sampled from a distribution with a linear bias which increased the probability of reflection in the forward direction by a factor N_c relative to the backward direction.

(b) A polar angle biassing in the form of an inverse power of the cosine of the polar angle (μ^{-N_D}) was used to increase the probability of sampling at glancing angles.

(c) Correlated sampling of the azimuthal and polar angles was used, with stronger biassing being applied near the start of the leg than near its exit.

It was found that the optimum choice of biassing functions increased the efficiency of a three-legged duct calculation by a factor 60. Polar angle biassing was most effective, and surprisingly correlation of the azimuthal and polar angle sampling did not improve efficiency.

(ii) The method of splitting and Russian roulette applied at each point of reflection was examined. The importance function used was independent of energy and was an exponential function of the distance along each leg of the duct ($e^{\alpha z}$). The function was adjusted in trial runs in order to give an approximately uniform flow of particles along the duct. In a three-legged problem with a mouth source the use of splitting improved the efficiency by a factor of 500.

(iii) With the high intergroup transfer probabilities in the albedos it is usually a problem to obtain accurate results in the high energy groups. There is a straightforward way of avoiding this difficulty if the emergent angular distribution in the albedo is independent of energy since in this case the same set of particle tracks may be used for all groups and the group dependence from the other terms in the albedo can be taken into account by carrying a separate particle weight for each group. This "group correlation" approach has been extended to albedos in which the angular distribution does vary with energy, when these variations are allowed for by means of additional weighting factors.

Table I summarises the relative efficiencies of RANSORD calculations for the three-legged ORNL duct using the various angle biassing and splitting options. It can be seen that for this case it was splitting which was the most powerful technique, and this enabled the thermal neutron calculation described above to be completed in 3 minutes on an IBM 360/75 machine. The group correlation technique was used in the calculation for the GLEEP rectangular duct, in which the Monte Carlo results in Figure 6 were obtained in 1 minute. The increase in efficiency was estimated here as a factor 3. Thus, although the major improvement in efficiency achieved with this method occurs at high energies, the calculation of low energy fluxes is also accelerated significantly.

8 SUMMARY

The special features required of Monte Carlo codes to be used by shield designers have been identified as a flexible mode of construction, efficient operation, and ease of application. In the scheme described in this paper the flexibility is provided by the WRS modular coding system, which facilitates the assembly of Monte Carlo codes and their linking with the approximate methods required for many practical applications, and allows alterations or additions to be made without the need for major reprogramming. The requirements for speed and for economy of storage have influenced not only the variance reduction methods but also the choice of simplified treatments of geometry, neutron cross section data, and albedo data. The need to facilitate the task of the programme users has led to the development of automatic variance reduction facilities. It has also set a limit on the degree to which cross-section data can be simplified, to ensure that the user is not left with a choice of parameters such as the number of groups or the cross section averaging procedures, which may be problem dependent.

The aim of providing Monte Carlo methods which can be used efficiently by engineers for routine shield design calculations on commercial reactors presents considerable problems. It is believed, however, that the techniques described in this paper represent significant progress towards this goal.

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TABLE I

Relative Efficiencies of the RANSORD Acceleration Techniques for a Three-Legged 3 ft x 3 ft Concrete Duct Geometry

Importance Splitting	Reflected angle biassing			Relative Efficiency
	Polar angle N_D value	Azimuthal angle N_c value	Correlation	
yes	0	1	no	500
yes	1.6	100	yes	160
no	1.0	1	no	65
no	1.5	5	no	65
no	0	1000	no	25
no	1.5	5	yes	18
no	0	10	no	17
no	0	100	no	17
no	1.6	1000	no	11
no	1.6	100	no	6
no	1.7	10	yes	4
no	1.7	100	yes	4
no	0	2	no	4
no	1.6	1	no	3
no	1.5	1	no	2
no	0	1	no	1

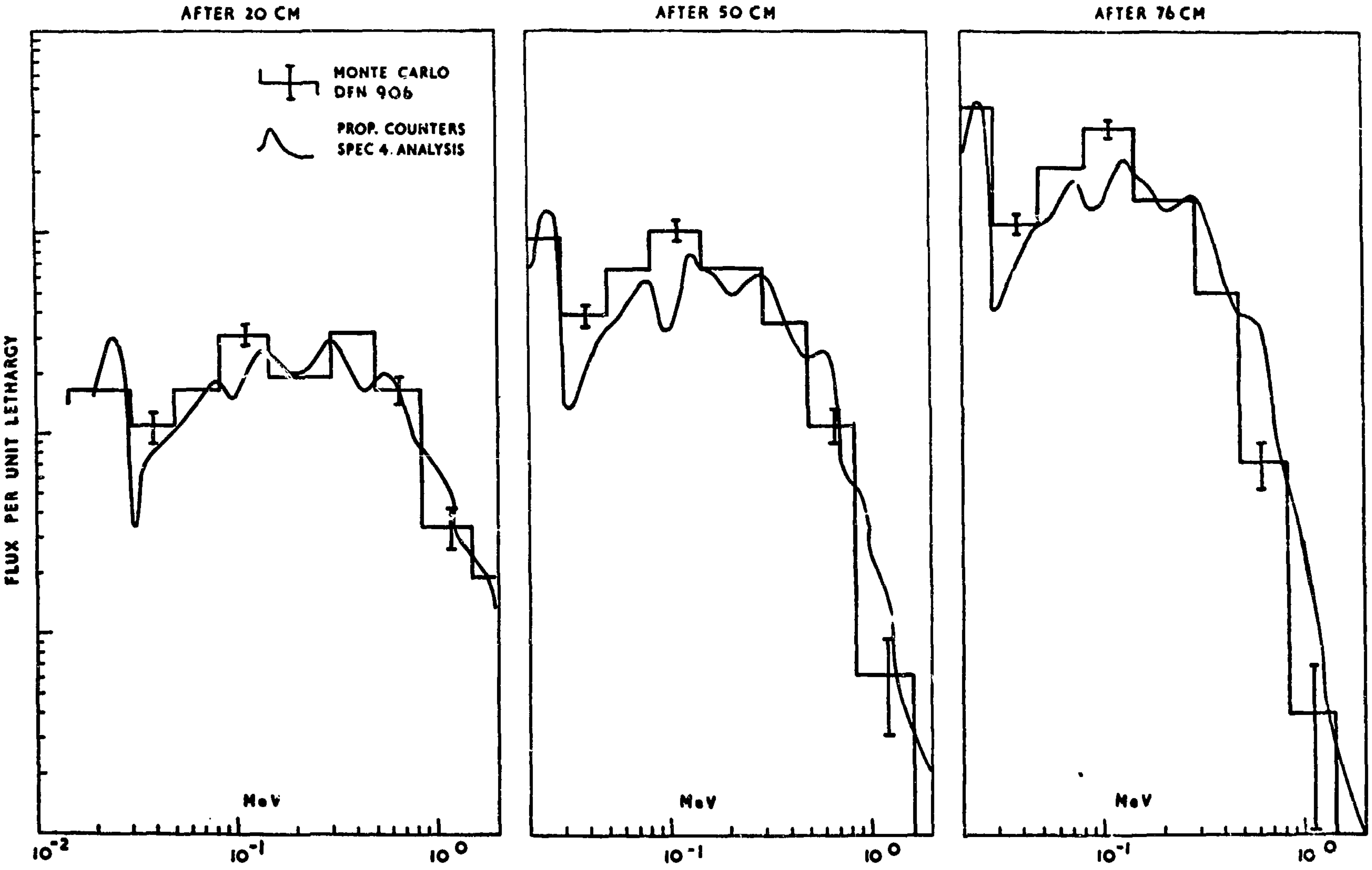

Fig. 1. Comparison of measured and predicted neutron spectra in a mild steel shield in ASPIS.

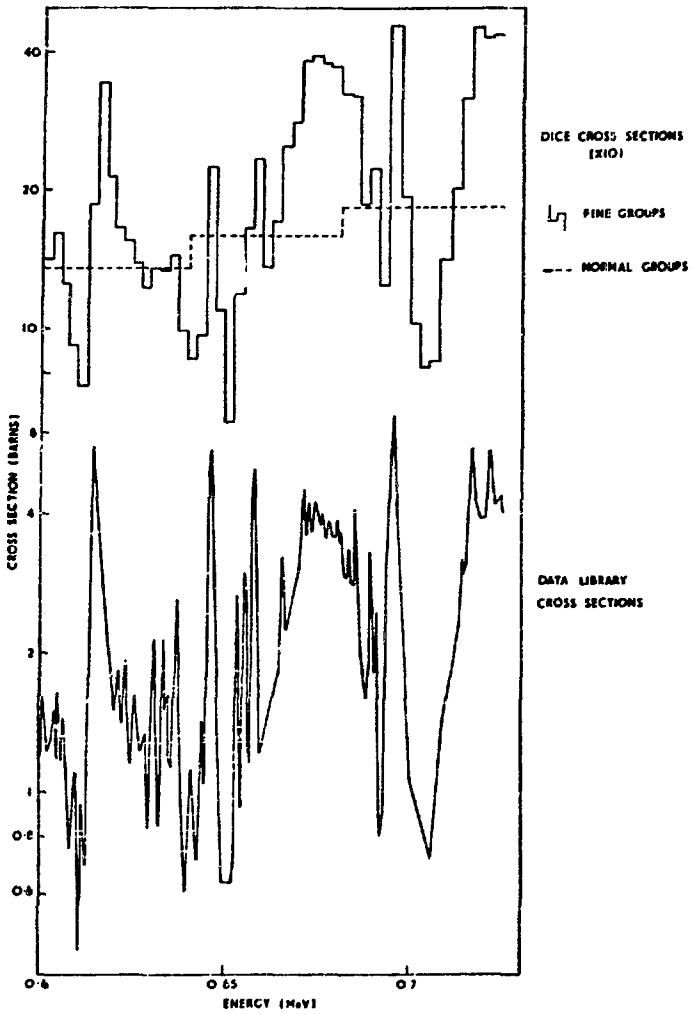

Fig. 2

Total cross section for iron.

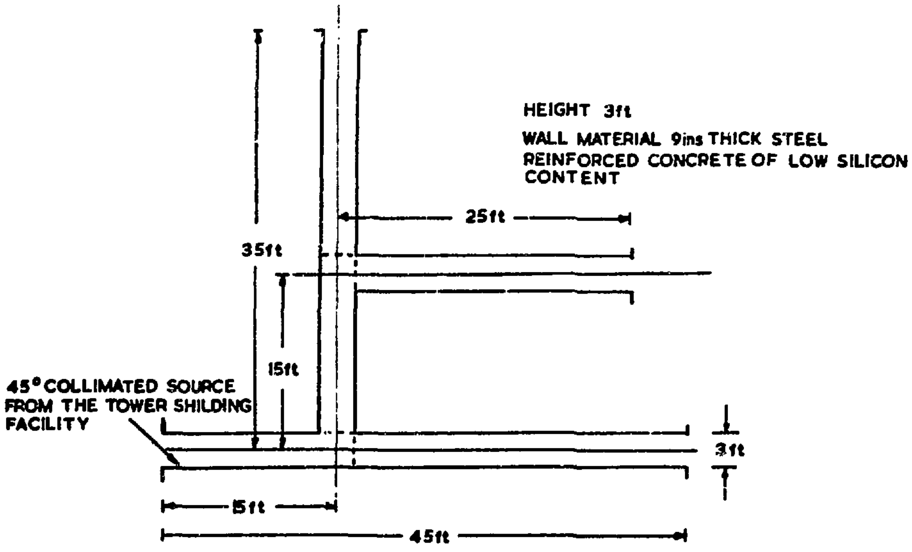
HEIGHT 3ft
WALL MATERIAL 9ins THICK STEEL REINFORCED CONCRETE OF LOW SILICON CONTENT
25ft
35ft
15ft
45° COLLIMATED SOURCE FROM THE TOWER SHILDING FACILITY
3ft
15ft
45ft

Fig. 3. Geometry of the ORNL concrete ducts (ORNL-4147).

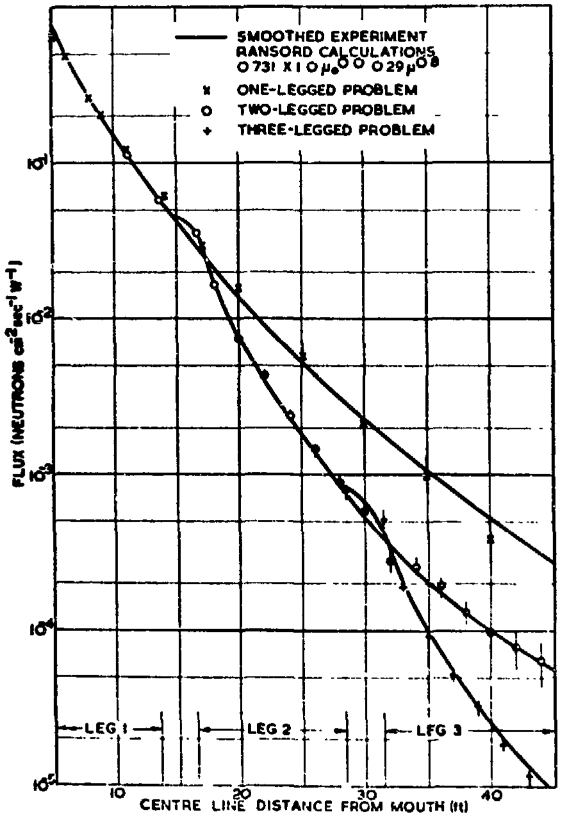

Fig. 4. Comparison of RANSORD predictions with measurements of the thermal neutron flux in the ORNL ducts due to incident thermal neutrons.

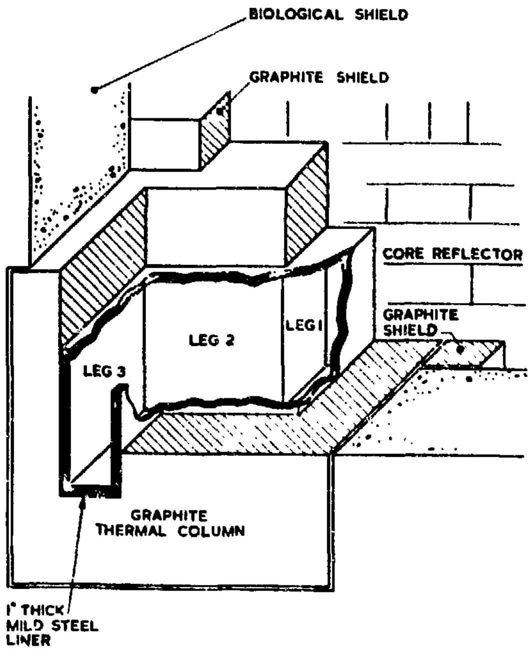

Fig. 5. Three-legged steel-lined duct in GLEEP thermal column.

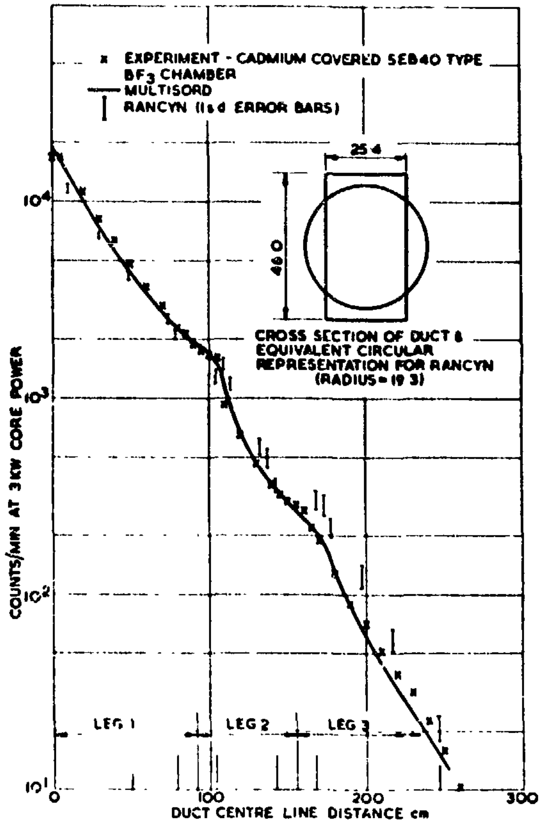

Fig. 6. Comparison of RANCYN with MULTISORD for a three-legged duct in the GLEEP thermal column.

DISCUSSION

Gelbard: There was a question raised initially in this talk as to whether general geometry routines were substantially more expensive to use than specialized geometry routines. Does anyone have any information on this subject?

Whitesides: Since one of the most extensively used general geometry routines (aside from routines of combinatorial type) was written at Oak Ridge, our experience might be of some interest. We find that general geometry routines generally run four to five times longer than specialized routines. That is quite a penalty to pay to use a generalized geometry routine. I believe that Mal Kalos is better qualified to comment on the combinatorial routines. but we find them quite a bit faster than the generalized routines for the relatively simple problems in which we have used them.

Gelbard: Did you say that the combinatorial routines were quite a bit faster than the general geometry routines that you have been using?

Whitesides: For the problems that we have run, that seems to be the case.

Gelbard: I would think of them as general routines, not specialized routines.

Kalos: The combinatorial geometry code has the property (as such codes should) that when it is required to treat a slab, it does so very well. It does not investigate to see whether a slab is, perhaps, a general n-*th* degree polynomial, or whatever. It treats slabs in a rather good way, though not perhaps as well as possible for infinite slabs in all cases. It is possible to have your cake and eat it too. It is possible to make reasonable compromises and I am glad to hear we have done a reasonable job in combinatorial geometry.

Whitesides: I was speaking of combinatorial geometry, as opposed to the GEOM subroutines of the O5R which most people are using. GEOM solves a general equation for every surface, and you may not have to do this, as Mal Kalos says, in combinatorial geometry. You solve only what you need to solve.

Gelbard: At Argonne we don't have any information on this subject at this point. But we ought to very soon because our original VIM code has a very specialized geometry for ZPPR lattices and we are now supplementing this with the combinatorial geometry capability. We will be interested to see what sort of comparisons we get.

Borgwaldt: We have a general geometry routine, I think like that in O5R. But we identify simple surfaces, like planes orthogonal to the x-y and z axes, and cylinders parallel to the z axis. Since they are identified separately, we get fast execution speeds for such surfaces, and normally only a very small number of general planes or general second-order surfaces are really used.

Coveyou: I was wondering about that factor of 4. That is the execution time for the geometry itself? What is a typical figure for the increase in running time for the problem?

Whitesides: I am not sure I know ...

Kalos: In a lot of problems, in our experience, tracking through the geometry takes a very large fraction of the running time — at least half, perhaps more.

Whitesides: Yes, that is right.

Gelbard: What is it in RECAP? Is it about 40%? I think that you mentioned that earlier.

Gast: Yes, that is correct.

Gelbard: So, one-half is not unusual for a wide range of codes.

Kalos: I would like to add one comment about the use of complex geometry routines. In particular, in combinatorial geometry, the running time, the speed with which you treat a complex geometry, can well depend on how you set the problem up. For example, you may have a particularly complex domain which is not encountered very often and which may require a great deal of computation. If you use the simple device of putting it in a box, then you never have to deal with the surfaces in this domain unless you first encounter the box. The geometry computations will, then, speed up considerably. I don't know how to give general prescriptions for the average user, but a word to the wise will go a long way.

Gelbard: The other suggestion that has been mentioned is that simple surfaces be identified specifically in general geometry.

Coveyou: When I designed this sort of routine originally it was based on a block and zone concept, so that you in fact never did use the more complex parts of the routine unless they were needed. Has that feature been dropped?

Whitesides: No it has not been dropped, obviously. But the problem is, as Kalos correctly pointed out, that the efficiency of the routine in a specific case depends on the care and time you invest in writing out the geometry description. In general, most people find that it is easier to let the machine solve the geometry problem than to try to treat the geometry carefully themselves.

Gelbard: I would like to rush the discussion today, because I want to stick strictly to schedule and would like to cover some other questions. The biasing that you discussed initially was one where the machine adjusted the biasing so that you got equal density particles in equal volume of phase space?

Grimstone: Yes.

Gelbard: Have you had any opportunity to notice what effect this has on the error estimates? Have you had any trouble with error estimates with this sort of biasing.

Grimstone: No, we have not really looked at this in any great detail.

Kalos: I want to ask first of all a technical question about this adaptive procedure. When you use this method, do you start with some sort of guess as to what would be a good set of weights, or do you start with flat weights and go on from there?

Grimstone: We can do both; but I think in most applications we have, in fact, started with flat weights.

Kalos: So that means that your information grows, diffuses out slowly from the source, and it also means that you have to execute some sort of cycle, stopping, taking a tally of what has happened, and improving and going on. About how many such bootstraps seem to be necessary in a penetration problem where you have an attenuation of, say, 10^6?

Grimstone: Generally we make weight readjustments after every particle history, and do this throughout the entire calculation.

Kalos: Then the procedure is biased, your answers are biased.

Gelbard: You recall that he said that the arrangement settled after 5 minutes of computation, that although one continues to adjust the weights in principle, in practice it is claimed that the adjustment process settles after 5 minutes.

Kalos: So that, in practice, he is claiming that, very likely, the bias is small. I don't deny that.

Gelbard: This does depend on the settling time.

Grimstone: Presumably the bias would be smaller if we were to discard that first 5 minutes of history, which we don't, in fact, do at the moment.

Kalos: If you did that, then it would be unbiased.

Grimstone: Or almost unbiased ...

Kalos: No it would be unbiased, completely unbiased if you discarded the settling period and did not readjust weights afterwards.

Grimstone: If we continued to refine the weights somewhat then it would be somewhat biased, but probably not to a serious extent.

Kalos: I regard the fact that you are able to bootstrap from zero information to a reasonably satisfactory scheme as a significant triumph. In the very early days we tried manually to do things like this and our experience seemed discouraging. I am very encouraged and hope that we can do some experiments along similar lines. We have had some ideas about bootstrapping which are not quite the same as yours, but they rely on one's ability to do this kind of thing, and I think that your success means that we will have success.

Coveyou: Have you performed the experiment of doing this kind of calculation twice, and comparing the weights you get to see if they vary very much from one run to another.

Grimstone: Yes, I have tried to see how rapidly the weights appear to be converging. The weights that we use are, in fact, very closely related to, and very similar in properties to the flux estimates themselves, and therefore behave in roughly the same way.

Coveyou: I wonder whether such a procedure has, shall we say, metastable states. Would you get a set of weights on one run, and yet another set of weights and another set of answers if you were to rerun the whole problem again, with a different set of starting weights and random numbers? I am wondering if it is sufficient to rely on the fact that the weights seem to have settled down.

Grimstone: Well when I say they settle down what I mean by that is that they might only have reached, say, within a factor of 2 of their final values. I am not putting any very stringent convergence criteria on the weights.

Gelbard: I want to direct a brief question to Whitesides. In Grimstone's study of the effect of cross sections, it was found that the cross sections for iron in a big hunk of iron did not have to be represented very accurately. I recall Monte Carlo studies of this sort at Oak Ridge, and I seem to remember that they came to other conclusions. Is that not true?

Whitesides: That is correct. It just depends upon what sort of problem you are looking at. If you are looking at a deep penetration problem through iron, and you have many neutrons in the vicinity of the windows, they are going to stream through. One thing that I have personally been concerned about for some time (and this applies to criticality problems where you have heavy metal reflectors) is that it is very, very difficult, I believe, to define a multigroup set that is going to work. You are simply going to run into streaming through windows when you least expect it, and when this streaming might cause you the most difficulty.

Gelbard: The problem that was described here, was it not also a problem of penetration through a large chunk of iron?

Grimstone: That is right, yes.

Gelbard: So it is not really clear why the conclusions are so different. The Oak Ridge conclusion has been that you need an accurate cross section representation.

Whitesides: Obviously you can get a set that would give you the right answer.

Gelbard: But the windows all disappeared in the smooth set that Grimstone used.

Whitesides: That is so.

Gelbard: If you can close these windows with impunity, then the cross-section problem becomes very much easier. The S_n method then becomes a much more important competitor. We don't have time to discuss this, but I think it is really important to people in our business to think of the role of other computational methods. If windows don't matter too much, S_n becomes a tool which is much more valuable.