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ABSTRACT

Monte Carlo methods for analysing radiation transport are well established, although the ease of use can vary markedly between different software packages. This paper briefly reviews the present status of the MCBEND Monte Carlo code and how it is has been developed to satisfy the requirements of the non-specialist user. It then discusses some of the ways in which MCBEND can be used to increase understanding of the performance of radiation systems by conducting virtual experiments.

Keywords: MCBEND, Monte Carlo, radiation transport, neutron detector, nuclear logging.

1. INTRODUCTION

Over the last decade, the Monte Carlo method for solving radiation transport problems has moved from a reference method, against which more approximate calculations could be tested, to the first choice for performing many design and assessment calculations ranging from the routine to the extremely complex. This has been brought about mainly as a result of two separate factors. Firstly, the development of automated acceleration techniques in the late-eighties, which greatly simplified the preparation of case data and removed much of the black-art previously associated with the method. The second factor was the arrival of the modern workstation, which has provided the user with a massive, yet inexpensive, computer resource for individual use. This has enabled the full power of the Monte Carlo method to be unleashed. By using Monte Carlo software the designer now has a method capable of solving most practical problems associated with radiation transport. Furthermore the method is rigorous and, within constraints imposed by material tolerances and subjective modelling approximations, its accuracy is limited only by the knowledge of the basic cross-section data.

No matter how advanced the techniques and computers are, the power of the Monte Carlo method is of little relevance to the would-be Monte Carlo analyst if it is inaccessible. Accordingly, Monte Carlo developers have invested in making their products easier to use by the non-specialist so that they can solve today's problem and not have to wrestle with the method. A goal for the developer is to provide a robust software package that suits today's flexible work-force; suitably trained users should be able to retain their productivity and accuracy even though they might not have used the software for a period of some time. Modern working practises sit uneasily with the resident full time guru or expert in running a particular software package. This model is being replaced by one of more widespread use, with Monte Carlo software becoming one of a number of tools that can assist its user to achieve his technical objectives.

This paper discusses some of the ways in which the MCBEND Monte Carlo code can be used to increase understanding of the performance of a particular system by conducting virtual experiments. The attractions of these experiments are clear: they are totally flexible, safe and inexpensive. Whilst it might be argued that other computational methods could also be used in this way the ability of Monte Carlo to fully model 3D systems sets it apart. First we will briefly discuss the capabilities of MCBEND, its current status and the way it is has been developed to satisfy the requirements of the non-specialist user

2. THE MCBEND MONTE CARLO CODE

The functionalities of the current generation of major Monte Carlo codes used in the analysis of radiation transport are very similar although the codes ease of use can be markedly different. A basic description of MCBEND is provided for completeness and by way of introduction to the following sections.

MCBEND[1] is a general geometry, point energy Monte Carlo code used for deep penetration problems in shielding and radiation transport, and is one of the ANSWERS suite of codes for Reactor Physics, Shielding and Criticality. It may be used for neutron, gamma-ray, electron/positron and coupled calculations. The neutron data are presented in 8220 groups and are derived from the UK Nuclear Data Library, JEF-2.2 or ENDF/B-VI compilations. This fine group treatment has explicit representation of the energy/angle laws. The gamma-ray data are described in a continuous energy scheme and are based upon the UKNDL compilations. Coupled (n,γ) calculations are performed by running the neutron calculation and writing details of the neutron collisions to a dump file[2]. This is then combined with a gamma-ray production library to produce the source for the gamma-ray calculation. Multi-group data are also available for neutron, gamma-ray or coupled calculations.

The model is built using the techniques of combinatorial geometry with the system being specified as a series of Parts which are then assembled into the complete model[3]. The Parts are dimensionally defined within their own local co-ordinate system. They can be included, individually or in groups, within other parts to form new parts. This process can be repeated over and over. Thus the user can build a MCBEND geometry model as it is done in real life by assembling individual components to form larger components or completed systems. A benefit of the method is that the user can construct unique libraries of tested parts, i.e. models of fuel elements, instruments, logging tools, etc., for inclusion in larger geometric models. The use of Parts also decreases the QA burden in team projects.

An extension to the geometry modelling is the Secure Geometry (SG) option. This provides a facility whereby a model of a commercially sensitive item, such as an oil well logging tool, can be made available to third party users, in an encrypted form, as a Part for incorporation into the users own calculational model of the surrounding environment. In this way the design of the Part is not revealed but the user has the benefit of an approved model. In addition to the geometry description, SG Parts can contain all other information relating to the component. For the case of the logging tool this includes source description, material description, splitting information, detector description, and scoring requirements.

The source specification of MCBEND is very flexible, with freely orientated source bodies, built-in source spectra, and powerful weighting algorithms. The code's variance reduction techniques are based on splitting and Russian roulette with energy dependent importances specified in a separate orthogonal mesh and being provided by an adjoint diffusion calculation which is performed as an integral part of the MCBEND run[4]; the module performing this function being known as MAGIC. Extra techniques designed for the acceleration of streaming calculations are also available[4].

Several quantities may be scored in a MCBEND calculation. The basic tally is the volume-averaged flux or response, but facilities exist to score sensitivity, angular fluxes and currents, heat or charge deposition and pulse height distribution. A simple point estimator is also available.

Clear and informative input data and documentation are an integral part of the MCBEND package. For the user guide a simple input syntax, based upon a flow diagram format, has been in successful use for many years. The guide permits a quick and easy assimilation of the input requirements and gives detailed notes to clarify specific items. The user guide is supported by an expanding range of introductory texts and applications guides. Diagnostic information and geometry display of the MCBEND model are provided by the VISTA suite of graphics packages[3,5]

The validation base for MCBEND is broad and covers all the areas in which it has been used. The validation range includes highly specified experimental benchmarks, many of which were performed at AEA Winfrith[6] using standard radiation metrology techniques and advanced neutron spectrometry techniques[7]. It also includes validation against measurement on operating plant, whether this be associated with the nuclear fuel cycle or commercial applications of radiation in industry.

In the past year MCBEND has undergone development on several fronts ranging from fundamental methods development to further improving the image and user-friendliness of the code. In all cases the aim has been to enhance the productivity of the user through improved functionality and ease of use. A paper at the ANS Radiation Protection and Shielding Topical Meeting[5], 21-25 April 1996, described some of the most recent developments. These include the development of:

> a capability for performing adjoint calculations for neutrons using point energy cross-section data. With the new method, there are many situations where significant gains in efficiency can be achieved over calculations in forward mode, without any loss of accuracy;

the use of diffusion theory to provide a rapid integrated scoping capability within MCBEND. The switch between diffusion and Monte Carlo methods requires minimal user effort, so a series of scoping calculations can be easily followed by a definitive Monte Carlo calculation.;

two new GUI based tools for the manipulation of the code's results and for the display of paths taken by the Monte Carlo particles through the system. These tools add to the existing range of VISTA graphics products for geometry visualisation.

3. MONTE CARLO EXPERIMENTS

In this section we look at a few examples of how Monte Carlo methods can be used to improve the interpretation of experimental results and system performance.

There are several features of Monte Carlo Method that lend it to this type of investigative study. The ability to model complex three-dimensional structures can remove, or minimise approximations. The separability of the method arising from the independence of each particle track permits impractical, but very useful, virtual experiments to be performed. For instance, if the contribution to the score from certain interactions in a defined region is required. When used in conjunction with MCBEND’s adjoint, sensitivity, and staged calculation capabilities it provides a powerful diagnostic capability as is demonstrated in the following examples which would have been difficult, impractical or impossible to complete in any other way.

3.1 The determination of energy/angle response function of a hand-held cylindrical neutron dose-meter.

When developing a neutron dose-meter it is common practice to take a detector which is sensitive to low energy neutrons and to surround it with combinations of moderating and absorbing materials to alter its response. The arrangements of the latter are adjusted to tune the energy dependence of the response to neutrons incident on the outer surface of the instrument so that it approximates to that of the dose conversion factor. This process is greatly facilitated if calculations can be used to show the effects of changes to the configuration. They are also valuable in providing interpolation when the instrument is only calibrated at selected energies. Alternatively when no calibration of the energy dependence is available the results of calculations can be adopted when the accuracy of the theoretical methods has been established.

An example of the application of the MCBEND code in the interpretation of measurements made outside a spent fuel transport flask with such a partially calibrated instrument is described by Locke[8]. The detector in question was a cylindrical He^3 counter which had been surrounded by paraffin wax in order to enhance its response to fast neutrons. The volume of gas within the counter was 100mm long and 45mm in diameter with a pressure of 3 atmospheres. It was surrounded on all sides by 100mm of paraffin encased in a 1mm thick steel can apart from the 51mm diameter channel at one end which provided access for the cable. Calibration of this instrument had been performed with a Cf^{252} source in air so that there was a relationship between the measured count rate and a known flux of neutrons with a spectrum corresponding to that of the fission source. The variation of the neutron fluxes outside a cylindrical transport flask loaded with spent fuel from a pressurised water reactor had been measured with this instrument and the requirement was to relate the resulting count-rates to the neutron dose-rates. The spectra outside a flask composed of a thick steel wall and a layer of resin will be very different from that in the calibration experiment so that it was necessary to establish the energy dependence of the response. Secondly, as the instrument was cylindrical with measurements being made with its axis parallel to that of the flask, there will be a variation of its response with the neutron’s angle of incidence. MCBEND was applied to provide both of these dependencies.

One approach to the calculation of the responses would be to set up models of the flask and its fuel elements with representations of the counter being included at each of the measurement positions. This presents a problem for a Monte Carlo calculation because the volume of the counter is then only a very small fraction of that of the whole model so that there is a low probability of a neutron track passing through it and statistical uncertainties on the results would be high. It is therefore preferable to calculate the neutron fluxes at positions in air outside the flask in a single MCBEND run and to then fold these with the counter response functions. The latter could be derived by considering a wide range of mono-energetic parallel beams incident upon the counter at various angles. This would involve a very large number of cases. The alternative is to perform an adjoint calculation and to score the adjoint currents at the surface of the instrument in a number of energy groups and angular bins. These can then be folded with the fluxes outside the flask calculated in similar energy and angle ranges. This approach was adopted.

The adjoint calculation was performed with MCBEND with a source specified in the volume of the helium gas with a strength per unit volume and spectrum given by the macroscopic cross-section for the $He^3(n,p)$ reaction. The adjoint currents were then be combined with the forward fluxes to give the count rates. The formula that was employed was

$$\text{RESPONSE} = \iiint \Phi(E,\Omega,x)\Phi^*(E,\Omega,x)\mu dAdEd\Omega$$

where

$\Phi(E,\Omega,x)$	=	Neutron flux per unit energy per unit solid angle at energy E and direction Ω at a position x on the surface of the instrument,
$\Phi^*(E,\Omega,x)$	=	the corresponding adjoint flux,
μ	=	cosine of the angle between W and the normal to the surface at x,
dA angle	=	an element of the surface area andthe integration is taken over the area of the instrument, the solid 2π, and the full energy range.

The forward fluxes are assumed to be uniform over the area of the instrument and the adjoint values are scored as currents integrated over three separate areas of the cylindrical surface and the two end faces. The cosine term is thus included. The integration over angle is reduced to a summation over the angular bins which is simplified further because there is no azimuthal dependence. The integration over energy is then a summation over the angular bins. The adjoint calculation with MCBEND gave the currents in 10 equal 9^o intervals of the polar angle, i.e. the angle with the axis of the counter, and 100 energy groups in the range $1x10^{-10}$MeV to 14.9MeV. In the one calculation it was thus possible to produce a very detailed response function which were to be folded with the forward fluxes to give the count-rates.

The theoretical count-rate for the calibration experiment with the neutron spectrum from Californium being incident on the cylindrical surface of the instrument at 90^o to its axis was then derived. It was found to be higher than the measured value, the discrepancy being attributed to modelling of the gas in the counter and a lower active length than the overall physical value. The ratio between the two was then used to normalise the calculated response function.

The forward fluxes in the 100 energy groups and 10 angular bins as calculated at 39 positions outside the flask were then folded with the response function to give the corresponding count rates for the instrument. The ratio of these to the dose-rates from the calculation enabled the measurements to be expressed as neutron dose-rates. It was found that the angular dependence led to a 43% change in this ratio as the angular distribution became more forward peaked when the counter was moved from the flask surface to a position at 1.81 metres.

The MCBEND calculation was thus able to provide a more detailed response function than would be available from measurements alone and this enabled the measurements of detector response surrounding the fuel transport flask to be interpreted in a meaningful manner.

3.2 Sensitivity studies at the design tolerance level for a gamma-ray nuclear logging tool.

Gamma-Ray Density Sondes are commonly used in petrophysical logging for the in-situ measurement of the bulk density of the rock formation immediately surrounding the oil-well borehole.

MCBEND's ability to model gamma-ray transport has been applied to the interpretation of the design and performance of such density tools[9,10]. The complex geometry of the tool and formation, including source and detector collimators, can make the scoring of tool response (pulse height distributions from gamma-ray interactions in the crystal), an inefficient and time consuming calculation. MCBEND's Forced Flight option[4] was specifically designed to improve the efficiency of the analysis of collimated systems, and involves the addition to the normal Monte Carlo tracking of a deterministic - or "forced" - flight from collision sites to the collimator. When applied to the analysis of typical collimated gamma-density tools increases of a factor of 30 in the figure of merit efficiency have been obtained.

As part of an AEA research club sponsored by oil and gas companies, logging companies and the CEC a systematic range of studies was carried out to validate MCBEND for use with gamma-ray density tools by comparisons with a series of experimental benchmarks. The validation programme started with a simple bare NaI detector and mono-energetic gamma-ray source in air and ranged progressively through more complicated configurations to a full-sized reference mock-up of a commercial density tool in realistic environments.

Good agreement was found between experiment and absolute calculations with the exception of the full size mock-up where C/M ratios of between 0.84 and 0.91 were recorded for clean hole conditions. Detector responses are very sensitive to small changes (of the order of fractions of mm) in key tool parameters, e.g. source and detector location, collimator size. An inspection of the construction and assembly tolerances showed that the overall position of the active source pellet was ±0.3mm. MCBEND calculations demonstrated that this had a ±4% effect on the detector count-rates. Similar analyses were completed for the position of the NaI crystals within their housings, the thickness of the cylindrical steel tool wall and borehole liner. Compounding these tolerances advantageously into a revised model demonstrated that C/M ratios of between 0.94 and 0.99 for clean hole conditions could be obtained. These were consistent with other benchmark experiments in the series.

Whilst discrepancies remain between calculation and experiment the exercise demonstrated conclusively the ability of MCBEND to calculate accurately the sensitivity of the tool response to small changes of tool design. This type of information at the design stage can be used to set tolerances to ensure optimal consistency between the response of different tools of the same design.

3.3 Various analyses of Pulsed-Neutron Logging tool response.

Monte Carlo modelling is now widely used to assist with the characterisation of nuclear logging tool response. These tools are calibrated using a mixture of experimental results from test pits and theoretical results from Monte Carlo simulations. The use of Monte Carlo allows the tool response to be characterised for situations which are difficult or impossible to simulate experimentally, such as formations containing multiphase fluid.

3.3.1

One recent application of MCBEND has been to investigate the response of Pulsed Neutron Capture tools (PNC). These tools measure the thermal absorption cross-section (sigma) of the rock formation to monitor well production by distinguishing saltwater (high sigma) and oil (low sigma). A typical PNC tool contains an accelerator neutron source that emits bursts of 14MeV neutrons lasting some 100 microseconds. The interactions of the neutrons with materials surrounding the tool and with the tool itself produce gamma-rays that are recorded by detectors placed at locations within the tool that are ‘near’ and ‘far’ from the source. The decay of the resulting gamma-ray signal is used to measure the thermal absorption cross-section of the rock formation

However, the apparent (or measured) sigma value determined by the tool measurement is not usually the same as the true value due to the varying effects of the borehole contents on the thermal neutron distribution, and correction algorithms must be applied. MCBEND has been used to calculate apparent sigma values for a wide range of borehole and formation conditions, most of which are not accessible experimentally. The results were analysed to assess the dependence of the error in apparent sigma on the borehole and formation conditions and to produce suitable correction algorithms. This type of Monte Carlo analysis cannot claim to be new[11] but the use of MCBEND has greatly simplified the process so that non-specialists can apply the techniques.

3.3.2

Carbon/Oxygen tools use the same pulsed neutron source as PNC tools with a shorter burst of 20 microseconds. They detect the characteristic gamma-rays produced from inelastic scatter of fast neutron with carbon and oxygen nuclei. This provides information on the hydrocarbon content of the fluids in the rock formation.

By using Monte Carlo simulations of a PNC tool adapted to also operate as a C/O tool Peeters[12] et al have demonstrated that operation of such a tool in horizontal three-phase production-logging wells can provide a measurement of oil, water and gas ratios in the borehole. This is particularly useful for assessing gas locks and water traps in horizontal wells that can reduce production flow. The investigation required the Monte Carlo estimation of the tool response to different oil/water/gas fractions in a cased well. Three separate parameters were studied: the ratio of near to far detector gamma count-rates, the ratio of gammas produced by inelastic scatter in carbon and oxygen and the thermal neutron capture cross-section of the composite borehole fluid (derived from a double exponential fit to the decay of the gamma signal). These parameters can respectively be related to gas, oil and water in the borehole. A multivariate analysis was used to determine the relationship between the three nuclear parameters and the fluid fractions. Experimental assessment of the algorithm in a flow loop demonstrated the validity of the method giving measurements of the water fraction with an accuracy of 7%. Field tests with the new tool are now underway.

3.3.3

MCBEND has also been used to determine the depth of investigation of these pulsed neutron tools under different operating conditions and locations within the borehole by dividing the borehole and formation into a set of concentric annuli and calculating the fraction of the signal which comes from gamma-rays born in each annulus. This task in MCBEND is achieved by simply sampling only those gamma-production reactions that occur in the annulus and tracking them back to the detector to score the contribution to the response. This type of virtual experiment[13] has replaced cumbersome experiments of the past[14] and has given new insight into the sensitivity of the tool to the borehole, casing and cement. For short time gates the formation contribution to the signal can typically be as low as 10 to 30% but rises to between 30 and 70% for longer time gates.

3.4 Pipeline Assay.

The technique of simplifying the analysis of a complicated system by splitting the calculation into several stages linked at physical interfaces in the model is well known. It also provides an efficient route for the analysis of design variations or to determine sensitivity of results to parametric changes.

Determination of the effects of changing the material compositions of parts of a system is sometimes required. A particular case is that of nuclear logging devices which are passed through sea floor pipelines to detect whether they are supported by sediment or whether the sediment has been eroded leaving the pipeline unsupported and possibly stressed. In such cases it is laborious to perform complete calculations for each tool/pipeline/sediment configuration, especially as only small changes in response might be expected. The so-called "black albedo" technique is therefore used.

Firstly, an interface is specified at the outer surface of the pipe. The interface is specified as an albedo material with a very low probability of reflection - hence the name of the technique. The particles hitting the interface effectively form a first crossing current and are used as the source terms for a series of second-stage calculations which model the external systems and, in this example, the subsequent transport of radiation back to the tool detector. This method isolates those particles which will be affected by changes in the material surrounding the pipe. The particles which reach the detector without passing through the pipe wall are not modelled so the method is also free from any uncertainties in the background signal. Because the tracking of particles to the interface is performed only once, the overall efficiency of the calculations is increased. Furthermore, as the first stage of each calculation is common, the statistical uncertainties in the interface source for the second stages are fully correlated and can be cancelled from the analysis. Thus the differences in the results of the second stage may be directly related to differences in the configurations.

4. SUMMARY.

The Monte Carlo method is well established and is now in routine use. The early problems of acceleration to achieve unbiased results in a reasonable time have been resolved. Monte Carlo's 3D modelling capability and its ability to allow the user to break down the radiation transport processes into component parts form a powerful diagnostic and design tool which has been demonstrated by way of several examples of "virtual experiments" which would have been difficult or impossible to achieve in reality.

The features of the Monte Carlo code MCBEND have been explained. However, it is the benefit to the user of increased productivity with MCBEND that sets it apart from other Monte Carlo software. With a few days of training, the newcomer to MCBEND can use the straightforward geometry preparation system to confidently set up a practical case and, using the technique of automatic acceleration, obtain a reliable design estimate. When problems do arise the user can turn to the ANSWERS support service which is manned by experts in the application of the software who will offer advice and support.

The development programme for MCBEND is focused firmly on enhancing the productivity of the user through improved functionality and ease of use. It has been designed for non-specialists and not software developers. Analysts are now starting to use MCBEND for 'what if' calculations rather than just for 'once off' calculations. To aid the analyst in this task the May 96 release of the MCBEND includes the ability to parameterise the input and to loop calculations. In this way analysts can perform calculations for several different scenarios through one job launch.

What if.......

5. ACKNOWLEDGEMENTS

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