Extension of the MCBEND Monte Carlo Code to Perform Adjoint Calculations using Point Energy Data

Malcolm Grimstone

Abstract

In radiation transport calculations there are many situations where the adjoint mode of solution can be more efficient than the conventional forward method. One example is a case where the size of the detector is small compared with that of the source; another is the calculation of detector responses corresponding to a changing source distribution in an otherwise stable system. Multigroup adjoint methods are commonly used, and the MCBEND Monte Carlo code has had such a capability for many years. However, such methods involve the approximations of cross-section averaging and simplified representation of the angular distribution of scattering. MCBEND has now been extended to perform adjoint calculations using point energy neutron data. The new facility enables users of MCBEND to choose the most efficient mode of operation for their problem without having to sacrifice the accuracy of the point energy data representation.

The method which has been adopted is to cast the adjoint transport equation into a form which resembles the forward equation but contains transformed definitions of the cross-sections and the secondary energy/angle distributions. A one-group treatment is used for thermal neutrons. The transformed data are held in a special library which is used for adjoint MCBEND runs.

To verify the method, detector responses have been calculated by running MCBEND in both forward and adjoint modes and showing that the results are the same. The paper includes examples of such calculations for simple test problems and for shielding experiments, together with a demonstration of the use of the method to calculate detector reaction rates in a surveillance capsule in the radial shield of a PWR. In this case the adjoint option provides plant operators with an efficient method of determining the detector responses corresponding to changing core conditions during the reactor lifetime.

1. INTRODUCTION

MCBEND[1] is a general geometry Monte Carlo code used for radiation transport problems involving neutrons, gamma-rays or electrons/positrons and for coupled calculations. Point energy data are normally used, although it does provide the option to use multigroup data. There are some situations where the adjoint mode of solution can be more efficient than the conventional forward method. One example is a case where the size of the detector is small compared with that of the source; another is the calculation of detector responses corresponding to a number of different source distributions in the same system. MCBEND has, for some time, included the capability of performing calculations in adjoint mode, but only with multigroup data. Accordingly, MCBEND has now been extended to perform neutron calculations in adjoint mode using point energy data, thus enabling users to choose the most efficient mode of operation for their problem without having to sacrifice the accuracy of the point energy data representation.

The following sections outline the method which has been adopted and describe how this has been implemented in the code. Results are then given for some simple verification tests and for some examples of more practical applications; the accuracy and efficiency of the method are discussed.

2. POINT ENERGY ADJOINT MONTE CARLO METHOD

The adjoint transport equation may be written in the following form:

$$-\mathbf{W}.\tilde{\mathbf{N}}\Phi^*(\mathbf{x},E,\mathbf{W})+\Sigma_t(\mathbf{x},E)\Phi^*(\mathbf{x},E,\mathbf{W})=$$
$$\int\sum_{n,r} r_n(\mathbf{x})n_{n,r}(E)\,s_{n,r}(E)P_{n,r}(E\to E',\,\mathbf{W}\to\mathbf{W}')\Phi^*(\mathbf{x},E',\mathbf{W}')\,dE'\,d\mathbf{W}'+S^*(\mathbf{x},E,\mathbf{W})$$

In the integral term, n and r are the nuclide and reaction indices and r is an atomic number density. The adjoint source term S^* is normally equal to the response function for the detector of interest.

A common feature of point energy adjoint Monte Carlo techniques[2,3,4] is the reconstruction of the adjoint equation so that it looks as similar as possible to the forward equation, thus minimising the changes which have to be made to the Monte Carlo procedure. In MCBEND the restructured equation has the form

$$\mathbf{W}.\tilde{\mathbf{N}}\Phi^+(\mathbf{x},E,\mathbf{W})+\Sigma_t(\mathbf{x},E)\Phi^+(\mathbf{x},E,\mathbf{W})=$$
$$\int\sum_{n,r} r_n(\mathbf{x})n^+_{n,r}(E')\,s^+_{n,r}(E')P^+_{n,r}(E'\to E,\,\mathbf{W}'\to\mathbf{W})\Phi^+(\mathbf{x},E',\mathbf{W}')\,dE'\,d\mathbf{W}'+S^+(\mathbf{x},E,\mathbf{W})$$

where

$$\Phi^+(\mathbf{x},E,\mathbf{W})=\frac{1}{E}\Phi^*(\mathbf{x},E,-\mathbf{W})$$

$$S^+(\mathbf{x},E,\mathbf{W})=\frac{1}{E}S^*(\mathbf{x},E,-\mathbf{W})$$

and (omitting the subscripts for simplicity)

$$s^+(E')=\int s(E)P(E\to E',\mathbf{W}\to\mathbf{W}')\frac{E'}{E}\,dE\,d\mathbf{W}$$

$$n^+(E')=\frac{\int n(E)\,s(E)P(E\to E',\mathbf{W}\to\mathbf{W}')\frac{E'}{E}\,dE\,d\mathbf{W}}{s^+(E')}$$

$$P^+(E'\to E,\mathbf{W}'\to\mathbf{W})=\frac{n(E)\,s(E)P(E\to E',\mathbf{W}\to\mathbf{W}')\frac{E'}{E}}{n^+(E')\,s^+(E')}$$

The weighting factor $1/E$ improves the efficiency of the adjoint solution by producing better behaved secondary energy/angle distributions and by making Φ^+ into a more "flux-like" quantity. Two other refinements have been applied to the basic method described above. Firstly, the microscopic adjoint partial cross-sections s^+ are scaled so that they sum to the true microscopic total cross-section. This is necessary to allow the adjoint transport equation to be solved by a Monte Carlo procedure analogous to the forward case. A compensating factor is applied to the particle weight at each collision. Secondly, the adjoint secondary energy/angle distributions are defined using only the slowly varying part of the cross-section; otherwise these distributions would contain rapid fluctuations due to resonances. Once again, compensation is made through an adjustment of the particle weight. The method, as implemented, does not allow fission to be treated explicitly. It is therefore limited to the (default) MCBEND option in which fission is treated as capture.

3. METHOD FOR THERMAL NEUTRONS

In forward MCBEND calculations, the standard treatment of thermal neutron scattering is a bound atom model for some light nuclides and a free atom model for all other nuclides. It would be a substantial task to develop an adjoint version of this thermal treatment, so for the initial implementation it was decided to adopt a simple one-group model which should nevertheless be adequate for many shielding applications. This has been implemented as the only available method in adjoint MCBEND cases, and it is also provided as an alternative to the standard treatment in forward cases to enable comparisons to be made. It operates as follows.

In a forward calculation, neutrons are slowed down using the normal collision processing methods until their energy falls below a thermal cut-off. At that stage they enter the thermal group, where they remain for the rest of

their life. Within this group they "forget" their exact energy and undergo absorption or linearly anisotropic scattering as defined by thermally averaged values of the cross-sections and the mean scattering cosine.

In an adjoint calculation, an adjoint particle born in the thermal group will generally undergo a number of scatters within the group and will then be scattered out of the group. After this, it will be speeded up by the normal adjoint collision processing. The angular distribution for scattering within the thermal group is the same as for a forward calculation. The additional data required for adjoint cases are the probability of scattering out of the group and the secondary energy/angle distributions for such scatters. These data are calculated from the basic one-group parameters at run time on the assumption that (in the equivalent forward process) neutrons enter the thermal group only by elastic scattering and that this scattering is isotropic in the Centre of Mass system. These assumptions are usually true and, in any case, they represent only small approximations which are acceptable in a simple one-group treatment.

4. IMPLEMENTATION WITHIN MCBEND

The point energy adjoint method has been implemented as an option within the neutron collision processing module of MCBEND. The method has been formulated in such a way as to keep the required changes to a minimum.

New input data options have been provided to assist the user in specifying the source and scoring data required for an adjoint calculation. For example, the adjoint source spectrum may be specified by giving the name of one of the responses in MCBEND's library of response functions. MCBEND's facility for calculating the importances which control variance reduction has been extended to generate importances for an adjoint case by means of a forward diffusion calculation. Finally, new scoring and editing facilities have been added to enable detector responses to be derived by integrating the product of the adjoint flux and the source.

Adjoint versions of the three main MCBEND neutron data libraries have been produced. These are derived from different evaluated data libraries: UK Nuclear Data Library (UKNDL), JEF-2.2 and ENDF/B-VI. The transformations of the cross-sections and the secondary distributions described in Section 2 have been applied to each of these normal (forward) MCBEND libraries to produce a corresponding "adjoint MCBEND library".

5. VERIFICATION

A number of cases have been run for uniform infinite media or very simple geometries to test the adjoint collision processing procedures within MCBEND and the data in the various adjoint MCBEND libraries which have been generated. In each case the objective is to calculate a certain detector response, and this is done by performing both forward and adjoint runs so that the results can be checked for consistency. Table 1 gives details of these test cases. Figure 1 illustrates the 3D geometry of Case 8. The 3D geometry of Cases 6 and 7 is similar, but all regions contain the same material. In each case the source has a 1/E spectrum and a strength of 1 n/cc/sec. The detector cross-section is a constant 1.0 within the range shown in the table.

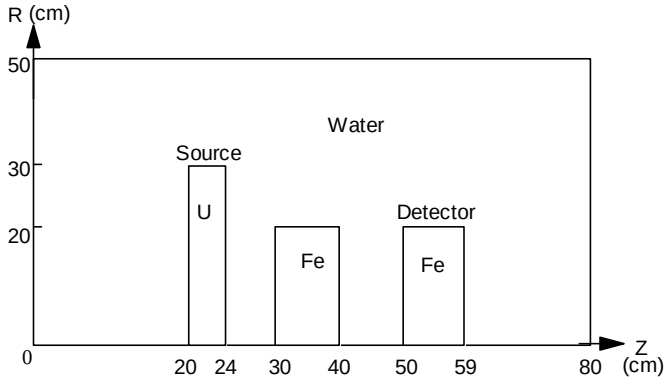

Figure 1. Geometry for Test Case 8

Table 1. Details of verification test cases

Case	Geometry	Materials	Data	Source	Detector
1	Infinite medium	H	UKNDL	1.74-14.6MeV	0.0709-1.5eV
2	Infinite medium	C 1.6g/cc + Fe56 7.8g/cc mixed 50:50 by volume	JEF2	1.74-14.6MeV	0.0709-1.5eV
3	Infinite medium	H	UKNDL	Thermal	Thermal
4	Infinite medium	H	JEF2	0.64-14.6MeV	Thermal
5	Infinite medium	C 1.6g/cc + Fe56 7.8g/cc mixed 70:30 by volume	ENDFB6	0.64-14.6MeV	0-1.5eV
6	3D	H 0.1119 g/cc in all zones	ENDFB6	0.64-14.6MeV	Thermal
7	3D	H_2O 1.0 g/cc + Fe 7.8 g/cc mixed 70:30 by volume in all zones	UKNDL	0.64-14.6MeV	0.55-4eV
8	3D (Fig. 1)	Source zone: U 18.7 g/cc (5% U235 by atoms) Detector and intermediate zone: Fe 7.8 g/cc Outer zone: H_2O 1.0 g/cc	JEF2	0.64-14.6MeV	0-1.5eV

Table 2 shows the forward and adjoint results obtained. In all cases the forward and adjoint results agree within 2 standard deviations. There is also no overall + or - bias in the differences. The numerical agreement is therefore considered satisfactory.

The last column of the table compares the efficiency of the adjoint and forward calculations. It shows the ratio of the Figures of Merit for the adjoint and forward calculations, where FOM is given by $(s^2t)^{-1}$, s being the standard deviation and t the running time. The geometries of these test cases do not particularly favour either the forward or the adjoint approach, being either infinite media or 3D systems in which the source and detector regions have equal volumes, so any observed differences in efficiency are associated mainly with energy effects. It can be seen that the differences in efficiency are within a factor 3 either way, except in two cases. In these cases, 2 and 5, the adjoint method is very much less efficient. Both of these involve a mixture of C and Fe56 as a uniform infinite medium, and it is believed that the problem is caused by large weight changes during adjoint collisions at the energies of the deep minima in the Fe56 cross-section. The method will be examined to see if its efficiency can be improved in such cases, but it can be seen that other cases (7 and 8) which involve regions of iron in 3D systems do not suffer in the same way.

Table 2. Results of verification tests

Case	Forward result	St. dev.	Adjoint Result	St. dev.	Difference (sd units)	Relative FOM (adj/fwd)
1	1.728E 0	0.9%	1.741E 0	0.8%	+0.6	0.63
2	1.723E+1	1.3%	1.676E+1	2.4%	-1.0	0.007
3	5.149E+1	1.2%	4.997E+1	1.2%	-1.7	1.0
4	5.026E+1	1.0%	5.007E+1	0.9%	-0.3	0.31
5	3.023E+1	0.8%	3.077E+1	3.8%	+0.5	0.003
6	1.956E-1	1.0%	1.992E-1	0.7%	+1.5	2.0
7	3.527E-3	1.0%	3.520E-3	1.0%	-0.1	1.0
8	1.553E-2	1.0%	1.520E-2	0.9%	-1.6	0.57

6. APPLICATION TO TWO SHIELDING EXPERIMENTS

6.1 NESDIP2

A simulated PWR radial shield was studied in the NESDIP2 experiment conducted at Winfrith[5]. The adjoint method has been used to calculate the S32(n,p)P32 reaction rate at a position near the outer face of the simulated pressure vessel corresponding to a cavity dosimetry position. In Table 3 the result is compared with that of a forward MCBEND calculation and with the measurement. The nuclear data used for these calculations were derived from the UKNDL.

Table 3. S32(n,p)P32 reaction rate in NESDIP2 cavity position

	Reaction Rate	St. Dev. %	C/M
Measurement	2.02E-26	5.0	
Forward calculation	1.897E-26	1.0	0.94
Adjoint calculation	1.867E-26	0.6	0.92
Adjoint/Forward	0.984	1.2	

The difference of 1.6% between the forward and adjoint results is within 2 standard deviations, as are the differences between the calculations and measurements.

6.2 RADIAL SHIELD MOCK-UP IN DIMPLE

An experiment in the DIMPLE reactor at Winfrith simulated a corner section of the core of a PWR together with the radial shield[6]. The adjoint method has been used to calculate the S32(n,p)P32 reaction rate at the inner surface of the simulated pressure vessel. In this case the point energy adjoint result (using UKNDL data) has been compared with a multigroup adjoint calculation using the 100 group EURLIB data. The results are shown in Table 4.

Table 4. S32(n,p)P32 reaction rate in DIMPLE experiment

	Reaction Rate	St. Dev. %	C/M
Measurement	1.226E-21	5.0	
Multigroup adjoint calculation	1.048E-21	0.5	0.85
Point energy adjoint calculation	1.143E-21	0.9	0.93
Point/Multigroup	1.091	1.0	

Compared with the multigroup method, the point energy adjoint method gives significantly improved agreement with the measurement in this case. From the standard deviations and the running times (which were not the same), it was estimated that the point energy method would take about 30% longer than the multigroup method to achieve the same standard deviation. This is a small penalty considering the greater accuracy of the point energy method.

7. APPLICATION TO A PWR SHIELDING CALCULATION

7.1 BACKGROUND

The H B Robinson Unit 2 station is a three-loop 665MW(e) Westinghouse PWR owned by the Carolina Power and Light Company and located at Hartsville, South Carolina, USA. An extensive range of measurements was carried out during cycle 9 using special dosimetry introduced into the surveillance position in the downcomer annulus and into the reactor cavity. These measurements provide a means of validating MCBEND for radial shield calculations on PWRs, and a number of comparisons with MCBEND calculations have been carried out in recent years [7,8].

The use of adjoint calculations for such applications could offer advantages, both because the detectors are small in volume relative to the source over the reactor core and because there is a need to calculate the change in the detector responses due to the changing source distribution during and between cycles.

Some further MCBEND calculations for this system have therefore been carried out using the new point energy adjoint option. They have been compared both with MCBEND calculations in forward mode and with the measurements.

7.2 FORWARD CALCULATIONS

A plan view of the MCBEND model is shown in Figure 2. In MCBEND calculations for this type of system, separate runs are usually performed to obtain results in the surveillance capsule and in the cavity, this being done so that the particle splitting can be directed towards the region of interest. However, the reaction rates in all the detectors at the given position are usually calculated in the same run. The importance function used to control particle splitting is calculated by the code using an adjoint diffusion solution, in which the source is made uniform in energy with the aim of obtaining adequate statistical accuracy both for high and low energy detectors.

The present calculations have been restricted to one position, the surveillance capsule, and to two detectors, the high energy reaction Ni58(n,p) and the low energy reaction Fe58(n,γ).

The source was modelled using an XYZ mesh over the reactor core, the fission neutron source strengths being mid-cycle values. The proportions of fissions from uranium and plutonium were specified over the mesh, so that account could be taken of the different fission spectra. The main scoring region was the surveillance capsule, which is located in the water between the thermal shield and the pressure vessel. The MCBEND library response functions (IRDF-90 values) were used for the Ni58(n,p) and Fe58(n,γ) detectors. The MCBEND nuclear data library derived from ENDF/B-VI data was used.

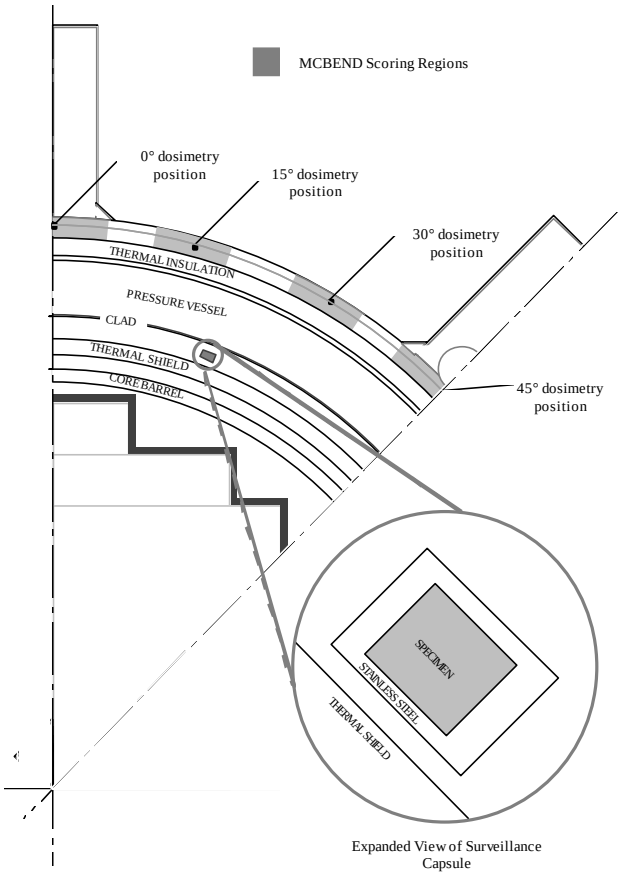

Figure 2. H B Robinson radial shield model

7.3 ADJOINT CALCULATIONS

Reaction rates for the same two detectors at the surveillance position have been calculated using the adjoint method. In this case a separate run was required for each detector. The source region for these adjoint runs was the surveillance capsule. The source spectrum was identified with the cross-sections for the Ni58(n,p) or Fe58(n,γ) reaction, for which the MCBEND library response functions were used. The scoring region for the adjoint runs was the reactor core. The detector response is the integral of the product of the adjoint function and the source strength. MCBEND provides scoring and editing facilities which enable this result to be obtained. Importances for variance reduction were calculated by the code using a forward diffusion solution.

7.4 RESULTS

The measured and calculated results, expressed as end-of cycle activations, are compared in Table 5 for Ni58(n,p) and Table 6 for Fe58(n,γ).

Table 5. Ni58(n,p) activation at surveillance position

	Activation dps/a	St. Dev. %	C/M
Measurement	2.58E-15	10	
Forward calculation	2.508E-15	0.4	0.97
Adjoint calculation	2.474E-15	0.4	0.96
Adjoint/Forward	0.986	0.6	

For Fe58(n,p), the forward and adjoint results agree within 1.4%. This difference, although small, is just over 2 standard deviations and is therefore statistically significant; it is of the order that would be expected from the error associated with the representation of the data in the forward and adjoint forms of the MCBEND nuclear data library. The calculated results are lower than the measurement by 3% and 4%. This is well within the uncertainty of 10% on the measurement.

Table 6. Fe58(n, g) activation at surveillance position

	Activation dps/a	St. Dev. %	C/M
Measurement	2.06E-14	12	
Forward calculation (Detailed thermal)	1.952E-14	1.8	0.95
Forward calculation (1-gp thermal)	1.948E-14	1.7	0.95
Adjoint calculation (1-gp thermal)	1.938E-14	1.9	0.94
1-gp/Detailed	0.998	2.5	
Adjoint/Forward	0.995	2.5	

For Fe58(n,γ), the forward and adjoint calculations using the one-group thermal treatment agree within the statistical uncertainties. A further forward calculation was performed to assess the difference between the detailed and one-group thermal treatments, and although the very close agreement is probably fortuitous in view of the statistical uncertainty, the result shows that any error associated with the one-group treatment is unlikely to be greater than 5% in this case. The calculated results are lower than the measurement but the differences are within the uncertainties.

7.5 EFFICIENCY

The results shown in the previous section were obtained with the following running times (on a SUN UltraSparc2 work station):

A forward run of 36 hours gave st. dev. 0.4% for Ni58(n,p) and 1.7% for Fe58(n,γ).

An adjoint run of 2.5 hours gave st. dev. 0.4% for Ni58(n,p).

An adjoint run of 10 hours gave st. dev. 1.9% for Fe58(n,γ).

In general the relative efficiency of using forward or adjoint runs depends on the number of detectors and the number of different source distributions which are to be considered. The present example has only two detectors and one source distribution. Additional detectors (at the same position) could be calculated to about the same statistical accuracy in a single forward run, but each would need a separate adjoint run. On the other hand, results arising from additional source distributions could be calculated to about the same accuracy from the same adjoint runs, but each would require a separate forward run.

As an example, suppose that there is a requirement to calculate reaction rates for 10 detectors (5 high energy and 5 low energy) arising from 10 different source distributions. On the basis of the running times shown above, the total times needed to obtain standard deviations of about 0.4% for high energy detectors and 1.7% for low energy detectors would be as follows:

Forward: 10 runs of 36 hours = 360 hours

Adjoint: 5 runs of 2.5 hours + 5 runs of 12.5 hours = 75 hours

So in this example, the adjoint method would be about 5 times more efficient.

8. SUMMARY

Facilities for performing point energy adjoint calculations for neutrons have been implemented in MCBEND. A range of verification tests have been performed and the application of the method to a radial shield calculation for a PWR has been demonstrated. This option offers improved efficiency and convenience for some common applications. For example, it can provide PWR plant operators with an efficient method of calculating neutron fluences in pressure vessels and in surveillance capsules, taking account of changing core conditions during the reactor lifetime.

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