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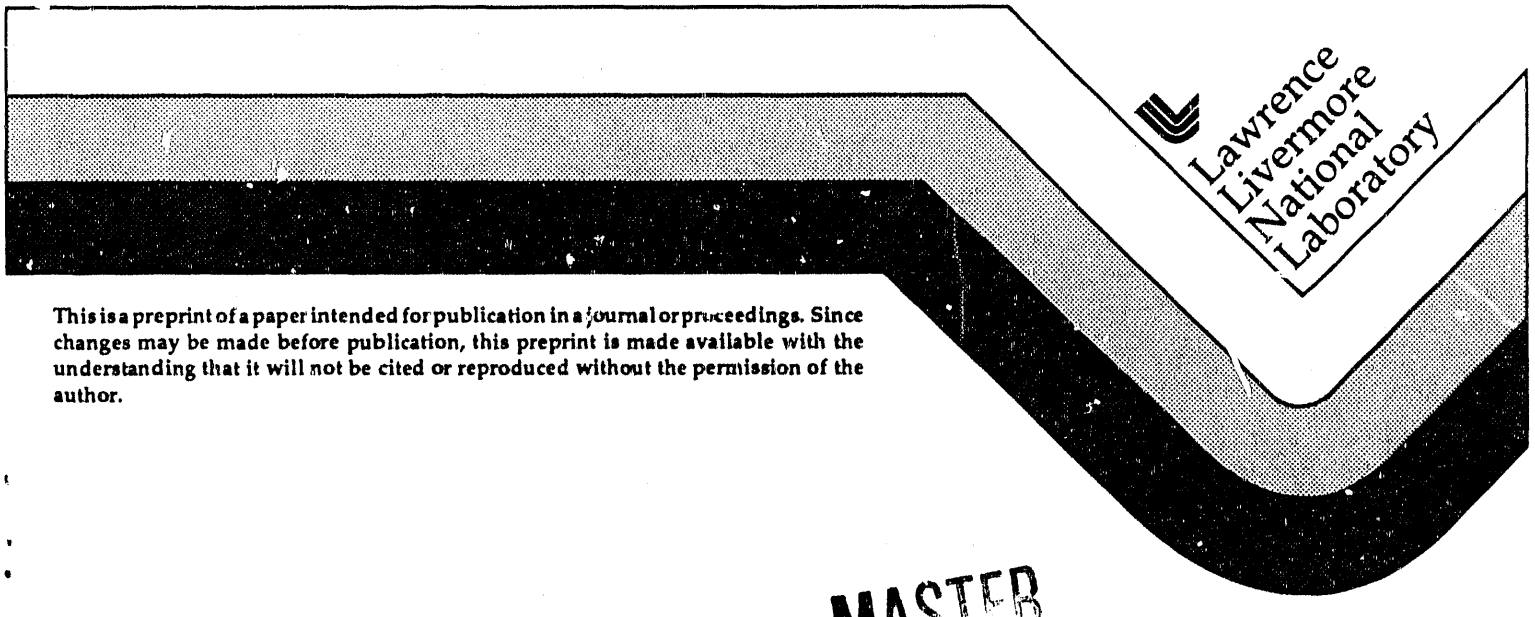

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RESPONSE MATRIX MONTE CARLO FOR ELECTRON TRANSPORT

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ABSTRACT

A Response Matrix Monte Carlo (RMMC) method has been developed for solving electron transport problems. This method was born of the need to have a reliable, computationally efficient transport method for low energy electrons (below a few hundred keV) in all materials. Today, condensed history methods are used which reduce the computation time by modeling the combined effect of many collisions but fail at low energy because of the assumptions required to characterize the electron scattering. Analog Monte Carlo simulations are prohibitively expensive since electrons undergo coulombic scattering with little state change after a collision. The RMMC method attempts to combine the accuracy of an analog Monte Carlo simulation with the speed of the condensed history methods. The combined effect of many collisions is modeled, like condensed history, except it is precalculated via an analog Monte Carlo simulation. This avoids the scattering kernel assumptions associated with condensed history methods. Results show good agreement between the RMMC method and analog Monte Carlo.

INTRODUCTION

A Response Matrix Monte Carlo (RMMC) method has been developed for electron transport calculations in finite media. This new method is based on using energy, angle, and position probability distribution functions (PDFs) which are constructed from an analog Monte Carlo simulation over a small region (local calculation). Local calculations for different incident energies and region sizes generate PDFs for use in a global Monte Carlo calculation. In the global calculation, random samples from the PDFs are used to simulate the transport of electrons by updating electron energy, angle, and position. Unlike deterministic response matrix techniques, this method does not depend on *a priori* knowledge of global geometry. The geometry of the local calculation is independent of the overall geometry being analyzed. Hence, local calculations need to be performed only once so a data base can be constructed for different materials.

Electron transport problems are complicated by the extremely anisotropic coulombic scattering cross section and the very small energy loss associated with individual electron interactions. Condensed history methods, presently used for electron transport problems, combine the effects of many collisions into a composite effect that is more easily modeled in a Monte Carlo code. Generalizations about the scattering kernel and energy loss per collision are required to predict the composite effect. Low energy electron transport (below a few hundred keV) is ill-suited for condensed history because the scattering angle and energy loss are greater than at high energies. The RMMC method can be used as a replacement for condensed history methods especially at low energies.

ELECTRON INTERACTIONS

Electron interactions fall under two categories: inelastic scatter where the electron changes energy and direction, and elastic scatter, where only the direction changes. Inelastic events include ionization and excitation which alter the target atom by knocking out or exciting a bound electron. The target atom can relax or decay to produce secondary radiation in the form of Auger electrons or x-rays. When electrons impinge upon a material, a multiplication in the electron population occurs complicating the transport.

Coulombic interactions with the charged atomic nucleus have negligible effect on electron energy since the nucleus is many time heavier than an electron but the interactions can change the electrons direction. As energy decreases, the elastic scattering cross section dominates. Figure 1 shows the average scattering cosine associated with a single elastic scattering event (μ is the cosine of the scattering angle). Because elastic scatter is extremely anisotropic especially at high energies, Legendre moments would be ineffective in describing the angular dependence unless hundreds of moments were used.

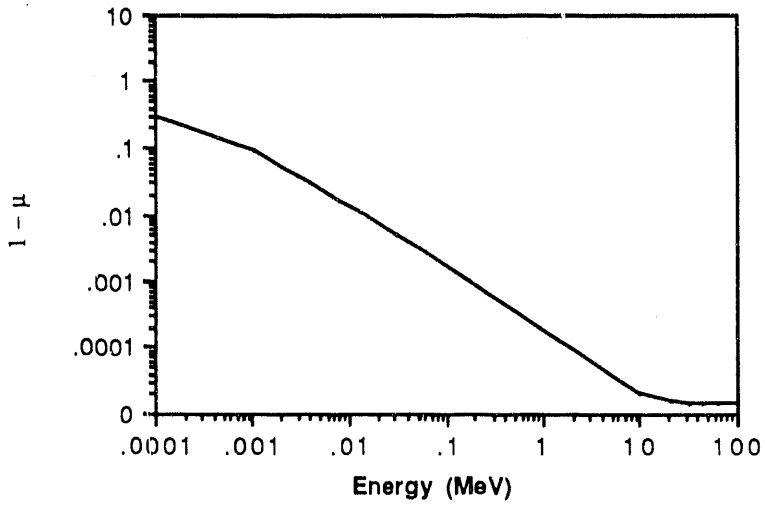

Fig. 1. Mean scattering angle verses electron kinetic energy.

Table 1 shows the total interaction cross section [1-4] compared to total photon interaction cross sections as a function of energy. The electron cross sections are up to five orders of magnitude larger than the photon cross sections while the average energy loss per collision are sometimes five orders of magnitude lower. Total electron cross section refers to the sum of ionization, bremsstrahlung, and elastic scattering cross sections. Excitation cross sections, if included, would increase the difference between photons and electrons even more. Hence, electron transport does not lend itself to photon transport techniques.

TABLE 1. Cross sections and energy losses for electron and photon interactions.

Energy (MeV)	Electron total σ (barns)	Electron Fractional ΔE/E	Photon total σ (barns)
10000	3.25E6	2.0E-5	1.4192
1000	3.31E6	2.0E-5	1.3579
100	3.42E6	2.0E-5	1.1268
10	4.19E6	2.6E-5	1.0365
1.0	9.05E6	3.9E-5	2.7510
0.1	3.90E7	1 8E-4	7.6413
0.01	1.07E8	1.5E-3	1167.2
0.001	6.03E8	0.011	5.2837E4
0.0001	1.09E9	0.052	5.7659E6

ELECTRON TRANSPORT METHODS

Analog Monte Carlo

Analog Monte Carlo simulations for electron transport are prohibitively time consuming for all but the thinnest geometries since an electron undergoes thousands of collisions while traveling a fraction of its range. An analog Monte Carlo code has been written for generating input for the RMMC method and to test the accuracy of some condensed history models. Cross sections for ionization, elastic scatter and bremsstrahlung events were compiled into a data base and used in the analog simulation. Excitation events were modeled with a stopping power since excitation cross sections were unavailable at the time of this work. All cross sections are listed in continuous energy format (EPDL format type) for all electron interactions and distributions describing angle after elastic scatter, knock-on electron energy, and bremsstrahlung photon energy are tabulated for several incident energies.

Equal probability bin structure describing the distributions requires a large amount of storage due to the extremely small energy and angle changes. In addition, table look-up methods are very slow. Sampling speed is important since the Monte Carlo code will sample for thousands of collisions. The Alias method [6] was chosen as the sampling scheme for the analog Monte Carlo code since it uses the same energy and angle spacing as does the tables yet allows for faster sampling compared to table look-up. Statistical interpolation is used for energies between those of the tabulated distributions. Distributions for different incident energies are listed so that between these energies a decision is made about which distribution to sample. The decision for interpolation is based on Eq. 1 for a linear relation in electron energy (E).

$$R = \frac{E_i - E}{E_i - E_{i-1}} \qquad (E_{i-1}<E<E_i) \tag{1}$$

if $R \geq \xi$ then sample from the E_i distribution

if $R < \xi$ then sample from the E_{i-1} distribution

ξ = random variable $\in [0,1)$

Condensed History

To avoid the computational requirements of an analog Monte Carlo simulation, condensed history methods were developed. Many condensed history theories exist describing energy and direction distributions for electrons that have traveled a short path-length. Theories by Moliere [7] and Goudsmit & Saunderson [8] are used to describe the electron direction while the theory by Landau [9] describe the exit energy distribution. The combination of these theories gives a complete description of the electron direction and energy after a certain path-length. [7]

The idea behind condensed history methods is that PDFs representing energy and direction can be generated to describe the effect of many collisions over a short path-length. In a Monte Carlo code these PDFs can be sampled to reconstruct electron histories over a larger region. Thus, individual events are replaced by sampling from a PDF that represents the result of a large number of collisions in the Monte Carlo code. Assumptions that limit the electron scattering are required since the PDFs are obtained analytically. Moliere assumed small angle scatter for individual collisions to obtain an expression for the angle distribution after several collisions. The theory of Goudsmit & Saunderson uses the small angle approximation by claiming the number of collisions is given by a Poisson distribution (Eq. 2). This is only true when the physical dimension is equivalent to the path-length traveled by the electron.

$$P(n) = e^{-\Sigma_t d} (\Sigma_t d)^n / n! \qquad (2)$$

Where:

P(n)= probability of **n** collisions

d = distance traveled

Σ_t= total macroscopic cross section

Figure 2 shows that this condition can be met only if each collision causes no angle change, ie. small angle approximation.

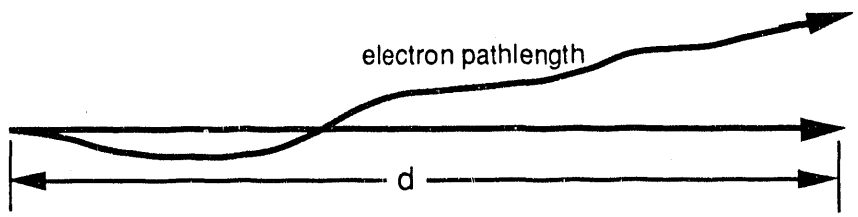

Fig. 2. Path-length not equal to the straight ahead distance.

The use of the small angle assumption implies that the theories are based on conditions which do not exist at low energy since the mean scattering angle increases exponentially with decreasing energy (see Fig. 1). In light of the assumptions used, the condensed history theories are outside their range of validity at low energies. The energy where the condensed history methods fail is dependent upon material thickness and atomic number.

Response Matrix Method

Like the condensed history theories, the RMMC method develops PDFs for direction and energy which represent the effect of many collisions. The RMMC method generates these distributions using an analog Monte Carlo simulation. Position distributions are also constructed since the electrons are not assumed to go straight, giving the advantage of producing PDFs which are valid for any energy. The RMMC method consists of two codes, an analog Monte Carlo code to generate the PDFs (local calculation) and a RMMC code that uses these PDFs to step through a large problem (global calculation).

Local calculation. The local calculation is used to generate PDFs via an analog Monte Carlo simulation of electron transport over a small region. PDFs for energy, direction, and position are constructed and assumed independent of one another so that storage is reduced by avoiding coupled energy-direction-position distributions. Decoupling the variables introduces inaccuracies in the global calculation. Local region shape determines the extent of the coupling between energy and direction with position. Slab geometry local regions are not suited for construction of independent PDFs because the strong relation of energy on exit position. Electrons can suffer a variety of different histories in the slab geometry since those escaping straight do not encounter as many collisions as those exiting at a corner.

The ideal shape would be a surface of equal path-lengths, where all exiting electrons have traveled the same distance allowing energy and position to be nearly decoupled. Spherical geometry provides a good approximation to the equal path-length surface. Hemisphere local calculations were chosen for this work because the problems of interest are beams incident upon flat surfaces. In addition, few electrons scatter in the backward direction making it computationally inefficient to track a few renegade electrons in the reverse direction since little additional information is gained. The hemisphere surfaces were divided into sections where energy and angle PDFs were constructed by tallying the electrons that exit a particular section, see Fig. 3.

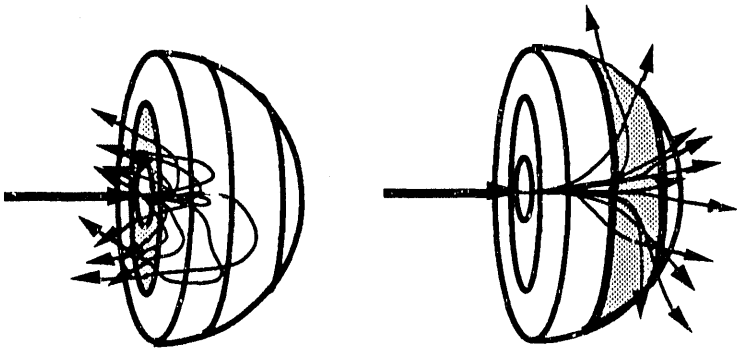

Fig. 3. Sectioned hemisphere used for the local calculations.

Tallying over a surface section preserves some of the coupling of position with energy and angle. Three dimensional quantities such as direction and position require a close investigation to reveal symmetry which can reduce the number of coupled tallies. The exit position PDF has an

obvious symmetry because the cross sections are azimuthally symmetric; the exit position angle (φ) is enough to describe the exit position (Fig. 4). The exit direction's subtle symmetry was discovered after detailed study. The exit direction is symmetric about the n-τ plain where n is the surface normal and τ is tangent to the hemisphere and intersects the incident axis.

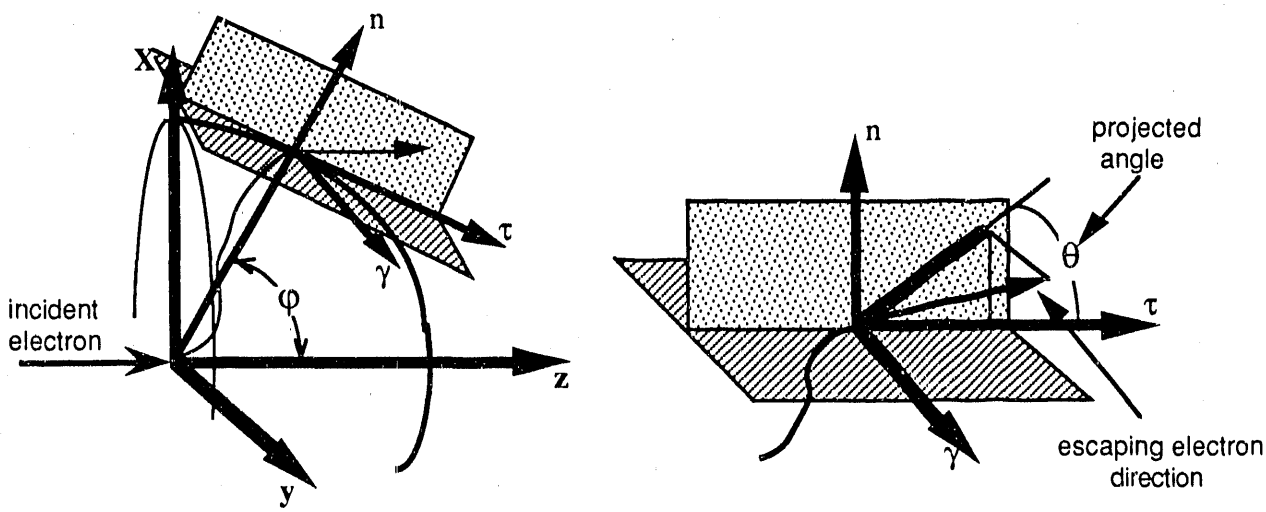

Fig. 4. Exit position and exit direction symmetry.

A PDF representing the electron projected angle onto the n-τ plain was required to describe exiting direction. The direction in the n-γ plain can be approximated by a Gaussian with a small width. These two direction cosines can be used to reconstruct the third direction cosine; hence, only one PDF is required to describe the 3-D direction.

The local calculations are done only once since the data can be saved and used again. PDFs for full and half radius hemispheres are constructed in an single calculation.

Global calculation. Once the PDFs from several local calculations for different incident energies and sizes are constructed, the global calculation can proceed. Statistical interpolation is used for electron energies between energies where PDFs are tabulated. The global simulation begins by sampling an exit position cosine and placing it randomly in azimuth on the hemisphere. This position indicates which of the divided surface sections should be used when sampling from the energy and exit direction PDFs. Once the energy and direction are updated by sampling from the correct PDFs for the surface section, the new electron state is fully described.

This process is continued until the electron encounters a boundary or the energy falls below a cutoff energy. Figure 5 shows what a single electron history might look like in the global calculation.

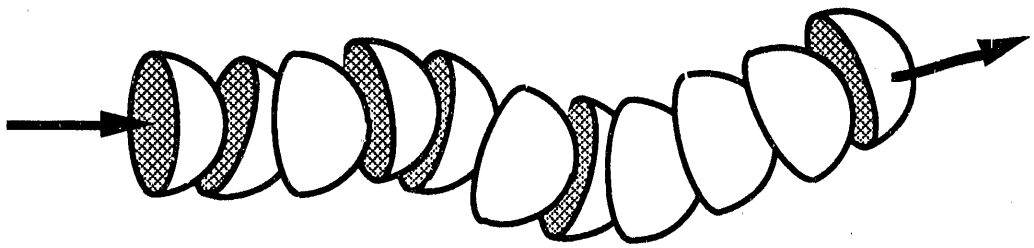

Fig. 5. A single electron history in the global calculation.

Boundaries cannot be matched exactly with hemispheres but are approximated by using smaller hemispheres. When a boundary is crossed, the sampled exit position is used to indicate the direction of exit from the global calculation and the energy loss is taken as a fraction of the sampled energy loss. A linear relation between energy loss and distance to the boundary is assumed.

RESULTS

Results were analyzed in a two step process: first, the analog Monte Carlo results were compared to those from MCNP4 [10] (a condensed history code) to establish the accuracy of the analog Monte Carlo method and secondly the RMMC results were compared to the analog and condensed history results.

Validity of the Analog Monte Carlo Code

The validity of the analog Monte Carlo code had to be established before it could be used to generate PDFs for use in the RMMC method. Hence, the analog code results were compared to MCNP4 results for high energy electron transport, where condensed history methods are valid. Exit energy spectra for electrons traveling through a slab of aluminum are shown in Fig.6.

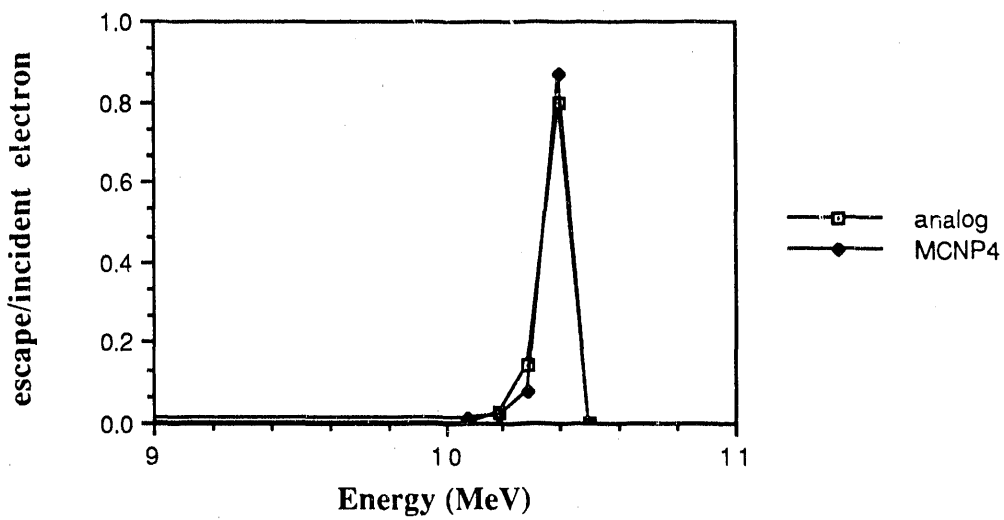

Fig. 6. Transmitted energy spectra for MCNP4 compared to analog Monte Carlo for 10.5 MeV electrons normally incident on 0.04 cm of aluminum.

The results from both codes were within statistical uncertainty in Fig. 6. The codes were also tested for saturation backscatter amount using 102 keV electrons normally incident upon a thick aluminum target. Both the analog Monte Carlo code and MCNP4 obtained 14.8 % (± .1) backscatter which agrees exactly with experimental data from Darlington, *et al.*.[11]

Validity of the RMMC Code

At the time of this writing, results for the RMMC method are unavailable based on full analog simulation data. However, work using a simpler analog Monte Carlo code to generate PDFs show excellent agreement between the RMMC method and the simplified analog simulation. The analog code used in this comparison was based on a stopping power for energy loss and a screened Ruterford cross section to describe the scattering. Figure 7 shows the energy spectra for both codes for transmitted and backscattered electrons from a gold target. The RMMC code and the simple analog Monte Carlo code compared well for different energies and material types.

Table 2 shows the computer time requirement per history for the full analog Monte Carlo code and MCNP4 on a Cray YMP. An order of magnitude more time is required for the analog Monte Carlo simulation over the MCNP4 results. Timings for the RMMC method based on the PDFs generated from the simplified analog Monte Carlo code will remain the same when the new PDFs are constructed. Comparisons between the RMMC speed and the simple analog Monte Carlo code show RMMC is 10 times faster on average. The RMMC cpu requirement is a linear function of the number of hemispheres required to traverse a material. The full analog code requires 4-5 times more than the simple analog simulation so it is expected that the RMMC method be 40 times faster than a full analog Monte Carlo.

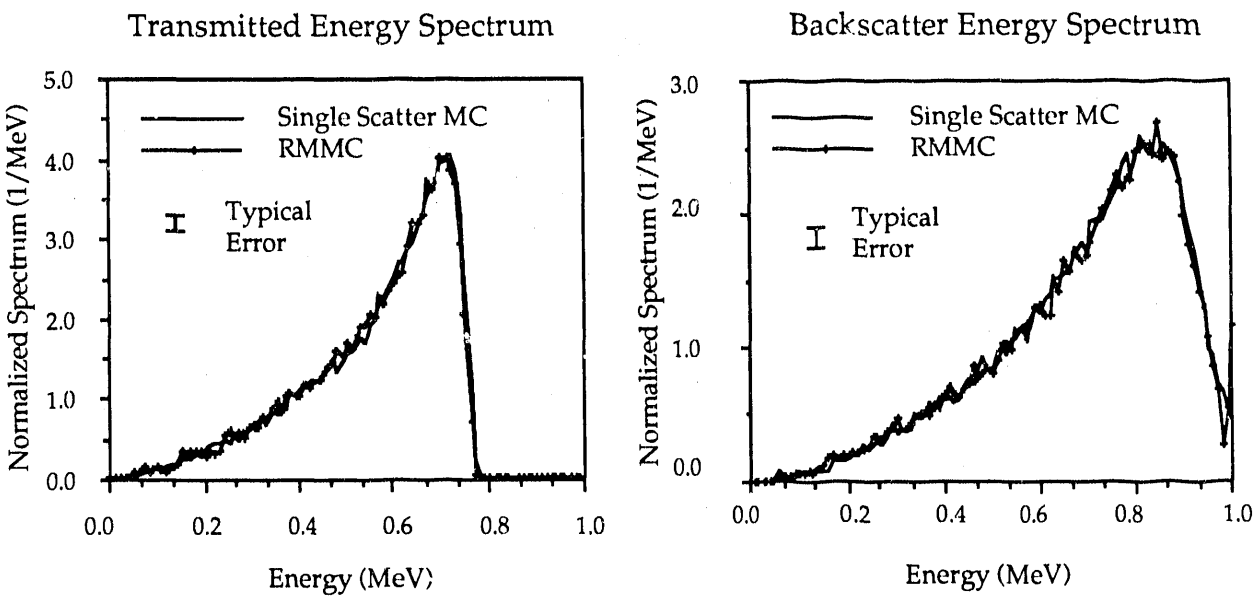

Fig. 7. RMMC vs simple analog Monte Carlo for 1 MeV electrons normally incident on a 0.01 cm slab of gold.

TABLE 2. CPU requirement for analog Monte Carlo, RMMC, and MCNP4 per source electron on a Cray YMP.

Problem Description	Analog M.C.	MCNP4
102 keV electrons on a .002 cm. Al slab	13.3 msec	1.797 msec
102 keV electrons on a .005 cm. Al slab	32.6 msec	7.38 msec
300 keV electrons on a .008 cm. C slab	35.3 msec	5.32 msec

CONCLUSIONS

The RMMC method was successfully used to reproduce analog Monte Carlo results in a fraction if the time. Once the local calculations generate the PDFs, the RMMC method can reuse them to greatly reduce the time requirements for electron transport calculations. Since the RMMC method is based on an analog simulation to generate the PDFs, it has the potential of being more accurate than condensed history methods particularly at low energies. No assumptions of small angle scatter are required for the RMMC method so material type and energy should not effect the validity of the results. This method can be used to replace condensed history methods in many situations. Condensed history methods can be used for high energy transport, while low energy electrons can be transported using the RMMC method. The RMMC method will be at least as fast as the condensed history methods since it uses precalculated PDFs in the global calculation; condensed history methods construct PDFs during the calculation. Comparisons using the full analog simulation PDFs are underway and should compare well with condensed history. Energies where the condensed history results differ from the RMMC results will give insight on the applicable energy range for condensed history methods.

ACKNOWLEDGEMENTS

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