27
7-2-79
24 to 51 TIS

SAND78-1780
Unlimited Release

MASTER

A Versatile Numerical Method for Electron Slowing-Down Spectral Calculations

Jim E. Morel, John A. Halbleib, Sr.

Sandia Laboratories

SF 2900 Q(7-73)

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

SAND78-1780
Unlimited Release
Printed May 1979

A VERSATILE NUMERICAL METHOD FOR ELECTRON SLOWING-DOWN SPECTRAL
CALCULATIONS*

J. E. Morel and J. A. Halbleib, Sr.
Theoretical Division, 4231
Simulation Research Department, 4230
Sandia Laboratories**
Albuquerque, New Mexico 87185

ABSTRACT

A collocation method is presented for the calculation of electron slowing-down spectra. The primary advantage of this approach is its versatility. Unlike the well-known Spencer-Fano technique, this method does not require an analytically integrable expression which closely approximates the scattering kernel in the region of small energy transfers. Computational results are given which demonstrate the effectiveness of the technique. User instructions for a computer program which implements the collocation method are given in Appendix A.

NOTICE

This document is prepared as part of the work performed under contract DE-AC04-76DP00789, between the U. S. Department of Energy and Sandia Corporation. The U. S. Government is authorized to reproduce and reprints for government purposes not withstanding any copyright notation that may appear hereon.

*This work is supported by the U. S. Department of Energy under Contract No. DE-AC04-76DP00789.

**A U. S. DOE facility.

I. INTRODUCTION

The purpose of this report is to present a collocation method for the calculation of infinite-medium electron slowing down spectra. By this we mean the energy spectrum of the electron flux due to a uniformly distributed source of electrons in an infinite homogeneous medium. Such calculations are useful for a variety of purposes. The infinite-medium spectrum is generally representative of the spectrum in the interior of a finite homogeneous medium when the dimensions of the medium are large with respect to the range of the most energetic source electrons. For instance, infinite-medium calculations are often used to provide the spectrum due to photoelectron production in a region small with respect to the mean-free-path of the incident photons, but large with respect to the maximum range of the photoelectrons. When spatial effects are important, large complex Monte Carlo codes[1] must generally be used to perform the calculations. However, it is often the case that spatial effects are only important at the higher energies in a calculation. Thus an increase in computational efficiency can be achieved by performing a Monte Carlo calculation at the higher energies and coupling it to an infinite medium calculation at the lower energies.

One of the first numerical methods for the calculation of electron slowing down spectra was proposed by Spencer and Pano[2] in 1954. Since that time, their technique has prevailed as the standard technique for such calculations. The major strength

of our method lies in its versatility. Its applicability is essentially independent of the functional form of the scattering kernel. Conversely, the Spencer-Fano technique is predicated upon the existence of an analytically integrable expression which very closely approximates the scattering kernel when the initial and final electron energies are nearly equal. A research program is currently being carried out here at Sandia regarding the application of discrete ordinates methods to electron transport calculations. A portion of this program involves the development and testing of approximate inelastic electron-electron scattering cross sections. Infinite-medium spectral calculations present a simple and efficient means of performing preliminary testing of such approximate cross sections. Unfortunately, the Spencer-Fano method is quite cumbersome to use with a large number of distinct cross sections. This is why we were motivated to develop a more versatile method. In addition, because a production computer code for performing infinite-medium electron spectral calculations is not currently available at Sandia, we were motivated to write such a code based upon our collocation technique.

In Section II we discuss the spectral equation and its general solution using our technique as well as certain other existing techniques. In Section III we develop the theory in detail for electron calculations. Computational results are presented in Section IV, and conclusions given in Section V. Appendix A gives user instructions for the computer code which implements our method.

II. GENERAL THEORY

II.A. The Boltzmann Equation

The Boltzmann equation for the slowing-down flux spectrum can be expressed as follows:

$$\sigma_s(E) \phi(E) - \int_E^{E_{\max}} \sigma_s(E', E) \phi(E') dE' = Q(E), \quad (1)$$

where,

$\phi(E)dE$ $\equiv$ the particle flux corresponding to particles with energies between E and $E+dE$

$\sigma_s(E', E)dE \equiv$ the scattering kernel describing the probability per unit path length that a particle with initial energy E' will scatter with a final energy between E and $E+dE$.

We assume that $\sigma_s(E', E) = 0$ for $E > E'$.

$\sigma_s(E)$ $\equiv$ the probability per unit pathlength that a particle with initial energy E will undergo a scattering interaction. Note that

$$\sigma_s(E) = \int_0^E \sigma_s(E, E'') dE'' . \quad (2)$$

$Q(E)dE \equiv$ the source of particles with energies between E and $E+dE$.

$E_{\max}$ $\equiv$ the maximum source energy.

An integral form of Eq. (1) can be derived which is more amenable to numerical solution. We begin by integrating Eq. (1) as follows:

$$\int_E^{E_{\max}} \sigma_s(E'') \phi(E'') dE'' - \int_E^{E_{\max}} \int_E^{E_{\max}} \sigma_s(E', E'') \phi(E') dE' dE'' = \int_E^{E_{\max}} Q(E'') dE'' . \quad (3)$$

The quadrature weights are labelled with two indices because the effective interval of integration (and thus the quadrature weights) changes as a function of the index i .

Note that to solve for the flux value at E_i , only the flux values at energies above E_i are required:

$$\phi(E_i) = \left(\sum_{j=1}^i Q(E_j) w_{ij} - \sum_{j=1}^{i-1} K(E_j, E_i) \phi(E_j) w_{ij} \right) / (K(E_i, E_i) w_{ii}), \quad (7)$$

$i=2, N$.

A value for $\phi(E_1)$ must be obtained by other methods which we will discuss later. Once this value has been obtained, the remaining flux values can be obtained successively using Eq. (7).

II.C. The Spencer-Fano Technique

Difficulties arise in applying the standard quadrature method to the electron spectral problem because the electron kernel is nearly singular in the region where $E' \approx E$. Thus an unacceptably fine energy mesh must be used in order to properly evaluate the integral on the left side of Eq. (5). To circumvent this difficulty, Spencer and Fano defined another kernel, $\bar{K}(E', E)$, which was analytically integrable in E' and closely approximated $K(E', E)$ for $E' \approx E$. In particular, the following criterion was satisfied

$$\int_E^{E+\delta} \{K(E', E) - \bar{K}(E', E)\} dE' \approx 0, \text{ for } \delta \ll E. \quad (8)$$

They then re-expressed Eq. (5) as follows:

$$\int_E^{E_{\max}} \bar{K}(E;E) \phi(E) dE' + \int_E^{E_{\max}} \{K(E;E) \phi(E') - \bar{K}(E;E) \phi(E)\} dE' = \int_E^{E_{\max}} Q(E') dE'. \quad (9)$$

The first integral on the left side of Eq. (9) can be analytically evaluated and the second integral has an integrand which is much better behaved than the integrand on the left side of Eq. (5) due to the continuity of $\phi(E)$ and condition (8). Thus Eq. (9) is much more amenable to the standard quadrature method than is Eq. (5) whenever the integral kernel is ill-behaved about $E' \approx E$. This is the central theme of the *Spencer-Fano* approach.

II.D. A Collocation Technique

Collocation methods, like quadrature, finite-difference, and finite-element methods, constitute a general class of methods for the solution of integral and differential equations.[3] Most equations of physical interest can be expressed as

$$L \phi(\vec{x}) = q(\vec{x}), \quad (10)$$

where

L = a linear operator,

$\phi(x)$ = the solution,

$q(x)$ = a source or driving function.

A collocation solution for such an equation is generally constructed in the following way. First, the solution and the

driving function are assumed to be expressible in terms of a linear combination of N basis functions

$$\phi(\vec{x}) = \sum_{i=1}^N \phi_i B_i(\vec{x}), \quad (11a)$$

$$q(\vec{x}) = \sum_{i=1}^N q_i B_i(\vec{x}). \quad (11b)$$

Under this assumption, the solution is uniquely defined by the expression coefficients, $\{\phi_i\}_{i=1}^N$. A linear system of equations for these coefficients is then obtained simply by requiring that the original equation be exactly satisfied at N distinct points,

$$L \phi(\vec{x}_i) = q(\vec{x}_i), \quad i = 1, N. \quad (12)$$

Equation (12) reflects the fact that all collocation methods are based upon pointwise approximations.

Our particular collocation method is based upon the use of a set of piecewise linear basis functions to describe the flux solution. Suppose that a solution to Eq. (5) is desired over the interval $(E_{\min}, E_{\max})$. Let $\{E_j\}_{j=1}^N$ denote a discrete energy mesh with $E_1 = E_{\max}$ and $E_N = E_{\min}$. The flux solution, $\phi(E)$, is assumed to be representable by

$$\phi(E) = \sum_{j=1}^N \phi(E_j) B_j(E), \quad (13)$$

where

$$B_1(E) = (E - E_2)/(E_1 - E_2), \quad E \in (E_2, E_1), \\ = 0 \text{ otherwise.}$$

$$\begin{aligned}
B_j(E) &= (E_{j-1} - E)/(E_{j-1} - E_j), \quad E \in (E_j, E_{j-1}), \quad j = 2, N-1 \\
&= (E - E_{j+1})/(E_j - E_{j+1}), \quad E \in (E_{j+1}, E_j), \\
&= 0 \text{ otherwise.}
\end{aligned}$$

$$\begin{aligned}
B_N(E) &= (E_{N-1} - E)/(E_{N-1} - E_N), \quad E \in (E_N, E_{N-1}), \\
&= 0 \text{ otherwise.}
\end{aligned}$$

Note that the use of this basis set is equivalent to linearly interpolating the discrete flux values.

Substituting expression (13) into Eq. (5) and assuming that the source function can be similarly expressed yields

$$\sum_{j=1}^N \phi(E_j) \int_E^{E_1} K(E', E) B_j(E') dE' = \sum_{j=1}^N Q(E_j) \int_E^{E_1} B_j(E') dE'. \quad (14)$$

The equation for the discrete flux values is obtained by requiring the above equation to hold at the points of interpolation. The result is,

$$\sum_{j=1}^N \phi(E_j) \int_{E_i}^{E_1} K(E', E_i) B_j(E') dE' = \sum_{j=1}^N Q(E_j) \int_{E_i}^{E_1} B_j(E') dE', \quad (15)$$

$$i = 2, N.$$

Note that a value of $i = 1$ is not included in Eq. (15) simply because it is indeterminate for that first value. Thus, like Eq. (6), an initial flux value must be obtained by other means. Since each $B_j(E)$ is non-zero only on (E_{j+1}, E_{j-1}) , the summation

over the index j can be terminated at $j = i$, the upper limit of integration can be changed to E_{j-1} , and the lower limit of integration can be changed to $\alpha_i \equiv \max(E_1, E_{j+1})$. Thus

$$\sum_{j=1}^i \phi(E_j) \int_{\alpha_i}^{E_{j-1}} K(E', E_i) B_j(E') dE' \quad (16)$$

$$= \sum_{j=1}^i Q(E_j) \int_{\alpha_i}^{E_{j-1}} B_j(E') dE', \quad i = 2, N.$$

Equation (13) can be conveniently re-expressed as follows:

$$\sum_{j=1}^i \phi(E_j) w_{ij}^* = \sum_{j=1}^i Q(E_j) w_{ij}, \quad i = 2, N, \quad (17a)$$

$$w_{ij}^* \equiv \int_{\alpha_i}^{E_{j-1}} K(E', E_i) B_j(E') dE', \quad (17b)$$

$$w_{ij} \equiv \int_{\alpha_i}^{E_{j-1}} B_j(E') dE'. \quad (17c)$$

Note that both the downscatter and source integrals are exactly calculated with the quadrature weights defined in Eqs. (17b) and (17c), respectively. Thus the number of mesh points required for a calculation is dependent only upon the adequacy of the corresponding basis function expansions for the flux solution and source function. An ill-behaved scattering kernel does not necessarily imply the necessity of a large number of mesh points as it does with the standard approach. This is an important characteristic of our collocation method.

The source weights given in Eq. (17c), can be analytically evaluated and are in fact simply equal to the composite trapezoidal rule quadrature weights. In general, the downscatter weights, given in Eq. (17b), cannot be analytically evaluated. However, they can be evaluated numerically. We have found that modern adaptive integration algorithms [4] can be very effective for these types of integrals.

It is significant to note that if the differential kernel cannot be analytically integrated to obtain the integral kernel defined by expression (4), the downscatter weights can be re-expressed in terms of the differential kernel:

$$w_{ij}^* \equiv \int_{\alpha_i}^{E_j-1} \int_0^{E_i} \sigma_s(E', E'') B_j(E') dE' dE'' \quad (18)$$

The resulting double integrals can also be evaluated numerically.

Like Eq. (6), Eq. (17a) corresponds to a lower triangular system of linear equations. Hence the flux value at any energy E_i depends only upon the flux values at energies above E_i . Once the first flux value is obtained, the remaining values can be successively obtained using the equation

$$\phi(E_i) = \left(\sum_{j=1}^i Q(E_j) w_{ij} - \sum_{j=1}^{i-1} \phi(E_j) w_{ij}^* \right) / w_{ii}^*, \quad (19)$$

$$i=2, N.$$

An expression for the initial flux value can be found by a simple manipulation of Eq. (5). In particular, we divide both sides of the equation by a common quantity to obtain

$$\frac{\int_E^{E_{\max}} K(E'E) \phi(E') dE'}{\int_E^{E_{\max}} K(E'E) dE'} = \frac{\int_E^{E_{\max}} Q(E') dE'}{\int_E^{E_{\max}} K(E'E) dE'} \quad (20)$$

If we interpret the kernel as a weight function, we find that the left side of Eq. (20) is simply the weighted average value of the flux between $E_{\max}$ and E . It follows then that

$$\phi(E_{\max}) = \lim_{E \rightarrow E_{\max}} \frac{\int_E^{E_{\max}} Q(E') dE'}{\int_E^{E_{\max}} K(E'E) dE'} \quad (21)$$

In practice we have found that a single evaluation of expression (21) with $E = 0.95E_{\max}$ is generally sufficient for electron calculations. The integrals can be easily evaluated using adaptive numerical integration algorithms. This initial value scheme is quite similar to the scheme proposed by Spencer and Fano [2], but it does not require an analytically integrable approximate kernel.

III. SPECIFIC THEORY FOR ELECTRON SPECTRAL CALCULATIONS

III.A. The Boltzmann Equation with Secondary Particles

Since we are primarily interested in electron spectra with source energies below 1.0 MeV, bremsstrahlung will be completely neglected in our treatment. However we shall include secondary electron production as it is quite important at the low energies. Equation (5) can be altered to include secondary particle production as follows:

$$\int_E^{E_{\max}} K(E', E) \phi(E') dE' = \int_E^{E_{\max}} K_P(E', E) \phi(E') dE' + \int_E^{E_{\max}} Q(E') dE', \quad (22)$$

where,

$K_P(E', E) dE \equiv$ the probability per unit path length that a particle with initial energy E' will produce a secondary particle with an energy greater than E .

III.B. Electron Cross Sections

Møller has derived a relativistic differential cross section for inelastic electron-electron scattering [5] which is

$$\sigma_M(E', E) = (2\pi Z N_a r_0^2 / (A\beta^2)) \{ 1.0 / (E' - E)^2 + 1.0 / E^2 + 1.0 / (E' + 1)^2 \\ - ((2.0 + 1.0/E') / (E' + 1.0)^2) (1.0 / (E' - E) + 1.0/E) \} ,$$

for $E \leq (0.5E', E')$,

$$= 0 \text{ otherwise,} \quad (23)$$

where,

$Z \equiv$ atomic number of the transport medium,

$N_a \equiv$ Avagadro's number,

$r_0 \equiv$ classical electron radius,

$A \equiv$ atomic weight of the transport medium,

$\beta \equiv V'/c = \{E'(E'+2)\}^{1/2} / (E+1),$

$E' \equiv$ incident electron kinetic energy in mc^2
(electron rest mass) units,

$E \equiv$ emergent electron kinetic energy in mc^2 units.

This cross section expresses the probability per unit path length (g/cm^2) per unit emergent energy that a primary electron with initial energy E' will emerge from a scattering interaction with an energy between E and $E+dE$. The primary electron is defined to be that electron which emerges from the interaction with the larger fraction of the incident energy. This is why the cross section is defined to be zero for fractional energy losses greater than 0.5. Because the energy lost by the primary is equal to the energy of the secondary, the differential cross section for secondary electron production, $c_p(E',E)$, can be expressed as

$$\sigma_p(E',E) = \sigma_M(E',E' - E) , \text{ for } E \in (0.0, 0.5E') , \quad (24)$$

$$= 0, \text{ otherwise.}$$

This cross section represents the probability per unit path-length per unit secondary energy that a primary electron with initial energy E' will produce a secondary electron with an energy between E and $E+dE$.

The Møller cross section rigorously applies only to scattering between free electrons. Hence it is applicable only if the energy of the secondary electron is much greater than the maximum binding energy of the transport medium. Unfortunately, detailed information on the true behavior of the cross section at low secondary energies is not generally available. However, accurate expressions for a transport quantity known as the stopping power are available. This quantity, denoted by $S(E)$, is related to the differential cross section in the following way:

$$S(E') = \int_0^{E'} \sigma_s(E', E) (E' - E) dE \quad (25)$$

It can easily be seen that the stopping power is simply the average energy loss per unit pathlength, or equivalently, the average energy loss per interaction multiplied by the total interaction probability per unit pathlength. It is possible to calculate the electron stopping power without explicit knowledge of the differential cross section. Rohrlich and Carlson [6] give a relativistic expression for the electron stopping power which can be expressed as

$$S(E) = (2\pi N_a r_0^2 / A\beta^2) \{ \ln[E^2(E + 2)/(2I_0^2)] + f(E) \}, \quad (26)$$

$$f(E) = 1 - \beta^2 - (2E + 1)/(E + 1)^2 \ln(2) + \frac{1}{8} E^2/(E + 1)^2,$$

where E is the electron energy in mc^2 units, I_0 is the mean ionization potential of the medium in mc^2 units and all other terms are

as given in expression (22). This expression has units of $mc^2/(g/cm^2)$ and is valid whenever $E \gg I_0$.

Spencer and Fano [2] have argued that a reasonable approximation to the true cross section can be obtained by modifying the Møller cross section about $E' \approx E$ so as to make the stopping power (as defined by expression (25)) of the modified cross section equal to that given by expression (26). In particular, if we denote the modified cross section by $\sigma_M^*(E', E)$, then

$$\begin{aligned}\sigma_M^*(E', E) &= \sigma_M(E', E), \text{ for } E \in (0.5E', E' - \bar{\gamma}(E')), \quad (27a) \\ &= 0 \text{ otherwise}\end{aligned}$$

where

$$\bar{\gamma}(E') = I_0^2 \exp(\beta^2) / (2.0E'(E' + 2.0)). \quad (27b)$$

In order to insure the conservation of both particles and energy, we similarly define a modified cross section for secondary electron production

$$\begin{aligned}\sigma_p^*(E', E) &= \sigma_p^*(E', E' - E), \text{ for } E \in (\bar{\gamma}(E'), 0.5E'), \quad (28) \\ &= 0 \text{ otherwise.}\end{aligned}$$

The integral scattering kernel appearing in Eq. (22), $K(E', E)$, can be expressed as

$$\begin{aligned}
K(E', E) &= \int_{0.5E'}^E \sigma_M^*(E', E'') dE'', \\
&= (2\pi Z N_a r_0^2 / (A\beta^2)) \left\{ 1.0 / (E' - E) - 1.0 / E + (E - 0.5E') / (E' + 1.0)^2 \right. \\
&\quad \left. - ((2.0 + 1.0/E') / (E' + 1.0)^2) \ln(E / (E' - E)) \right\}, \\
&\quad \text{for } E \in (0.5E', E' - \bar{\gamma}(E')), \\
&= K(E', E' - \bar{\gamma}(E')), \text{ for } E \in (E' - \bar{\gamma}(E'), E'), \\
&= 0 \text{ otherwise.}
\end{aligned} \tag{29}$$

The integral secondary production kernel appearing in equation (22), $K_p(E', E)$, can be similarly expressed as

$$\begin{aligned}
K_p(E', E) &= \int_E^{0.5E'} \sigma_F^*(E', E) dE, \\
&= K(E', E' - E), \text{ for } E \in (\bar{\gamma}(E'), 0.5E'), \\
&= K(E', E' - \bar{\gamma}(E')), \text{ for } E \in (0.0, \bar{\gamma}(E')), \\
&= 0 \text{ otherwise.}
\end{aligned} \tag{30}$$

III.C. The Approximate Electron Spectral Equations

Due to the nature of the electron cross sections and the fact that electron spectra tend to change rapidly at low energies due to a build up of secondary electrons, it is convenient to use a logarithmic energy grid of the form:

$$E_i = 2^{-\frac{1}{k}} E_{i-1} \quad i = 2, N \text{ and } k \geq 1, \quad (31)$$

where E_1 is the maximum source energy. The initial flux value is found by approximating expression (21) in the following manner:

$$\phi(E_1) = \frac{\int_{.95E_1}^{E_1} Q(E') dE'}{\int_{.95E_1}^{E_1} K(E', E) dE'} \quad (32)$$

Note that the secondary production kernel plays no role since $0.95 E_1 > 0.5 E_1$.

The discrete form of Eq. (22) can be expressed in a manner analogous to Eq. (17) as follows:

$$\phi(E_i) = \left(\sum_{j=1}^i Q(E_j) w_{ij} + \sum_{j=1}^{i-k} \phi(E_j) w_{ij}^+ - \sum_{j=i-k}^{i-1} \phi(E_j) w_{ij}^* \right) / w_{ii}^*, \quad (33a)$$

$$i = 2, N,$$

where,

$$w_{ij} \equiv \int_{\alpha_i}^{E_{j-1}} B_j(E') dE', \quad \alpha_i \equiv \max(E_i, E_{j+1}), \quad (33b)$$

$$w_{ij}^+ \equiv \int_{\gamma_i}^{E_{j-1}} K_p(E', E_i) B_j(E') dE', \quad \gamma_i \equiv \max(2E_i, E_{j+1}), \quad (33c)$$

$$w_{ij}^* \equiv \int_{\gamma_i}^{\zeta_i} K(E', E_i) B_j(E') dE', \quad \zeta_i \equiv \min(2E_i, E_{j-1}). \quad (33d)$$

The above integrals are to be considered as zero whenever the lower limit of integration is greater than the upper limit. This equation is then used to find the remaining flux values.

III.D. Validity of the Method

Expression (32) is intended to approximate the limit value given by expression (20). With a mono-energetic source, $Q(E) = \delta(E-E_1)$, the limit does not exist as the flux solution is singular at E_1 . However, Spencer and Fano[2] have shown that the singularity is logarithmic. Thus expression (32) can be used without inducing significant error into the calculation.

As previously noted, the modified Møller cross section is valid only when the energy loss of the primary electron is significantly greater than the maximum binding energy of the transport medium. Thus flux solutions at energies below the maximum binding energy must be viewed with limited confidence.

It can be shown that the expression given for $\bar{\gamma}(E)$ in Eq. (27b) is accurate only to first order in $\omega(E)$, where

$$\omega(E) = \bar{\gamma}(E)/E. \quad (34)$$

For sufficiently low E , completely erroneous values for $\bar{\gamma}(E)$ will be obtained. In particular, the expression for $\bar{\gamma}(E)$ is unbounded as $E \rightarrow 0.0$. It can be seen from expressions (23) and (27a) that if $\bar{\gamma}(E')$ is greater than $0.5E'$, the modified Møller cross section is identically zero. This is clearly incorrect. If we assume that $\exp(\beta^2) = 1.0$ in Eq. (27b), we find that an unacceptable value is obtained for $\bar{\gamma}(E)$ whenever $E < I_0/\sqrt{2}$. The maximum binding energy is always much greater than $I_0/\sqrt{2}$. Hence if the binding energy criterion is met, this difficulty will not be encountered. However, if for some reason it is desirable to

ignore the binding energy criterion, it must be remembered that at some energy below $I_0/\sqrt{2}$, the algorithm will yield completely inaccurate results.

IV. CALCULATIONS AND COMPARISONS

McGinnies[7] has performed a large number of electron spectral calculations using the Spencer-Fano technique. The modified Moller cross section is used by McGinnies to describe primary electron energy loss and secondary electron production. Bremsstrahlung is completely neglected. We have duplicated two particular calculations of McGinnies in order to verify our technique. The first calculation is for a unit monoenergetic source at approximately 1.0 MeV in Aluminum ($Z = 13.0$, $A = 28.0$, $I_0 = 163.0$ eV). The second calculation is for a unit monoenergetic source at approximately 1.0 MeV in lead ($Z = 82.0$, $A = 207.2$, $I_0 = 1180$ eV). In both our calculations and McGinnies' calculations, a logarithmic grid as given by expression (31) with $k=6$ was used. The source weights as given in Eq. (33c), and the downscatter weights as given in Eq. (33a) were calculated with an adaptive Simpson rule integration routine called SIMP[4] subject to a relative error criterion of 1%.

Our results for calculations 1 and 2 are compared with McGinnies' results in Tables I and II, respectively. Agreement is excellent in both cases. We are unable to compare the two methods with respect to running times, but our calculations 1 and 2 required approximately 12 and 8 seconds of CPU time respectively on a CDC-6600 computer.

Electron Energy (mc^2 units)	Collocation Method	Spencer-Fano
2.63	.370	--
1.81	.350	.352
1.28	.327	.326
.905	.307	.307
.640	.285	.284
.453	.260	.259
.320	.235	.234
.226	.213	.212
.160	.196	.195
.113	.184	.184
.0800	.179	.178
.0566	.179	.179
.0400	.186	.185
.0283	.197	.196
.0200	.213	.213
.0141	.235	.235
.0100	.264	.263
.00707	.300	.300
.00500	.348	.347
.00354	.411	.410
.00250	.496	.495
.00177	.618	.619
.00125	.805	.811
.000884	1.11	1.15

TABLE I: Comparison of collocation solution and Spencer-Fano solution for calculation 1. The solution data have units of flux/ $(mc^2 - \text{unit source})$.

Electron Energy (mc^2 units)	Collocation Method	Spencer-Fano
2.03	.594	--
1.81	.561	.557
1.28	.518	.517
.905	.494	.494
.640	.468	.467
.453	.439	.438
.320	.411	.411
.226	.390	.389
.160	.378	.378
.113	.379	.378
.0800	.409	.393
.0566	.424	.424
.0400	.473	.472
.0283	.544	.543
.0200	.646	.646
.0141	.793	.795

TABLE II: Comparison of the collocation solution and Spencer-Fano solution for calculation 2. The solution data have units of flux/(mc^2 - unit source).

V. Conclusions

The comparison of flux solutions given in Section IV demonstrates that our technique is capable of yielding accuracies comparable to that of the Spencer-Fano method when identical energy grids are used. The computing time required for a typical calculation on a modern computer (approximately 8-12 seconds of CPU time on a CDC-6600) demonstrates that our method is computationally inexpensive. Thus, taking all of these factors into account, we conclude that our technique is a valuable alternative to the Spencer-Fano method.

REFERENCES

1. Martin J. Berger, Meth. Comp Phys., I, (1963), 135.
2. L. V. Spencer and U. Fano, Phys. Rev., 93, (1954), 1172.
3. P. M. Prenter, Splines and Variational Methods, John Wiley and Sons, Inc., New York, 1975.
4. L. F. Shampine and R. C. Allen, Numerical Computing: An Introduction, W. B. Saunders Company, Philadelphia, 1973.
5. C. Møller, Z. Physik, 70, (1931), 686.
6. F. Rohrlich and B. C. Carlson, Phys. Rev., 93, (1954), 38.
7. R. T. McGinnies, Energy Spectrum Resulting from Electron Slowing Down, NBS Circular 597, (1959).

Appendix A

User Instructions for the IMES Code

The purpose of this Appendix is to provide user instructions for the computer code, IMES. This code was written to perform infinite-medium electron slowing-down spectral calculations and employs the solution algorithm described in the text of this report. It may be used on Sandia's CDC-7600, CYBER-176, or CDC-6600 computers. The control cards for the 7600 and CYBER-176 are as follows:

```
JOB
ACCOUNT
ATTACH (OLDPL, IMES)
FILE (OLDPL, RT=S)
UPDATE (F,L=0)
FTN (I=COMPILE, L=0)
LGO.
7/8/9
7/8/9
-----Input Data-----
6/7/8/9
```

The control cards for the 6600 are slightly different:

```
JOB
ACCOUNT
ATTACH (OLDPL, IMES)
UPDATE (F,L=0)
FTN (I=COMPILE, L=0)
COLLECT (LGO,FINLIB)
LGO.
7/8/9
7/8/9
-----Input Data-----
6/7/8/9
```

The input data instructions follow.

Card 1

Format (2E12.5, 4I4)

EO -- the maximum source energy in MeV.

RHO -- the density of the medium in g/cm³.

NE -- the total number of elements in the medium
 (< 5).

IFAC2 -- the electron energy grid is computed such
 that

$$E_{i+1} = E_i 2^{\frac{-1}{IFAC2}}, \quad i=1, NE-1, \quad E_1 = EO.$$

NMAX -- the total number of energy grid points (≤ 100).

KI -- Currently unused, but must be set to zero.

KS -- [E(KS), E(1)] is the interval over which the
 differential source spectrum is non-zero.
 Set to zero for a monoenergetic source at EO.

Card 2

Format (4E12.5)

Repeat card for each element, I = 1, NE.

CIE(I) -- The mean excitation energy of the ^Ith
 constituent element in eV.

ZE(I) -- the atomic number of the ^Ith element.

AI(I) -- the atomic weight of the ^Ith element.

WE(I) -- the weight fraction of the ^Ith element.

Card 3

Format (6E12.5)

If KS = 0, delete.

SRC(I) -- the differential source spectrum
 in units of particles/MeV,

I = 1, KS.

Multiple problems may be run by successively placing a data set for each problem in the input stream. The differential source spectrum is normalized to unity within the code before the calculation is carried out. As noted in the text, the Spencer-Fano kernel is inaccurate at low electron energies. If NMAX is chosen such that the last energy grid value is below the range of validity of the cross section, the code will appropriately decrease NMAX and print a diagnostic.

The code output includes all input variables, the energy grid values in both MeV and mc^2 units, and the flux spectrum in units of $\text{g}/(\text{cm}^2\text{-MeV})$, $\text{g}/(\text{cm}^2\text{-mc}^2)$, cm/MeV , and cm/mc^2 .

The card deck for successively running the two test calculations discussed in the text (1.0 MeV unit monoenergetic sources in aluminum and lead respectively) is given in Figure A1. The control cards are for the CDC-6600 computer. The solutions are given in Tables 1 and 2 respectively in the text.

17/09	100.0	82.0	207.2	1.0
1.0	11.35	1	8	10 9 0
13.0	13.6	20.0	1.0	
1.0	2.7	1	8 24 0 0	
17/09				
17/09				
00.				
COLLECT(CO.FIN,IB)				
FIN(CO.FIN,1-0)				
FOURIF(1-0)				
ATTACH(OUTP,INES)				
ACOUNT.				
00.				

Figure A1: Sample Problem Input Deck