CHAPTER II: A SEMIANALYTIC MONTE CARLO SOLUTION OF THE TRANSPORT EQUATION

I. INTRODUCTION

The solution of Boltzman transport equation for finite, heterogeneous systems with severe anisotropy in the scattering process is of practical interest even for one dimensional problems. In the present work a semianalytic technique is developed for the solution of the transport equation in one dimensional finite systems. The technique can be used to solve multiregion multivelocity transport problems with any degree of anisotropy, which may be varying with velocity. In the present approach, the space kernel is evaluated analytically whereas the energy-angle collision kernel is sampled randomly. This hybrid approach is then followed by an iterative method to solve the integral transport equation.

II. DERIVATION

The integral transport equation in one dimension can be written as

\[ \phi(x,B,u) = \phi_s(x,E,u) + \int \int \int dx'dE'du'T(x',x)C(B',E',u')\phi(x',E',u') \ldots \ldots (2.1) \]

In order to solve Eq. (2.1) numerically, space, energy and direction are divided in a number of mesh points. Space is divided into \( I \) intervals \( x_i \) (i=1,2,3...,I+1) between \( x_i = 0 \) and \( x_{I+1} = \text{total thickness of the slab} \). Similarly the energy range is divided into \( J \)
arbitrary groups at \( j=1,2,3,\ldots,J+1 \), and the direction cosines are divided into \( K \) intervals between \(-1\) and \(+1\).

Considering unit flux for a plane parallel beam given by

\[
\delta_{x_0} \delta_{E_j} \delta_{u^i} \delta_{\nu^o}
\]

incident on one side of a slab of nonmultiplying medium, the uncollided flux at space point \( x_1 \) is

\[
\varphi(x_1, E_j, u_k) = \exp \left[ - \sum_{l=1}^{L} \left\{ \sum_{j=1}^{J} \left( E_j - x_1 \right) / u_k \right\} \right] \delta_{u^i, u^o} \delta_{E_j} \delta_{\nu^o} \tag{2.2}
\]

Where \( \sum_{l=1}^{L} \) is the total cross-section of the \( l \)-th region.

Starting with this, the first iterated flux, i.e., the uncollided plus the first collision flux at \( x_1 \) becomes

\[
\varphi'(x_1, E_j, u_k) = \varphi(x_1, E_j, u_k) + \int \int \int dx' ds' du' \ T(x', x_1) \varphi(x', E_j, u', u_k)
\]

\[
\varphi'(x_1, E_j, u_k) = \delta_{E_j} \delta_{\nu^o} \delta_{u^i, u^o} \tag{2.3}
\]

In the next step to get \( \varphi''(x_1, E_j, u_k) \) the term \( \varphi'(x', E_j, u') \delta_{E_j} \delta_{\nu^o} \delta_{u^i, u^o} \) inside the integral in Eq. (2.3) is replaced by \( \varphi'(x', E_j, u') \) and the iteration is continued till convergence is achieved.

Integration over the space transmission kernel

For the sake of simplicity in notation, a single region with constant mesh width is considered in these derivations. Expressions for the more general case of multiple regions and variable mesh width can be readily obtained from them.
With a unit source of radiation of energy $E_1$ and direction cosine $u'$ located at $x'$, the fraction arriving per unit area at $x_1$ is
\[ \exp \left[ -\sum_{t} (B'(x_1-x'))/u' \right] \]. Therefore, the flux at $x_1$ is
\[ \exp \left[ -\sum_{t} (E'(x_1-x'))/u' \right] \]. Now, writing $\phi(x_{i-1}) = \phi(x_{i-1}, E_j, u_k)$ and $\phi(x_i) = \phi(x_i, E_j, u_k)$ and assuming the gradient of flux to be of exponential nature between two space mesh points, the flux $\phi(x')$ at any point $x'$ between $x_{i-1}$ and $x_i$ is given by
\[ \phi(x') = \phi(x_{i-1}) \exp \left[ -z(x'-x_{i-1}) \right] \] \[ \text{Where } z = \ln \left[ \phi(x_i)/\phi(x_{i-1}) \right]/(x_i-x_{i-1}) \] \[ \text{...(2.5)} \]

Thus, the number of collisions taking place in $dx'$ about $x'$ due to $\phi(x')$ is $\sum_{t} (B_j) \phi(x') dx'$ and number of particles coming out of the collisions in $du'$ about $u'$ and $dE'$ about $E'$ is
\[ \sum_{t} (E_j) \phi(x') C(E_j, E', u_k, u') dE' du' dx' \]
due to which the flux arriving at $x_1$ can be written as
\[ \sum_{t} (E_j) \phi(x') C(E_j, E', u_k, u') \exp \left[ -\sum_{t} (B'(x_1-x'))/u' \right] \mu' \] \[ \text{dE'} du' dx' \]

Integrating $x'$ between $x_{i-1}$ and $x_i$ we get the total flux arriving at $x_1$ from all the collisions between $x_{i-1}$ and $x_i$, made by the flux of energy $E_j$ and angle $u_k$ as (for $u' > 0$).
\[ \phi_T(x_1) = \sum_{t} (E_j) \phi(x') C(E_j, E', u_k, u') \exp \left[ -\sum_{t} (B'(x_1-x'))/u' \right] /\mu' \] \[ \mu' \] \[ dx' \]
\[ = \sum_{t} (E_j) \left\{ \phi(x_1) - \phi(x_{i-1}) \exp \left[ \sum_{t} (B')/u'(x_1-x_{i-1}) \right] \right\} / \left( \sum_{t} (E_j)/u'-z \right) \] \[ \text{...(2.6)} \]
and the flux arriving at $x_{i+1}$ ($i = 1, 2, \ldots, I-1$)

$$\varphi(x_{i+1}) = \varphi(x_i) \exp \left[ -\sum_{i} (S_i)(x_{i+1}-x_i)/u' \right]$$ \hspace{3cm} (2.7)

Similarly for $u < 0$

$$\varphi(x_{i-1}) = \sum_{B} \left\{ \varphi(x_i) \exp \left[ \sum_{E} (E_i)/u'(x_i-x_{i-1}) \right] \right\} / \left( \int (E_i)/u-z \right) \ldots (2.8)$$

and (for $i = 1, 2, \ldots, I-1$)

$$\varphi(x_{i-1}) = \varphi(x_{i-1}) \exp \left[ \sum_{E} (E_i)(x_{i-1}-x_{i-1})/u' \right]$$ \hspace{3cm} (2.9)

Integration over the collision kernel

Integration over the collision kernel is done by randomly sampling the energy and angle after scattering as per the scattering law, and is illustrated in the following:

(a) An isotropic scattering kernel

In this case the direction cosines of the scattered particles are distributed uniformly over -1 to +1, i.e.,

$$p(u\rightarrow u') = \frac{1}{2} \text{ for } -1 \leq u' \leq 1$$

and the direction after scattering can be estimated as

$$u' = 2R-1$$

where $R$ is a random number between 0 and 1.
(b) *any arbitrary scattering kernel*

In this case the general procedure for sampling from an arbitrary distribution is followed and \( u' \) can be obtained by solving

\[
\frac{\int p(u \rightarrow u')du'}{\int p(u \rightarrow u')du} = R
\]

(c) **Klein-Nishina Scattering Kernel**

Carlson\(^{(29)}\) has proposed a method for sampling based on an empirical fit for the inverse of the Klein-Nishina formula. In the case the scattered energy is estimated by

\[
E' = \frac{\frac{E}{1 + S} + 0.562S}{(E - S)(2 - S)R^2} \quad \text{for} \ E \leq 4 \quad (\sim 2 \text{ MeV})
\]

Where \( S = \frac{E}{1 + 0.5625} \)

Here \( E \) and \( E' \) are expressed in \( m_0c^2 \) units. Addition of a term \( \frac{1}{2}(E^2 - S^2)R^2(1 - R)^2 \) yields a reasonable good fit on the range \( 4 \leq E \leq 10 \).

The direction of the scattered photon can be obtained from

\[
u' = 1 + \frac{1}{E} - \frac{1}{E'}
\]

Kahn\(^{(30)}\) has proposed a method of sampling from the Klein-Nishina distribution based on rejection technique. But this method takes, on an average, 1.5 times more of Computer time than the method proposed by Carlson.
III. COMPUTATIONAL DETAILS

With cross-section and geometrical constants as input data, the formulations presented in Sec.II were solved in the following iterative manner.

The iteration starts with the calculation of flux at all space-energy-angle coordinates for a specified source, using the space transmission kernel. Then the collision densities at those points are calculated. The scattered energy-angle are sampled randomly from the proper distribution functions. In fact a stratified sampling technique is used to obtain five sets of scattered energy-angle for each incident energy-angle. The emergent densities at these five energy-angle points are used as a source for the next flux calculation with a weight of 1/5. The incident energy and angle are chosen randomly from the corresponding bins assuming a uniform distribution. This completes one iteration and the procedure is continued until the calculated fluxes in successive iterations agree within a preset convergence criterion.

In the basic procedure for iteration, the order in which energy, space and angle are iterated can be arbitrary. However, a variation in the basic iterative procedure has been found to be of advantage in situations where there is no upscattering of radiation. In this case iterations can be carried out sequentially group by group, starting from the highest energy group and from space and
angular points nearest to the source. After iterating for the equilibrium flux for a particular group, its contribution to all the lower energy groups is calculated and stored before proceeding to the next group. This procedure has been found to have faster convergence. The experience has been that about 5 to 6 iterations per group are needed by this method against 18 to 20 iterations for the basic (random order) iterative procedure. To obtain stability and also to have an estimate of the statistical spread of the estimated spectrum the result of the 6-th iteration is kept fixed and then 'one-more' iteration is done for five times, each time starting from the 6-th iteration results for all energy groups. The mean of the five sets are taken as the final spectrum and the standard deviations are calculated.

To get the optimum width of the spatial mesh the change in spectra has been studied as a function of spatial mesh width for different materials and source energies. Mesh width was varied from 0.2 to 6 m.f.p of the source energy. The spectrum converge faster inside the system than near the boundaries. For all the cases considered a mesh width up to 4 source mean free path has been found to be sufficient to obtain convergence within 5% which is the limit set by the random sampling method. However, for multiregion geometries at least one space mesh point has been found to be necessary within a region if the region happens to be thicker than one source mean free path.
The scattering kernel puts a necessary restriction on the size of the energy mesh interval. In the present case energy bins are so chosen that at least 50% of the particles with energies corresponding to the middle of the energy group are scattered out of the group in a collision. With this consideration the following energy mesh points for gammas were fixed (in MeV) as:

- 1.3-1.2, 1.2-0.7, 0.7-0.45, 0.45-0.3, 0.3-0.23, 0.23-0.19,
- 0.19-0.16, 0.16-0.14, 0.14-0.125, 0.125-0.11, 0.11-0.1,
- 0.1-0.09, 0.09-0.083, 0.083-0.077, 0.077-0.071, 0.071-0.066,
- 0.066-0.062, 0.062-0.0585, 0.0585-0.05525, 0.05525-0.0524,
- 0.0524-0.0498, 0.0498-0.047, 0.047-0.045, 0.045-0.043.

The lowest energy is fixed at 0.043 MeV because below this energy the energy of the photon does not change appreciably in a collision. Thus a large number of mesh points are required in this region to cover a relatively small interval of energy.

It was found convenient to use 8 points for \( u \) ranging from +1 to -1 at uniform intervals.

IV. RESULTS AND DISCUSSIONS

In the earlier sections a hybrid method for solving the integral transport equation is described. Here the results of studies on gamma ray transport with a plane parallel beam of energy 1.25 MeV incident normally on one dimensional slabs of different
materials are presented. The basic cross section data used are those of Hubbel\(^{(31)}\). Results are presented for evolution of spectra with iterations, convergence of the flux at different energy groups, and reflected, transmitted and internal spectra in a multilayer slab.

In the basic iteration procedure, each iteration corresponds to a collision generation of the radiation. Thus an iteration-wise study leads to the physical evolution of the spectrum. Though this is not a quantity that can be easily observed experimentally, it is presented here to obtain an insight into the behaviour of equilibrium spectra.

Fig. 1 shows the evolution of the spectrum integrated over all angles at a depth of 8 source mean free paths in a slab of water of 9 source mean free path thick. This point is chosen for presentation since it is intuitively obvious that the spectrum takes longer time to converge at a point further away from the source. The results of 10-th, 15-th and 20-th iterations are presented along with the final spectrum. It can be observed that the higher energy part of the spectrum (\(\gg 300 \text{ keV}\)) reaches saturation in about 10-15 collisions. The lower energy part takes around 20 collisions to reach saturation. Also the statistical fluctuations present in the spectra is evident.

In order to have an insight into the oscillatory nature of the convergence due to the random sampling of energy and angle, a
study of the convergence is made for some typical energy groups.
Figs. 2 and 3 show the convergence at mesh points \((i,j)\) where \(i\) indicates the space mesh point and \(j\) the energy mesh point for a slab of 9 source mean free path of water. Fig. 2 gives the result for the basic iteration procedure and Fig. 3 gives the results of the "improved" version used in the present case. It can be readily seen that while the iterations try to converge the spectrum the random sampling method disturbs it. This effect is more pronounced in the basic iteration procedure, which is expected to be so since in this case the converged flux is also unsettled by the randomness. It is, however, to be noted that this oscillation is not significant for the present method even in the 19th energy group (i.e. 0.0565 MeV to 0.05525 MeV) at the 9th space mesh point (i.e., 8 source mean free paths away from the surface where the beam is incident).

Figs. 4 to 8 give the spectra at different depths of a multilayer slab consisting of water, iron, concrete and lead. In Fig. 4, the spectrum at 0.0 cm in water gives the reflected spectrum of the system. This reflected spectrum is similar to what should be for a slab of water (9 m.f.p) which is also shown in the same figure but in a different scale. It can be observed from Fig. 5 that up to the interface of water/iron the spectrum is very much characteristic of the first region because of relatively small reflections from iron. Due to small photoelectric absorption in water there is a large buildup of scattered radiation,
showing a peak around 100 keV. Thus the spectrum incident on iron is rich in low energy part. The photoelectric absorption being higher in iron in low energy regions, the spectrum begins to harden with distance as the absorption of the low energy photons exceeds their generation by scattering. This "hardening" of the spectrum continues up to lead (Figs.6, 7 and 8) where the low energy part is completely cut off. Beyond this point the spectral behaviour is that of the lead system.

Some of the special features of the present method are:

The approach is essentially physical. Each iteration corresponds to the collision generation of the radiation and to the physical evolution of the spectrum.

The analytical treatment of the space transmission kernel allows solving deep penetration problems in an easier way. On the other hand, random sampling from the collision kernel, though introduces a little statistical uncertainty, enables the integration over complicated scattering kernels to be carried out in a very simplified manner.
Fig. 1 Iterative convergence of the spectrum in water at 8 m.f.p. from the Source.
Fig. 2 Iterative convergence of the flux in water at various energy groups at 8 m.f.p. from the Source.
Fig. 3 Iterative convergence of the flux in water at various energy groups at 8 m.f.p. from the Source.
Fig. 4 Gamma spectrum at various depths in a multilayer slab.
Fig. 5: Gamma spectrum at various depths in a multilayer slab.