Computational Medical Physics Working Group Workshop II, Sep 30 – Oct 3, 2007
University of Florida (UF), Gainesville, Florida USA on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

ELECTRON DOSE KERNELS TO ACCOUNT FOR SECONDARY PARTICLE TRANSPORT IN DETERMINISTIC SIMULATIONS

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ABSTRACT

For low energy photons, Charged Particle Equilibrium (CPE) usually exists within the patient treatment volume, in which case the photon absorbed dose *D* is equal to the collisional kerma *Kc*; however, this is not true for the dose buildup region near the surface of the patient, or at interfaces of dissimilar materials such as tissue/lung, where corrections for secondary electron transport may be significant. Moreover, as the energy of the ionizing radiation increases, the relative penetration power of the secondary charged particles increases more rapidly than the penetration power of the primary radiation, leading to CPE failure. This failure is caused by the small number of charged particles produced at initial penetration depths compared to deeper points along the primary radiation field direction.

In the case of low energy beams transporting through heterogeneous media, secondary electrons need not specifically be modeled using charged particle transport methods to accurately determine global dose distributions. Alternatively, at higher photon energies, this is not the case, and charged particle transport and corresponding interactions yielding energetic electrons must be considered over the problem phase space to yield an accurate dose distribution. This is readily treated in Monte Carlo codes, yet quite difficult to treat explicitly in deterministic codes due to the large optical thicknesses and added numerical complexities in reaching convergence in electron transport problems. To properly treat 3-D electron transport physics deterministically, yet still achieve reasonably fast and accurate whole body computation times using high energy photons, we are developing angular and energy dependent transport "electron dose kernels," or EDKs. These kernels are being derived via full physics Monte Carlo electron transport simulations, and upon integration into the PENTRAN-MP code system, will enable a very efficient and complete whole body dose, even in the case of high energy photon beams.

Using Monte Carlo calculations, we are generating electron dose kernels for pre-determined photon energy groups in terms of the energy deposited in voxel (i', j', k') as a result of the incident primary photons in a given energy group propagated from photon radiation in a nearby voxel (*i, j, k*). When producing these kernels, photons having energies lower than the limits of the energy group of interest will be 'cut off' to prevent a cascading contribution to the EDK for lower energy groups. These kernels will then be applied by noting the net current on each fine mesh, propogating the dose from charged particle electron transport (pre-computed using Monte Carlo) and projected along the current vector. . This is possible because the PENTRAN discrete ordinates code preserves angular information explicitly in process-scalable parallel data storage arrays.

1. Charged Particle Equilibrium

For low energy photons, Charged Particle Equilibrium (CPE) usually exists within the patient treatment volume, in which case the photon absorbed dose is equal to the collisional kerma. However, this is not true for the dose buildup region near the surface of the patient, or at interfaces of dissimilar materials such as tissue/lung, where corrections for secondary electron transport may be significant. Moreover, as the energy of the ionizing radiation increases, the penetration power of the secondary charged particles increases more rapidly than the penetration power of the primary radiation, leading to CPE failure. This failure is caused by the small number of charged particles produced at deeper penetration depths compared to initial points along the primary radiation field direction due to significant attenuation of the primary indirectly ionizing radiation, i.e. number of electrons produced at point P1 is smaller than the number of electrons produced at point P3, as indicated in Figure 1.

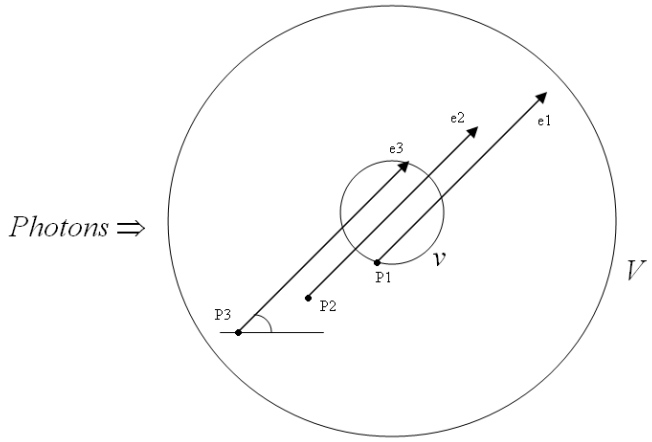

Figure 1: charged-particle equilibrium condition for an external source. The volume *V* contains a homogenous medium, uniformly irradiated throughout by indirectly ionizing radiation.

2. Limits of Charged Particle Equilibrium

Assuming that a maximum energy is transferred from a photon to an electron, then we can use this assumption to investigate a CPE requirement for a water phantom region, as defined earlier. Consider the continuous slowing down approximation range of the electron (R_{CSDA} **)**, and average range of the maximum energy electrons as function of energy. A comparison of those ranges to the thickness of water needed to attenuate different percentages of initial gamma rays is presented in Figures 2 and 3. Through inspection of these relationships, it is clear that CPE and use of a collisional kerma is quite valid for low energy photons. Moreover, one can decide what kind of tolerance is acceptable in applying a collisional kerma approximation for a dose calculation based on photon energy and a particular voxel size, i.e. to determine the CPE approximation limits. This also has been demonstrated in Table 1.

Table 1: Approximate thickness of water required to achieve various amounts of attenuation compared to maximum energy electron ranges generated by the same beam.

Photon Energy (MeV)	Range (cm) at which CPE is conserved by				Average range (cm)	R_{CSDA} (cm)
	1%	2%	3%	5%		
0.3	0.085	0.17	0.256	0.431	0.056	0.085
0.6	0.112	0.225	0.34	0.572	0.15	0.225
1.0	0.142	0.286	0.43	0.726	0.286	0.43
2.0	0.203	0.41	0.617	1.04	0.617	1.04

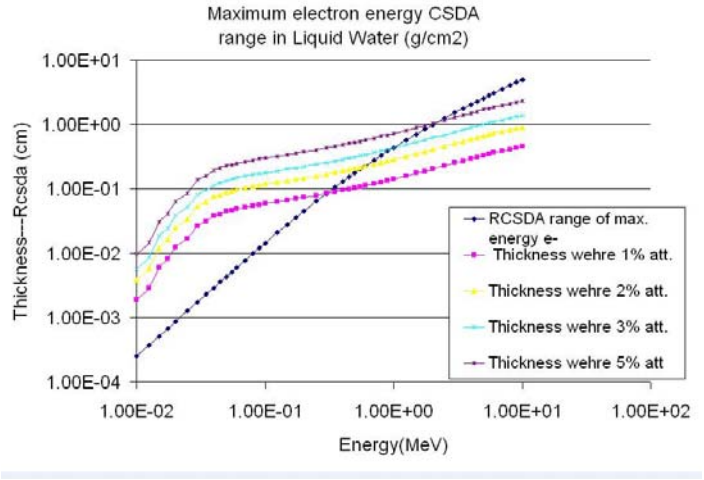

Figure 2: Comparison between thicknesses required to attenuate different percentages of primary photons and R_{CSDA} range for maximum energy secondary electrons produced by the same beam.

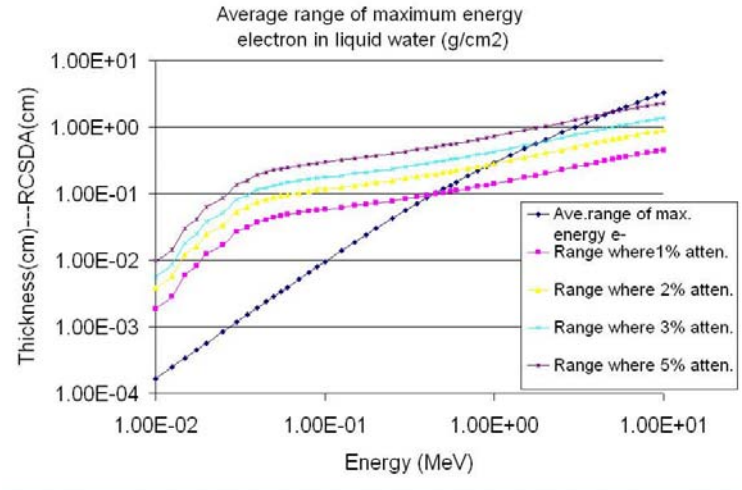

Figure 3: Comparison between thicknesses required to attenuate different percentages of primary photons and average range for maximum energy secondary electrons produced by the same beam.

With proper model discretization of the angle-energy-spatial transport phase space, and at low photon energies yielding primary and secondary electron interactions with small electron transport paths, 3-D S_N methods can be implemented to directly yield very accurate dose distributions. Therefore, the deterministically derived dose from a kerma approximation will be accurate up to the range of electron path lengths comparable to ranges smaller than the photon spatial S_N mesh grid interval in anatomical models (typically representative of the anatomical data voxel size).

At higher photon energies, this is not the case, and interactions yielding energetic electrons must account for the mechanism of electron transport through the problem phase space to deliver a dose after some electron transport distances. This is readily treated in Monte Carlo codes, and quite difficult to treat in deterministic codes. To properly treat the physics deterministically, yet still to achieve reasonably fast and accurate whole body computation times using high energy photons, energy dependent electron transport dose "kernels" can be pre-computed using Monte-Carlo to extremely low variances in various tissue media. These Electron Dose Kernels (EDKs) can then be implemented to enable direct attribution of the final equivalent dose initiated by photon "beamlets" placed in various tissue types and energies relative to a specific direction of photon travel. This will permit complete attribution of the dose ultimately due to electron straggling, where the EDK provides an "equivalent electron dose look-up table" for each photon "beamlet" in a discrete ordinates computation. Since the angular data is readily available and is explicitly stored in scalable parallel data arrays in the PENTRAN S_N code, this "electron kernel" treatment can be applied to effectively attribute dose from even high energy photons.

Issues surrounding limits of meshing, proper quadrature sets, cross section libraries, and differencing schemes have already been investigated in assessing what is typically required to yield accurate photon transport. Therefore, complete deterministic modeling of the integral doses in tissue due to photons is proposed in the following manner:

(i) Solve the 3-D neutral particle discrete ordinates equations over the complete problem phase space, including the anatomical voxelized patient phantom to render the global energy-group dependent angular photon fluence. Note completion of this task requires generation of an appropriate multigroup photon cross section library using the CEPXS (or similar) code, as well as an assessment of the appropriateness of the group bin structure, etc.

(ii) For each energy group (g) of photon average angular flux in each voxel for each S_N ordinate, compare the maximum electron range for an assumed photo-electron with the location and optical thickness ($\sigma_g \Delta x / \mu_m$) of the voxel (and associated material) under analysis. For electron ranges smaller than the size of the voxel and material containing it, attribute the dose delivered to that voxel using a standard kerma approximation. For electron ranges larger than the current voxel dimension, proceed to the next step.

(iii) Corresponding to each photon direction at each phase space location, determine the dose distribution in all connected and surrounding tissue voxels. This will include:

A. Convolving the primary photon fluence with a kernel that describes the transport and deposition of energy by secondary particles using pre-computed energy and density dependent Monte Carlo-based "electron dose kernels" (EDKs) for each angular flux in each energy group aliased to the deterministic calculation phase space.

B. Validating EDK approaches for dosimetry tested against full physics photon-electron Monte Carlo derived doses constructed using equivalent geometries for direct comaparison and validation

Step A can account for photon beamlet interactions (yielding electrons) that ultimately lead to a distributed, deposited dose as a function of angle, energy, and space in surrounding tissue, governed by the electron transport determined as a benchmark in step B.

(iv) Accumulate the total dose to each organ based on material type; report results.

It is worth noting that the basis of the existing convolution–superposition technique is a database of "energy deposition kernels" which are calculated using Monte Carlo techniques[1,2]. These kernels describe the spread of energy about the primary photon's point of interaction in the phantom with no regard to the incident photon angular component.
The goal of this work is to produce a methodology to estimate organ doses and attribute whole body doses incurred using CT based anatomical patient models coupled with 3-D deterministic discrete ordinates (S_N) radiation transport models. The angular data provided by the S_N method will be used as a guide in the dose mapping process to the surrounding voxels; this what which makes this approach novel.

3. Monte-Carlo Based Dose Kernels

Using Monte Carlo calculations, we are generating electron dose kernels for pre-determined photon energy groups in terms of the energy deposited in voxel (i', j', k') as a result of the incident primary photons in a given energy group propagated from a voxel (i, j, k). When producing these kernels, the photons of energies lower than the limits of the energy group will be cut off in order to prevent a cascading contribution to the EDK for lower energy groups. These kernels will then be applied using net current on a fine mesh and/or coarse mesh bases. This is possible because the PENTRAN discrete ordinates code preserves angular information explicitly in process-scalable parallel data storage arrays.
In addition, the fractional electron dose kernel in voxel (i, j, k) giving as EDF_g, due to a primary photon, can be determined in terms of initial photon energy for a particular energy group g. By partitioning the energy deposited in voxel (i, j, k), $EDK_g(i, j, k)$, into multiple energy bins, we can predict the fractional electron dose kernel contribution per unit photon flux per source particle:

$$EDF_g(i, j, k) = EDK_g(i, j, k) / \phi_g(i', j', k')$$

The dose rate can be obtained for the voxel at (i, j, k) by summing the product of $EDF_g(i, j, k)$, photon group energy g, and scalar flux $\phi_g(i, j, k)$, then dividing by the voxel mass M (i, j, k):

$$D(i, j, k) = \sum_g \sum_s [EDF_g\ (i, j, k)\ ]_s \phi(i, j, k)_g\ \ / M(i, j, k)$$

This procedure will enable detailed information to be obtained on the dose deposited in the model of study, which can be of great importance for fully understanding dose effects from a spectrum of secondary electrons.

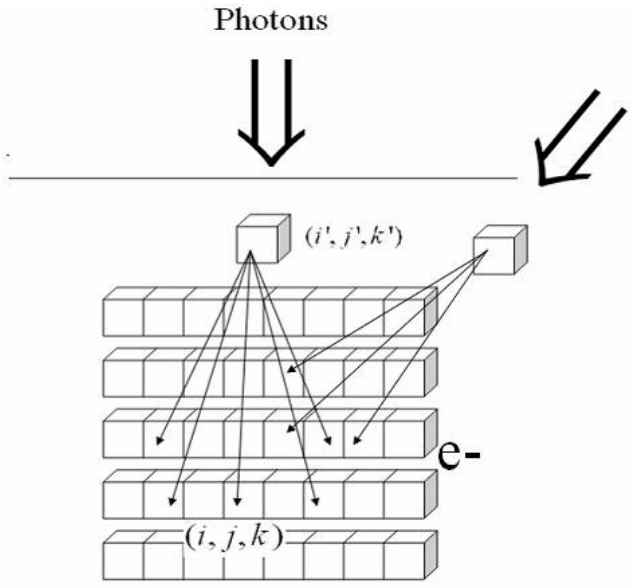

Figure 2. Procedure to produce EDK based on Monte Carlo Calculations

3.1 EDK Estimation Based on MCNP5

In the MCNP5 Monte Carlo code, there are three different methods by which one can tally to yield doses to be used for integrated organ dose calculations; these are achieved by using either F4, F6, or *F8 tallies, and each has a different basis for computing the dose[3]. To illustrate this, we compare doses computed using the F4, F6 and *F8 tallies to highlight the differences in these computations, and establish a procedure that ensures our electron kernels are calculated accurately, and the Monte Carlo transport and subsequent doses determined as a benchmark are completely based on a detailed physics treatment.

Figure (4-6) includes doses resulting from the use of an F4 volume flux tally method, using a "DE" Dose Energy and "DF" Dose Function Cards, compared to an F6 tally using both the photon-electron mode (p, e mode) and photon only (p mode) were all in good agreement.

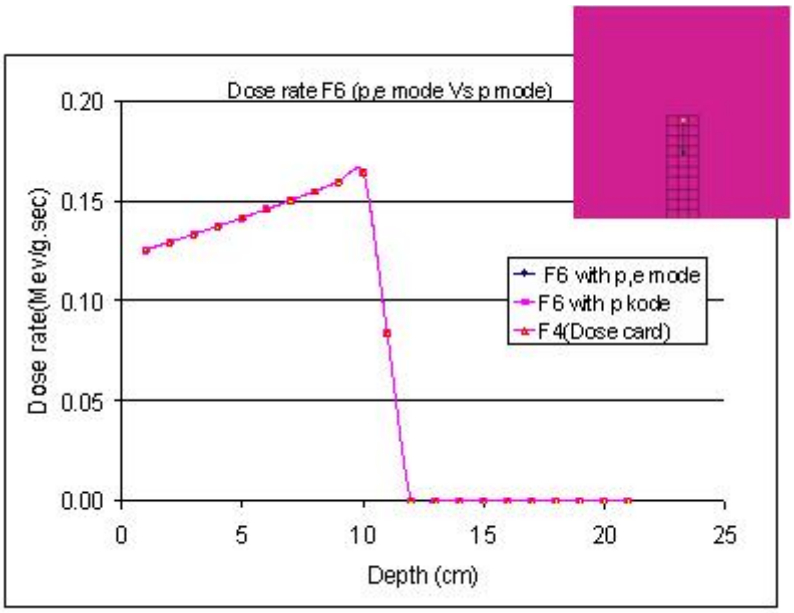

Figure 6: Comparison of between F6(p, e mode), F6 (p mode), and F4(DE, DF) tallies in MCNP5, statistical uncertainty was less than 1%

On the other hand, when comparing doses computed using *F8 using a full photon electon transport mode (p, e mode) and F6 derived dose tallies, the differences between these tallies for the example shown are relatively large (as given in Figure (4-7)). This is reasonable since the F6 tallies are derived from F4 tallies in MCNP, while F8 tallies are determined based on different physics from the F4 tallies[3].

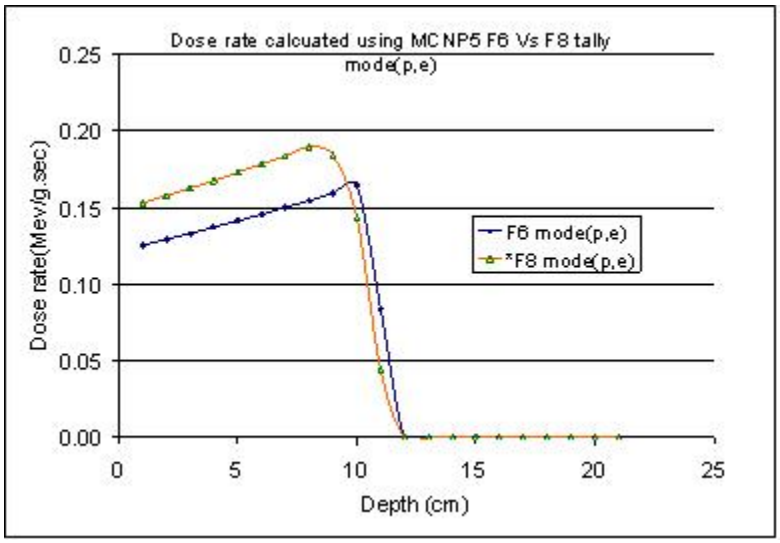

Figure 7: Comparison of between F6 (p, e mode) and *F8 (p mode) tallies in MCNP5, statistical uncertainty was less than 1%

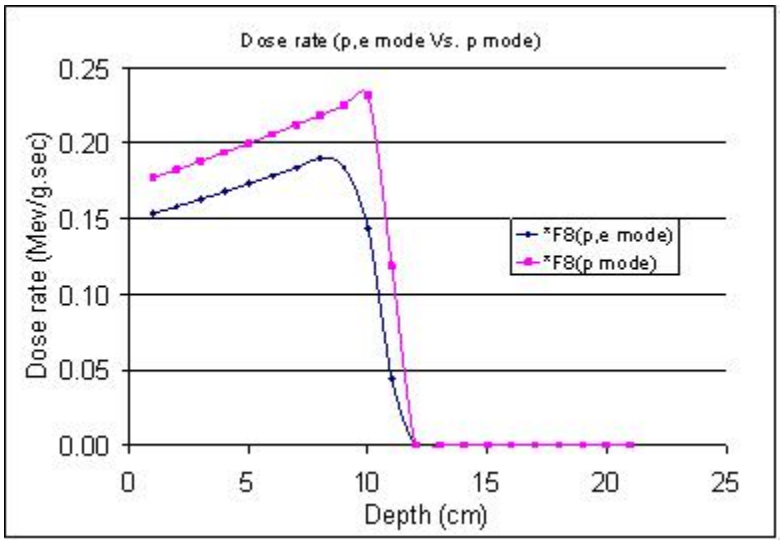

Figure 8: Comparison of between *F8 (p, e mode) and *F8 (p mode) tallies in MCNP5, statistical uncertainty was less than 1%

Moreover, when comparing *F8(p mode) and *F8(p, e mode), in Figure 4-8, there was a significant difference in the outcome for the same model. This is a result of the way different modes in MCNP5 are handled with regard to electron physics.. If electron transport is turned on (Mode P E), then all photon collisions except coherent scatter can create electrons that are banked for later transport. On the other hand, If electron transport is turned off (no 'e' on the MCNP5 Mode card), then a thick-target bremsstrahlung model (TTB) is used. This model generates electrons, but assumes that they are locally "slowed to rest"[3]. Any bremsstrahlung photons produced by the nontransported electrons are then banked for later transport. Thus electron-induced photons are not neglected, but the expensive electron transport step is omitted. (The TTB production model contains many approximations compared to models used in actual electron transport. In particular, the bremsstrahlung photons inherit the direction of the parent electron). The choice of which tally is to be used and the detailed physics treatment by which the Monte Carlo code is executed is essential to the success of this method. In conducting our EDK calculations, we will be using detailed physics treatment implementing a *F8(p, e mode) tally rather than an F4 tally method or F6 tally to insure accurate absorbed dose estimation (and not simply employing a collisional kerma). Table (4-2) is an example for fractional EDK using the *F8(p, e mode) tally.

3.2 Dose Calculations

The EDK method will serve as a critical link in a system that will accumulate the absorbed dose in each fine mesh for the following categories:

I. For low photon energies, where CPE conditions are met, the algorithm will apply a simple collisional kerma approximation based on pre calculated 3-D fluxes/fluences using the S_N methods. A deterministically derived dose will be accurate up to the

range of electron path lengths that are comparable to ranges smaller than the spatial S_N mesh grid interval in anatomical models (typically representative of the anatomic data voxel size).

II. At high energies were CPE satisfaction is not valid, our code system will accumulate the energy deposited in each voxel for each photon energy group and net current vector (ordinate) using the EDK method described here.

4. Conclusions

By following the EDK approach, the whole body dose from any incident photon beam (pencil, fan, areal, etc) applied to tissue resulting from any diagnostic imaging or therapy treatment can be readily determined based on a coupling of photon transport and application of the EDK methodology. This procedure can be readily accomplished by applying the PENTRAN parallel discrete ordinates code, since it is a parallel code design and stores, via partitioned parallel storage, all angular problem data. Since PENTRAN is based on a Cartesian geometry, CT voxel data can readily be mapped into the problem geometry to define the tissue and organ geometry structure. As a result, this research will render the first application of integrated electron transport kernels to properly account for the total dose in photon irradiation scenarios.

References

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