Investigation of various energy deposition kernel refinements for the convolution/superposition method

Jessie Y. Huang

The University of Texas Health Science Center Houston, Graduate School of Biomedical Sciences, Houston, Texas 77030 and Department of Radiation Physics, The University of Texas MD Anderson Cancer Center, 1515 Holcombe Boulevard, Houston, Texas 77030

David Eklund and Nathan L. Childress

Mobius Medical Systems, LP, Houston, Texas 77401

Rebecca M. Howell, Dragan Mirkovic, David S. Followill, and Stephen F. Kry^{a)}

The University of Texas Health Science Center Houston, Graduate School of Biomedical Sciences, Houston, Texas 77030 and Department of Radiation Physics, The University of Texas MD Anderson Cancer Center, 1515 Holcombe Boulevard, Houston, Texas 77030

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Purpose: Several simplifications used in clinical implementations of the convolution/superposition (C/S) method, specifically, density scaling of water kernels for heterogeneous media and use of a single polyenergetic kernel, lead to dose calculation inaccuracies. Although these weaknesses of the C/S method are known, it is not well known which of these simplifications has the largest effect on dose calculation accuracy in clinical situations. The purpose of this study was to generate and characterize high-resolution, polyenergetic, and material-specific energy deposition kernels (EDKs), as well as to investigate the dosimetric impact of implementing spatially variant polyenergetic and material-specific kernels in a collapsed cone C/S algorithm.

Methods: High-resolution, monoenergetic water EDKs and various material-specific EDKs were simulated using the EGSnrc Monte Carlo code. Polyenergetic kernels, reflecting the primary spectrum of a clinical 6 MV photon beam at different locations in a water phantom, were calculated for different depths, field sizes, and off-axis distances. To investigate the dosimetric impact of implementing spatially variant polyenergetic kernels, depth dose curves in water were calculated using two different implementations of the collapsed cone C/S method. The first method uses a single polyenergetic kernel, while the second method fully takes into account spectral changes in the convolution calculation. To investigate the dosimetric impact of implementing material-specific kernels, depth dose curves were calculated for a simplified titanium implant geometry using both a traditional C/S implementation that performs density scaling of water kernels and a novel implementation using material-specific kernels.

Results: For our high-resolution kernels, we found good agreement with the Mackie *et al.* kernels, with some differences near the interaction site for low photon energies (<500 keV). For our spatially variant polyenergetic kernels, we found that depth was the most dominant factor affecting the pattern of energy deposition; however, the effects of field size and off-axis distance were not negligible. For the material-specific kernels, we found that as the density of the material increased, more energy was deposited laterally by charged particles, as opposed to in the forward direction. Thus, density scaling of water kernels becomes a worse approximation as the density and the effective atomic number of the material differ more from water. Implementation of spatially variant, polyenergetic kernels increased the percent depth dose value at 25 cm depth by 2.1%–5.8% depending on the field size, while implementation of titanium kernels gave 4.9% higher dose upstream of the metal cavity (i.e., higher backscatter dose) and 8.2% lower dose downstream of the cavity.

Conclusions: Of the various kernel refinements investigated, inclusion of depth-dependent and metal-specific kernels into the C/S method has the greatest potential to improve dose calculation accuracy. Implementation of spatially variant polyenergetic kernels resulted in a harder depth dose curve and thus has the potential to affect beam modeling parameters obtained in the commissioning process. For metal implants, the C/S algorithms generally underestimate the dose upstream and overestimate the dose downstream of the implant. Implementation of a metal-specific kernel mitigated both of these errors. © 2013 American Association of Physicists in Medicine. [<http://dx.doi.org/10.1118/1.4831758>]

Key words: convolution/superposition, energy deposition kernel, kernel hardening, kernel scaling, heterogeneity correction

1. INTRODUCTION

Many modern radiation therapy treatment planning systems use the convolution/superposition method to perform photon dose calculations. The convolution/superposition (C/S) method involves the convolution of the total energy released per unit mass (TERMA), calculated by attenuating the primary fluence of the photon beam through the patient (or phantom) geometry, with an energy deposition kernel (EDK).^{1,2} The EDK describes the spatial distribution of energy deposition surrounding the site of a photon interaction. Mackie *et al.*³ generated EDKs for monoenergetic photons interacting in water by using the EGS Monte Carlo code. These kernels are currently used in the Pinnacle³ treatment planning system (Phillips Healthcare, Andover, MA), among others.

The accuracy of the C/S method as a whole is dependent not only on the accuracy of these energy deposition kernels but also on any simplifications or approximations applied to the kernels in the convolution calculation. In traditional implementations of C/S, a single, spatially invariant kernel is used for the entire dose calculation. This “effective mean kernel” is computed by combining monoenergetic kernels with relative weights based on the energy spectrum of the beam at a single location (e.g., at the surface of the patient, on the central axis). The “effective mean kernel” method ignores spectral changes of the photon beam throughout the patient geometry (e.g., beam hardening and off-axis softening) as well as spectral changes for different field sizes, and can lead to dose calculation inaccuracies.^{4–6} In fact, several studies have found that higher accuracy was achieved when beam hardening of the kernels was taken into account in the convolution calculation. Dose errors caused by using nonhardened kernels were found to be as high as 2%–5% on the central axis.^{4–6} Although Liu *et al.*⁶ suggested that their kernel interpolation method could be used to take into account the effects of off-axis softening, there have been no studies that have quantified the effects of kernel softening with larger field sizes and greater off-axis distances for a clinical photon beam.

A second simplification is density scaling of water kernels for dose calculations in heterogeneous media.⁷ It has been shown that this approximation can lead to dose calculation inaccuracies for material interfaces because the lateral scattering of electrons within the inhomogeneity is not accurately modeled.⁸ In fact, several studies have highlighted the limitations of the C/S method for media interfaces, especially for situations involving lateral charged particle disequilibrium in low-density media such as the lung.⁹ The weakness of C/S in calculating dose near material interfaces has important clinical implications for the treatment of patients with thoracic tumors, as well as patients with high-density metals near the treatment site (e.g., dental fillings). Notably, 1%–4% of radiation therapy patients have a prosthetic device that could affect their treatment.¹⁰ C/S algorithms have been shown to overestimate the dose downstream of a metal cavity and underestimate the dose upstream of the metal due to its inability to predict the increased backscatter caused by the metal heterogeneity.^{11,12} Because of the poor dose calculation accuracy near metal prostheses, the American Association

of Physicists in Medicine’s Task Group 63 recommends that beam arrangements be chosen to completely or partially avoid metal prostheses even when using modern dose calculation algorithms such as the C/S algorithm. However, this beam arrangement limitation may lead to nonoptimal dose distributions, causing unacceptably high dose to organs at risk.¹⁰ A more accurate dose calculation algorithm could allow greater flexibility in treatment planning and thus better quality treatment plans for these patients.

Although these limitations of the C/S method have been well documented, the relative importance of EDK refinements has not been explored. Determining which refinements are most important for accuracy allows for prioritization and therefore a more efficient implementation of these improvements into C/S algorithms. The purpose of this study is to generate and characterize high-resolution (i.e., those calculated with a greater number of angular and radial sample points), spatially variant, and material-specific EDKs. To this end, we performed Monte Carlo simulations to generate material-specific and high-resolution EDKs. Spatially variant polyenergetic kernels were calculated for various depths, field sizes, and off-axis distances for a clinical 6 MV photon beam. We also investigated the dosimetric impact of implementing polyenergetic and material-specific kernels using simple phantom geometries.

2. METHODS AND MATERIALS

2.A. Calculation of high-resolution kernels

The EDKnrc user code, part of the EGSnrc Monte Carlo simulation package, was used to generate high-resolution water kernels. The EDKnrc user code was derived from the EGS4 user code that was previously used to calculate water kernels by Mackie *et al.*^{3,13} For these simulations, monoenergetic photons moving along the z axis were forced to interact at the center of a 60 cm radius sphere of water, and the energy deposited in each voxel was recorded. Voxels were defined by the intersection of 48 spheres (radial bins) and 144 cones (angular bins), as opposed to the 24 spheres and 48 cones used by Mackie *et al.*³ The distance between radial boundaries was smaller near the interaction site (0.025 cm for the first few shells) and increased to 5 cm for the shells farthest from the interaction site in order to capture the higher energy deposition gradients near the origin. The angular spacing of cones was uniform (1.25° per angular bin). Twenty-two monoenergetic photon energies were simulated between 0.1 and 40 MeV. 100×10^6 histories were used for each simulation. Photon and electron cutoff energies (PCUT and ECUT) were set to 0.01 MeV, and the maximum fractional electron energy loss per step (ESTEPE) was 0.02.

The energy deposited in the simulation geometry was separated into primary and scatter kernels based on its origin (e.g., energy deposited due to interaction of a primary photon vs a scattered photon). For each high-resolution kernel, the total and the primary energy fraction were calculated. The total energy fraction, F_{tot} , is defined as the total energy deposited in the spherical phantom relative to the amount of incident

photon energy interacting at the origin and is obtained by summing the EDK over all voxels.³ Similarly, the primary energy fraction, F_{prim} , is defined as the sum over all voxels of the energy deposited from charged particles set in motion from primary photons only.

2.B. Calculation of polyenergetic kernels

The Monte Carlo package BEAMnrc¹⁴ was used to generate the primary photon spectrum from a 6-MV photon beam from a 2100 Clinac linear accelerator (Varian Medical Systems, Palo Alto, CA) at various locations in a water phantom. Our BEAMnrc accelerator model consisted of the target, primary collimator, flattening filter, and jaws, and has been previously validated against measurements.^{15,16} Particle phase space data were generated at five different depths ($d = 1.5, 5, 10, 15$, and 20 cm) in a water phantom for various field sizes (5×5 , 10×10 , and 20×20 cm²). Additionally, the primary photon spectra for various off-axis distances were obtained by scoring the phase space data in annular rings centered on the central axis. All phase space data were simulated with 10×10^6 electrons incident on the target, except for simulations taken at a depth of 20 cm, which were simulated with 35×10^6 incident electrons. The primary spectrum was isolated by excluding any photons that had interacted within the water phantom. These primary photon spectra were used to calculate the TERMA for each energy bin, which was then used as weighting factors for combining our high-resolution, monoenergetic water kernels into polyenergetic kernels that are specific to a given depth, field size, or off-axis distance.¹⁷

2.C. Calculation of material-specific kernels

Material-specific kernels were generated using EDKnrc, similar to the method used to generate our high-resolution water kernels, except that the simulation geometry consisted of a sphere of material rather than a sphere of water. For these simulations, the following ICRU materials¹⁸ were used: lung, bone, titanium, silver, and gold. These materials were chosen because they can be encountered in radiation therapy (e.g., gold fillings in head and neck treatment or a titanium hip prosthesis in prostate treatment). The simulation geometry consisted of 24 spheres and 48 cones, the original kernel resolution used by Mackie *et al.*³ However, the radii of the spheres were scaled on the basis of the density of the material such that the product of the radii and the density was the same for all materials (i.e., $r_{\text{lung}} \cdot \rho_{\text{lung}} = r_{\text{bone}} \cdot \rho_{\text{bone}}$). For each of the materials, monoenergetic kernels were calculated for various energies ranging from 100 keV to 8 MeV with 10×10^6 histories each (ECUT = PCUT = 10 keV and ESTEPE = 0.02). Additionally, polyenergetic material-specific kernels based on the spectrum of our clinical 6-MV photon beam (10×10 cm² field size, depth of 1.5 cm) were calculated and compared to the corresponding polyenergetic water kernel. This energy spectrum, calculated using the methods of Sec. 2.B, was chosen because it represents a reference energy spectrum.

2.D. Investigation of “pocket of material” kernels

A further issue associated with the implementation of material-specific kernels is that 60 g/cm² radius spheres of heterogeneities are unrealistic in terms of patient anatomy; rather, a smaller pocket of heterogeneity surrounded by tissue is usually encountered. To address this issue, we also investigated the impact of the size of the heterogeneity on the EDK. We considered two extremes: first, as described above, we considered a uniform 60 g/cm² radius sphere of the heterogeneous material. Second, we considered spheres where the heterogeneity comprised only the central 1 or 5 mm radius (at the interaction point), while the remainder of the sphere was comprised of water. Monoenergetic kernels were simulated with this geometry for 1.5 MeV photons for bone and titanium. These kernels will be referred to as “pocket of material” kernels.

2.E. Calculation of energy deposition kernel metrics

The effective depth of penetration $\bar{z}$, effective radial distance $\bar{r}$, and effective lateral distance $\bar{y}$ were calculated for each kernel in this study as these metrics have been previously used to characterize EDKs.^{3,19} These effective distances are a measure of the range of charged particles generated from primary photon interactions in the incident photon (z), the radial (r), and the lateral (y) directions. They describe how far away from the interaction site charged particles deposit energy as well as the spatial distribution of this energy. For instance, the ratio $\bar{y}/\bar{z}$ gives information about whether charged particles deposit energy more in the forward direction or the lateral direction and aids in describing the shape of the kernel. The effective distance in any given direction (z , r , or y) is essentially the expectation value of the primary EDK in that direction

$$\bar{d} = \sum_i \sum_j \frac{d(i, j) \varepsilon_{\text{prim}}(i, j)}{F_{\text{prim}}}, \quad (1)$$

where $\bar{d}$ indicates the effective distance to be calculated (z , r , or y), $d(i, j)$ is the pertinent distance from the origin to the center of the i, j th voxel, and $\varepsilon_{\text{prim}}(i, j)$ is the primary EDK for the i, j th voxel. To calculate $d(i, j)$, the geometric center was used to approximate the effective center of the voxel. For material-specific kernels, effective distances were also calculated using Eq. (1), with the density-scaled distance $\rho_{\text{mat}} \cdot d$ used in place of the physical distance d .

2.F. Investigation of dosimetric impact of kernel hardening and material-specific kernels

In order to investigate the dosimetric impact of implementing spatially variant polyenergetic kernels in the C/S method, depth dose curves for our clinical 6 MV photon beam were calculated using two different implementations of the collapsed cone C/S method (Mobius Medical Systems, Houston, TX):²⁰ one using a single polyenergetic kernel reflecting the surface spectrum (“single kernel” method) and one that represents the ideal case where all the spectral changes of the photon beam are fully taken into account. For the ideal case, a full convolution calculation using a monoenergetic kernel

is performed for each energy bin (“components” method).^{5,6} Depth doses were calculated using various field sizes (5×5 , 10×10 , and 20×20 cm²) using a $30 \times 30 \times 30$ cm³ water phantom.

In order to investigate the dosimetric impact of implementing material-specific kernels, a water phantom with a $4 \times 4 \times 4$ cm³ titanium cavity, representing a simplified hip prosthesis geometry, was used. The depth dose for this heterogeneous geometry was calculated using both a traditional C/S implementation that performs density scaling of water kernels and a novel implementation using titanium kernels for photon interactions occurring in the titanium cavity. The depth dose

was calculated for a field size of 10×10 cm² for our clinical 6 MV photon beam. The same calculation was also performed for a bone cavity phantom, with the same phantom geometry as the titanium phantom, using our bone kernels to describe photon interactions occurring in the bone cavity.

3. RESULTS

3.A. Calculation of high-resolution kernels

In general, there was very good agreement between our high-resolution kernels and those published by Mackie *et al.* This can be seen in Fig. 1 which shows the radial dose falloff for 1 and 10 MeV monoenergetic water kernels.³ The agreement between our high-resolution water kernels and the Mackie kernels was also confirmed by comparing various kernel metrics, including the total energy fraction F_{tot} , primary energy fraction F_{prim} , and effective distances $\bar{z}$, $\bar{r}$, and $\bar{y}$ (data not shown). Although the agreement was generally good, there were some differences for the lower photon energies (<500 keV), most likely attributable to improvements in the electron transport in the EGSnrc code compared to the EGS code used by Mackie *et al.*³ Mainegra-Hing *et al.*²¹ found differences in the two codes due to the different forcing algorithm and inclusion of Rayleigh scattering in EGSnrc, leading to differences in the EDKs near the interaction site, especially for lower photon energies (<500 keV).

3.B. Calculation of polyenergetic kernels

The various primary beam spectra generated from Monte Carlo simulations of a Varian Clinac 2100 accelerator are shown in Fig. 2. Notably, the mean energy of the beam

FIG. 1. Comparison of our high-resolution energy deposition kernels for water and Mackie *et al.*'s (Ref. 3) kernels for (a) 1 and (b) 10 MeV monoenergetic incident photons. Shown is the radial dose distribution averaged over selected angular intervals.

FIG. 2. Normalized primary photon spectra for a clinical 6-MV photon beam taken at various locations in a water phantom. The mean energy of the spectrum $\langle E \rangle$ is given in MeV. * indicates that the beam spectrum was taken over an annular region with an inner radius of $r = 0$ cm and an outer radius of $r = 2.5$ cm.

TABLE I. The effective depth of penetration $\bar{z}$, effective radial distance $\bar{r}$, and effective lateral distance $\bar{y}$ for polyenergetic energy deposition kernels calculated using the energy spectrum of the primary photon beam at various locations in a water phantom. The mean energy of the spectrum is also listed. In parenthesis is the % difference with respect to the polyenergetic kernel at $d = 1.5$ cm for a 10×10 cm² field (i.e., the reference spectrum).

Variable studied	Depth (cm)	Field size (cm $\times$ cm ²)	Portion of field	$\bar{z}$ (cm)	$\bar{r}$ (cm)	$\bar{y}$ (cm)	Mean energy (MeV)
Depth	1.5	10 $\times$ 10	Whole	0.327 (0.0%)	0.394 (0.0%)	0.220 (0.0%)	1.747
	5	10 $\times$ 10	Whole	0.342 (4.5%)	0.411 (4.3%)	0.228 (3.9%)	1.853
	10	10 $\times$ 10	Whole	0.361 (10.4%)	0.433 (9.9%)	0.239 (9.0%)	2.002
	15	10 $\times$ 10	Whole	0.379 (15.9%)	0.454 (15.2%)	0.250 (13.7%)	2.140
	20	10 $\times$ 10	Whole	0.397 (21.2%)	0.474 (20.2%)	0.259 (18.2%)	2.274
Field size	1.5	5 $\times$ 5	Whole	0.335 (2.3%)	0.403 (2.2%)	0.224 (2.0%)	1.801
	1.5	10 $\times$ 10	Whole	0.327 (0.0%)	0.394 (0.0%)	0.220 (0.0%)	1.747
	1.5	20 $\times$ 20	Whole	0.312 (−4.7%)	0.376 (−4.6%)	0.210 (−4.1%)	1.635
Off-axis distance	1.5	20 $\times$ 20	r[0, 2.5] ^a	0.331 (1.2%)	0.399 (1.1%)	0.222 (1.0%)	1.777
	1.5	20 $\times$ 20	r[2.5, 5]	0.325 (−0.6%)	0.392 (−0.6%)	0.218 (−0.5%)	1.736
	1.5	20 $\times$ 20	r[5, 7.5]	0.317 (−3.2%)	0.382 (−3.1%)	0.214 (−2.7%)	1.673
	1.5	20 $\times$ 20	r[7.5, 10]	0.308 (−6.0%)	0.372 (−5.7%)	0.208 (−5.1%)	1.609

^aIndicates that the beam spectrum was calculated over an annular region with an inner radius of $r = 0$ cm and an outer radius of $r = 2.5$ cm.

spectrum was most dependent on depth. However, there were noticeable spectral changes due to field size (i.e., the spectrum is softer for larger field sizes) and off-axis distance (i.e., the spectrum is softer for larger distances from the central axis). The mean energy of each simulated primary photon spectrum is shown in Table I, along with the effective distances ($\bar{z}$, $\bar{r}$, and $\bar{y}$) for each of the polyenergetic kernels. The data for spectral changes due to field size and off-axis distance shown in Table I are all for a depth of 1.5 cm. These two factors were also investigated at a depth of 20 cm, but the spectral differences due to field size and off-axis distance were less noticeable due to beam hardening at this depth. Although the spectral changes due to depth, field size, and off-axis distance are well understood, it is noteworthy that these spectral changes have caused noticeable changes in the effective distances used to characterize the polyenergetic kernels, indicating that the pattern of energy deposition is affected by these factors for a clinical photon beam.

3.C. Calculation of material-specific kernels

The density-weighted effective distances ($\rho_{\text{mat}} \cdot \bar{z}$, $\rho_{\text{mat}} \cdot \bar{r}$, and $\rho_{\text{mat}} \cdot \bar{y}$) calculated for the material-specific kernels are listed in Table II. As this table shows, the materials in this study have noticeably different values for the density-weighted effective distances. Notably, the density-weighted effective lateral distance $\rho_{\text{mat}} \cdot \bar{y}$ is different for different materials, and does not simply increase for materials of increasing density. The polyenergetic titanium kernel had the largest effective lateral distance (44% higher than the corresponding value for water). Furthermore, the ratio of $\bar{z}/\bar{y}$, which gives an indication of whether charged particles deposit more energy in the forward or the lateral direction, decreased by a factor of 3 in going from the lung to the gold polyenergetic kernel. This indicates that the shape of the kernels is changing as the density and the effective atomic number of the material is increased, with more energy being deposited in the lateral

TABLE II. The density-scaled effective depth of penetration $\rho_{\text{mat}} \cdot \bar{z}$, effective radial distance $\rho_{\text{mat}} \cdot \bar{r}$, and effective lateral distance $\rho_{\text{mat}} \cdot \bar{y}$ for material-specific energy deposition kernels for 300 keV monoenergetic photons and a 6-MV polyenergetic beam spectrum ($d = 1.5$ cm, 10×10 field size). In parenthesis is the % difference with respect to the relevant water kernel.

Incident energy	Material	Density (g/cm ³)	$\rho_{\text{mat}} \cdot \bar{z}$ (g/cm ²)	$\rho_{\text{mat}} \cdot \bar{r}$ (g/cm ²)	$\rho_{\text{mat}} \cdot \bar{y}$ (g/cm ²)	$\bar{z}/\bar{y}$
300 keV	Water	1.00	0.016 (0.0%)	0.025 (0.0%)	0.019 (0.0%)	0.858
	Lung	0.26	0.016 (0.0%)	0.025 (0.0%)	0.019 (0.0%)	0.858
	Bone	1.85	0.015 (−7.4%)	0.026 (1.6%)	0.021 (7.9%)	0.737
	Ti	4.54	0.013 (−20.9%)	0.027 (8.8%)	0.024 (26.3%)	0.538
	Ag	10.50	0.010 (−37.4%)	0.029 (16.3%)	0.027 (43.7%)	0.374
	Au	19.32	0.007 (−58.9%)	0.026 (2.4%)	0.025 (30.5%)	0.270
6 MV spectrum	Water	1.00	0.327 (0.0%)	0.394 (0.0%)	0.220 (0.0%)	1.491
	Lung	0.26	0.328 (0.3%)	0.395 (0.1%)	0.219 (−0.3%)	1.499
	Bone	1.85	0.327 (−0.1%)	0.417 (5.8%)	0.259 (17.9%)	1.263
	Ti	4.54	0.288 (−12.1%)	0.427 (8.3%)	0.315 (43.7%)	0.912
	Ag	10.50	0.190 (−42.1%)	0.350 (−11.2%)	0.294 (33.9%)	0.645
	Au	19.32	0.117 (−64.3%)	0.265 (−32.9%)	0.237 (8.1%)	0.493

FIG. 3. (a) and (b) Comparison of water, bone, and titanium monoenergetic kernels for 1.5 MeV incident photons. Shown is the radial dose distribution at selected angular intervals, where $\theta = 0^\circ$ is the forward direction, $\theta = 90^\circ$ is the lateral direction, and $\theta = 180^\circ$ is the backward direction.

direction as opposed to the forward direction. However, the lung kernel agrees well with the water kernel, indicating that lung has similar photon interaction and scattering properties as water. Figure 3 illustrates the differences between various 1.5 MeV monoenergetic, material-specific kernels. In comparison to water, it can be seen that the bone and titanium kernels deposit more dose in the backward ($\theta = 180^\circ$) and lateral ($\theta = 90^\circ$) directions and less dose in the forward direction ($\theta = 0^\circ$).

3.D. Investigation of “pocket of material” kernels

Figure 4 shows the radial dose falloff as a function of distance from the interaction site for our pure water, pure material, and “pocket of material” kernels for 1.5 MeV photons. We found that the dose distribution for our “pocket of material” kernels was generally very similar to that of the pure material kernels. Although there were small differences between the pure material kernels and the 1 mm radius “pocket of material kernels,” these differences were negligible when the size of the pocket was increased to a 5 mm radius. Notably, the “pocket of material” kernels always more closely resembled the pure material kernels than the water kernels, even for very small (1 mm radius) pockets of material.

3.E. Investigation of dosimetric impact of kernel hardening and material-specific kernels

Figure 5 shows percent depth dose (PDD) curves for a water phantom calculated using two different C/S implementations: one using a single polyenergetic kernel (“single kernel” method) and one that fully takes into account spectral changes in the photon beam (“components” method). The “components” method resulted in a harder PDD curve (i.e., larger PDD value at a given depth) than the “single kernel” method. The PDD value was 2.1%–5.8% larger at a depth of 25 cm and 1.0%–2.5% larger at a depth of 10 cm for the “components” method, with the discrepancy being larger for smaller field sizes.

Figure 6 shows PDD curves for the titanium cavity phantom and the bone cavity phantom calculated using both traditional density scaling of a water kernel, as well as a novel implementation using material-specific kernels. For the titanium cavity phantom, implementation of material-specific kernels resulted in 4.9% higher dose upstream of the metal (i.e., higher backscatter dose) and 8.2% lower dose downstream of the metal. Similar trends were found for the bone cavity phantom but the dose differences were of smaller magnitude. Materials-specific kernels resulted in 1.0% higher dose upstream and 1.5% lower dose downstream of the bone cavity.

4. DISCUSSION

In this study, we generated high-resolution, polyenergetic, and material-specific photon EDKs. Our high-resolution kernels agreed well with the original Mackie *et al.*³ kernels. However, we did observe differences near the interaction site for the lower photon energies (<500 keV), most likely attributable to improvements in electron transport in the EGSnrc code compared with the EGS code.²² Because the kernels were generally smoothly varying functions, interpolation of the kernels is likely a good approximation. Therefore, we believe that incorporating higher-resolution kernels into the C/S method will not appreciably improve the calculation accuracy, with the possible exception of near material interfaces and in the buildup region.

The impact of the photon spectrum used to calculate polyenergetic kernels was also investigated. Specifically, the

FIG. 4. Comparison of pure water, pure material, and “pocket of material” kernels for 1.5 MeV incident photons. (a) and (b) compare the radial dose distributions for 1 and 5 mm radius pockets of bone inside water, and (c) and (d) compare 1 and 5 mm radius pockets of titanium inside water in the forward ($\theta = 0^\circ$) and lateral ($\theta = 90^\circ$) directions.

effects of beam hardening with depth and beam softening with greater field size and off-axis distance were investigated. Among these three factors, beam hardening with depth was the most dominant. The effective depth of penetration of charged particles $\bar{z}$ for the polyenergetic kernels increased by 21%, going from a depth of 1.5 cm to a depth of 20 cm for a $10 \times 10 \text{ cm}^2$ field size (Table I). Metcalfe *et al.*¹⁷ also found that the effective range of charged particles increased for depth-hardened kernels in comparison to the surface kernel. Although the use of depth-dependent polyenergetic kernels has already been studied and shown to improve dose accuracy, no studies, to our knowledge, have investigated the effects of beam softening for larger field sizes and greater off-axis distances. Our data showed that the effective depth of

penetration of charged particles $\bar{z}$ can change as much as 7% for polyenergetic kernels calculated for various field sizes and off-axis distances (Table I). Although these spectral differences are smaller than those attributed to beam hardening with depth, they are still appreciable and taking them into account can improve dose calculation accuracy. We also found that the spectral differences due to field size and off-axis distance are smaller at greater depths due to beam hardening across the entire field. Therefore, kernel corrections for these factors may only be needed at shallower depths. We also compared the depth dose in a water phantom calculated with a single polyenergetic kernel against that calculated using the components method, which fully takes into account spectral changes in the photon beam. We found that the error associated with

FIG. 5. Percent depth dose curves for a water phantom calculated using a single polyenergetic kernel (“SK”) and the components method (“COMP”) for several field sizes.

not performing any type of kernel hardening correction is approximately 2%–6% for PDD values at a depth of 25 cm. These values are consistent with dose errors reported in previous studies.^{5,6} The disadvantage of the components method is the increased computation time. The components method increased the computation time by a factor of 8 in this study in comparison to the single kernel method. Liu *et al.*⁶ proposed a kernel hardening correction method, using interpolation to calculate the mean polyenergetic kernel as a function of depth, and found that this method was able to match the accuracy of the components method while only increasing the computation time by 50%. This kernel interpolation method may be a practical method of accounting for kernel hardening. However, because only spectral changes as a function of depth are taken into account, further studies need to be performed to look at the accuracy of this method off-axis.

It is also important to note that although the dose differences due to kernel hardening found in this study were fairly small, implementation of a kernel hardening correction can still have an impact on accuracy. For instance, in the TPS commissioning process, implementation of kernel hardening can potentially lead to beam model parameters that more closely reflect reality and thus a more accurate overall beam model. While our future work includes quantifying how the implementation of depth-hardened kernels affects various beam modeling parameters for fully commissioned beam models, this is outside the scope of the current study.

For our material-specific kernels, we found that the effective depths of penetration of charged particles were very similar for water and lung, indicating that the density scaling approximation is appropriate for this material. However, we found that as the density and effective atomic number differed more from water, the shape of the material-specific kernel also differed more from water. For higher density, higher Z materials, a greater proportion of the energy is deposited in the lateral direction. For our polyenergetic, material-specific

FIG. 6. Percent depth dose curves for the (a) bone cavity phantom and (b) titanium cavity phantom (heterogeneity extends from $z = 12$ to $z = 16$ cm) calculated using traditional density scaling of water kernels (“water kernels”) and novel implementation of material-specific kernels (“bone + water kernels” and “titanium + water kernels”).

kernels, the effective lateral range of charged particles in bone was 18% higher than that of water, and in titanium was 44% higher than that of water (Table II). Furthermore, we found that the shape of bone and especially metal kernels was poorly described by density scaling and thus density scaling may not be appropriate for these materials. Density scaling cannot accurately predict the lateral scatter and angular energy deposition caused by high- Z , high density materials. Woo and Cunningham⁸ also investigated the validity of the density scaling method and found it was too simple to adequately describe the scatter of electrons in different media and thus caused dose inaccuracies in regions greatly affected

by inhomogeneities. The inadequacy of the density scaling method for metals is a possible reason why the C/S method has been shown to be inaccurate near metal/tissue interfaces, overestimating the dose downstream and underestimating the backscatter dose upstream of metals. In this study, we found that the implementation of a metal-specific kernel resulted in increased backscatter dose and decreased dose downstream of a metal cavity, thus decreasing both of these dose errors associated with traditional C/S.

In reality, heterogeneities in patients are relatively small pockets within tissue, but these pockets are of different sizes depending on the situation. Developing distinct material kernels for pockets of different sizes would be impractical and difficult to implement. Fortunately, we found that the dose distribution from “pocket of material” kernels was very similar to that of pure material kernels. That is, implementing material-specific kernels simulated with large volumes of pure material (which are easy and consistent to calculate) are appropriate for describing pockets of material (which are realistic), and will give better accuracy than density scaling of water kernels.

Incorporating these kernel refinements into a commercial C/S algorithm increases the computation time.⁶ Thus, kernel refinements must be prioritized based on their relative importance. Based on our data, the differences in the kernels due to depth hardening is comparable to the differences between water and metal kernels. Of the various factors investigated, these two have the most dominant effects on the characteristics of the kernels, suggesting that incorporation of depth-specific and metal-specific kernels will give the greatest increase in accuracy. Incorporation of field size and off-axis position dependence will have some impact, comparable to implementation of bone kernels. These parameters should therefore be considered for inclusion into C/S algorithms as secondary refinements.

An issue that may arise in the implementation of material-specific kernels is the number of distinct materials to be included and how to handle intermediate-density materials (i.e., materials for which there is no material-specific kernel). To investigate this issue, we fit our polyenergetic material-specific kernels to the analytical function described by Ahnesjo.⁹ This analytical function describes the primary and scatter energy deposition components using a double exponential function with an inverse square correction for radial distance. Although our kernels were well described by this function, the fitting coefficients did not appear to have a predictable relationship with density, and thus material-specific kernels cannot be implemented by simply using an analytical function with fitting coefficients that scale with density. Practically, material-specific kernels will most likely be implemented such that the material kernel that is closest in density to the actual material found in the patient geometry is used. For instance, there would be a single metal kernel in the C/S algorithm and any material with a density above a certain threshold would use this kernel. This approximation will likely be an adequate one because, although the kernel shape does change in a complex way with respect to density, it does not change very drastically. Implementing a finite set

of material-specific kernels (i.e., water, bone, and metal kernels only) for patient geometries with many types of materials is also the subject of future research.

5. CONCLUSIONS

The use of depth-hardened and material-specific energy deposition kernels are refinements to the C/S method that have the potential to improve accuracy while taking advantage of the vast experience that clinicians and researchers have with this dose calculation algorithm. Density scaling of water kernels may be inadequate for describing the photon interaction characteristics of high-density, high Z metals. Implementation of a metal kernel in a collapsed cone C/S algorithm resulted in increased backscattered dose upstream of a metal cavity and lower dose downstream of the cavity, mitigating errors associated with traditional C/S. Taking into account spectral changes of the photon beam in the kernel convolution, namely, beam hardening with depth, resulted in a harder depth dose curve in water. Implementation of depth-hardening kernel correction has the potential to affect beam modeling parameters obtained in the treatment planning system commissioning process and thus the overall accuracy of the system.

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^{a)} Author to whom correspondence should be addressed. Electronic mail: sfkry@mdanderson.org; Telephone: (713) 745-8989; Fax: (713) 794-1364.

¹ T. R. Mackie, J. W. Scrimger, and J. J. Battista, “A convolution method of calculating dose for 15-MV x rays,” *Med. Phys.* **12**, 188–196 (1985).

² A. Ahnesjo, P. Andreo, and A. Brahme, “Calculation and application of point spread functions for treatment planning with high energy photon beams,” *Acta Oncol.* **26**, 49–56 (1987).

³ T. R. Mackie, A. F. Bielajew, D. W. Rogers, and J. J. Battista, “Generation of photon energy deposition kernels using the EGS Monte Carlo code,” *Phys. Med. Biol.* **33**, 1–20 (1988).

⁴ P. W. Hoban, D. C. Murray, and W. H. Round, “Photon beam convolution using polyenergetic energy deposition kernels,” *Phys. Med. Biol.* **39**, 669–685 (1994).

⁵ N. Papanikolaou, T. R. Mackie, C. Meger-Wells, M. Gehring, and P. Reckwerdt, “Investigation of the convolution method for polyenergetic spectra,” *Med. Phys.* **20**, 1327–1336 (1993).

⁶ H. H. Liu, T. R. Mackie, and E. C. McCullough, “Correcting kernel tilting and hardening in convolution/superposition dose calculations for clinical divergent and polychromatic photon beams,” *Med. Phys.* **24**, 1729–1741 (1997).

⁷ J. E. O'Connor, “The density scaling theorem applied to lateral electronic equilibrium,” *Med. Phys.* **11**, 678–680 (1984).

⁸ M. K. Woo and J. R. Cunningham, “The validity of the density scaling method in primary electron transport for photon and electron beams,” *Med. Phys.* **17**, 187–194 (1990).

- ⁹A. Ahnesjo, "Collapsed cone convolution of radiant energy for photon dose calculation in heterogeneous media," *Med. Phys.* **16**, 577–592 (1989).
- ¹⁰C. Reft, R. Alecu, I. J. Das, B. J. Gerbi, P. Keall, E. Lief, B. J. Mijneer, N. Papanikolaou, C. Sibata, and J. Van Dyk, "Dosimetric considerations for patients with HIP prostheses undergoing pelvic irradiation. Report of the AAPM Radiation Therapy Committee Task Group 63," *Med. Phys.* **30**, 1162–1182 (2003).
- ¹¹S. Spiridovich, L. Papiez, M. Langer, G. Sandison, and V. Thai, "High density dental materials and radiotherapy planning: Comparison of the dose predictions using superposition algorithm and fluence map Monte Carlo method with radiochromic film measurements," *Radiother. Oncol.* **81**, 309–314 (2006).
- ¹²E. Wieslander and T. Knoos, "Dose perturbation in the presence of metallic implants: Treatment planning system versus Monte Carlo simulations," *Phys. Med. Biol.* **48**, 3295–3305 (2003).
- ¹³D. W. O. Rogers, I. Kawrakow, J. P. Seuntjens, B. R. B. Walters, and E. Mainegra-Hing, "NRC User Codes for EGSnrc," Technical Report No. PIRS-702(RevB) (National Research Council of Canada, Ottawa, Canada, 2003).
- ¹⁴D. W. O. Rogers, B. Walters, and I. Kawrakow, "BEAMnrc Users Manual," NRCC Report No. PIRS-0509(A)revK (National Research Council of Canada, Ottawa, Canada, 2009).
- ¹⁵S. H. Cho, O. N. Vassiliev, S. Lee, H. H. Liu, G. S. Ibbott, and R. Mohan, "Reference photon dosimetry data and reference phase space data for the 6 MV photon beam from Varian Clinac 2100 series linear accelerators," *Med. Phys.* **32**, 137–148 (2005).
- ¹⁶O. N. Vassiliev, U. Titt, S. F. Kry, F. Ponisch, M. T. Gillin, and R. Mohan, "Monte Carlo study of photon fields from a flattening filter-free clinical accelerator," *Med. Phys.* **33**, 820–827 (2006).
- ¹⁷P. E. Metcalfe, P. W. Hoban, D. C. Murray, and W. H. Round, "Beam hardening of 10 MV radiotherapy x-rays: Analysis using a convolution/superposition method," *Phys. Med. Biol.* **35**, 1533–1549 (1990).
- ¹⁸ICRU, "Stopping powers for electrons and positrons," ICRU Report No. 37 (ICRU, Washington, DC, 1984).
- ¹⁹W. C. Roesch, "Dose for non-electronic equilibrium conditions," *Radiat. Res.* **9**, 399–410 (1958).
- ²⁰N. Childress, E. Stephens, D. Eklund, and M. Zhang, "Mobius3D White Paper: Dose calculation algorithm," Mobius Medical Systems, LP Rev. 0, 2012.
- ²¹E. Mainegra-Hing, D. W. Rogers, and I. Kawrakow, "Calculation of photon energy deposition kernels and electron dose point kernels in water," *Med. Phys.* **32**, 685–699 (2005).
- ²²I. Kawrakow, D. W. O. Rogers, E. Mainegra-Hing, F. Tessier, and B. R. B. Walters, "The EGSnrc Code System: Monte Carlo simulation of electron and photon transport," Report No. PIRS-701 (National Research Council of Canada, Ottawa, Canada, 2011).