Monte Carlo and Lambertian Light Guide Models of the Light Output from Scintillation Crystals at Megavoltage Energies

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Abstract

We have developed a new model of the light output from single crystal scintillators in megavoltage energy x-ray beams, as a function of depth of dose deposition. This is based on the concept of a Lambertian light guide model (LLG). This was evaluated in comparison with a Monte Carlo (MC) model of optical photon transport, previously developed and reported in the literature and which was used as a gold standard. The LLG model was developed as a means of enabling optimization of scintillator detector design. In both models the dose deposition and light propagation were decoupled, the scintillators were cuboids, split into a series of cells as a function of depth, with Lambertian side and entrance faces, and a specular exit face. The signal in a sensor placed 1 mm and 1000 mm beyond the exit face was calculated. Cesium iodide crystals of 1.5 and 3 mm square cross section and 1, 5 and 10 mm depth were modeled. Both models were also used to determine detector signal and optical gain factor as a function of CsI scintillator thickness, from 2 to 10 mm. Results showed a variation in light output with position of dose deposition of a factor of up to ~5, for long, thin scintillators (such as 10x1.5x1.5 mm³). For short fat scintillators (such as 1x3x3 mm³) the light output was more uniform with depth. MC and LLG generally agreed to within 5%. Results for a sensor distance of 1mm showed an increase in light output the closer the light originates to the exit face, whilst a distance of 1000 mm showed a decrease in light output the closer the light originates to the exit face. For a sensor distance of 1 mm, the study of signal as a function of scintillator thickness showed the ratio of signal for a 10 mm scintillator to that for a 2 mm scintillator, $S_{10/2}$, was 1.98, whereas, for the 1000 mm distance, the values were 3.00. The ratio of quantum efficiency (QE) between 10 mm and 2 mm thicknesses was 4.62. We

concluded that these models may be used for detector optimization, with the light guide model suitable for parametric study.

I. Introduction

Scintillators are used in many medical x-ray imaging applications. Their high light yield and high density make them ideal for applications involving imaging megavoltage energy x-rays, such as radiotherapy treatment beams¹⁻¹¹, diagnostic energy imaging^{12,13}, nuclear medicine^{14,15}, and for dosimetry with plastic scintillators^{16,17}.

However, the relationship between x-ray energy deposition in the scintillator and signal in a sensor is not straightforward. It depends on the spatial characteristics of energy deposition, the probability of light creation from this energy distribution, the transport of the optical photons within the scintillator and their probability of reaching the sensor. The sensor is a device which forms an image with light collected from the scintillator and may typically be an amorphous silicon flat panel imager^{12,18-22} or a camera^{3,6,7,8,23}.

In radiotherapy applications, the bremsstrahlung beam to be imaged is polychromatic, with a mean energy of typically between 1 and 8 MeV, with a component of energies as low as 50-100 keV²⁴. Thus different components of the x-ray spectrum may well yield different optical signals in the sensor per unit of input x-ray energy, due to variation in the penetration of the various x-ray energies.

An important new area of radiation therapy is image-guided radiotherapy (IGRT), in which radiological imaging is used to control the treatment process at each fraction. Imaging approaches include electronic portal imaging (EPI)^{25,26}, kilovoltage cone-beam CT (CBCT)²⁷, megavoltage CT (MVCT)^{1,2,6,7,9,28,29} and kilovoltage

fluoroscopy³⁰. This inevitably involves an x-ray dose, often to tissues outside the target. Additionally the lower the dose needed to form a useable image, the more efficient an IGRT intervention will be, or for a given dose, the better the photon statistics in the image will be. Hence there is the need to be able to optimize imaging systems for use in IGRT.

In this paper we consider the modeling and optimization of the light output from single crystal scintillators. A new model is presented based on a Lambertian light guide (LLG) model, defined as a light guide with Lambertian side faces. The results of the new model are compared with the results of a Monte Carlo (MC) model we presented previously⁶, with the MC model taken as the gold standard. The MC model was taken as gold standard, since it was in good agreement with experimental measurement⁶. The reason for developing the LLG model was to determine how fast and accurate an analytically based model could be in relation to the existing MC model. Furthermore the LLG model involves numerical integration and the accuracy and CPU time requirements are determined by the number of elements used in this integration. The dependency of these parameters was evaluated in comparison with the MC model.

The light output as a function of depth in the scintillation crystal is modeled and combined with the energy absorption characteristics of x-ray beams to yield signals in a sensor in close proximity to the exit face (1mm away, corresponding to a flat panel electronic portal imaging device, EPID) and remote from the exit face of the scintillator (1000 mm away corresponding to a camera based EPID). Two signal calculation approaches are discussed to enable optimization of detector design: one is

for calculating the signal for a given scintillator dimension for different x-ray spectra and the other is for studying effects of variations in detector thickness for a given spectrum. Results are presented for cesium iodide (CsI) and for megavoltage energy radiotherapy beams, although this approach is readily applicable to other scintillator materials and is expected to be valid for the kilovoltage energy range.

Novel aspects of the work presented here are:

1. the LLG model;
2. the analysis of light output as a function of depth of energy deposition in the scintillator;
3. the signal calculation approach for different energy spectra by combining component x-ray energy bins;
4. the study of variation in light output per cell with scintillator thickness;
5. the generation of light yield data for a sensor positioned close to the exit face of the scintillator (1 mm data).

II. Methods

A. X-ray and Optical Photon Modeling

In this work we decoupled the transport of x-rays and optical photons, i.e. ionizing radiation transport was modeled separately to optical photon transport. Hence in the models presented below, one Monte Carlo model was used to model ionizing radiation transport and another Monte Carlo (see section IIB) or the LLG (section IIC) model was used to describe light transport.

125 The system modeled is shown schematically in figure 1a. The scintillation crystal was
 modeled as a cuboid (or rectangular parallelepiped) with equal width and length sides
 (i.e. square cross-section). X-rays were normally incident on the entrance face. The
 scintillator was segmented in the depth direction, typically into 10 or 20 cells. X-ray
 dose deposition in each cell was modeled. The amount of light produced in each cell
 130 per incident x-ray was assumed to be proportional to the energy deposited in that cell.
 The light transport was modeled and used to determine how many optical photons
 reach a sensor placed at an arbitrary distance, in air, outside the exit face, which is
 opposite to the entrance face. This was done using the MC and LLG models described
 below, with the previously published MC model⁶ taken as the gold standard and the
 135 LLG model evaluated in comparison. In both models, the entrance face of the cuboid
 and four side faces were described as being Lambertian (i.e. a diffuse surface with
 luminous intensity proportional to the cosine of the angle of emission) and the exit
 face as a polished, specular plane. This set of face characteristics was chosen on the
 basis of our previous work which showed that a two-dimensional array of scintillators
 140 with this set of parameters may be constructed and produces a high light output⁶.
 Attenuation in the surfaces and volume and Fresnel refraction at the exit face of the
 crystal were modeled. Cells were numbered from 1 at the exit face to N_{cell} at the
 entrance face. It was assumed the sides of the crystals are optically isolated so that no
 light may enter from the side from similar crystals placed nearby.

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The x-ray dose deposited in cell N per incident x-ray is defined as $d(N)$. The number
 of optical photons produced in cell N by this dose (the light yield) is $y(N)$. $y(N)$ was
 determined by multiplying $d(N)$ by the product of the mass of the cell, m , and the light
 yield per unit of x-ray energy absorbed, g , which is a characteristic of the scintillator

150 material. These optical photons are then transported through the system until they are
either absorbed or pass through the exit face. If they pass through the exit face and
reach the sensor, they are detected and produce a signal $s(N)$. The conversion of light
to detected signal in the sensor was assumed to add negligible noise and hence was
not modeled. This is expected to be a good approximation as the noise added by this
155 gain stage is expected to be smaller than that from optical photon generation for
devices such as CCD cameras and amorphous silicon flat panel imagers. We define
 $\eta(N)$ as the percentage of optical photons launched in cell N that contribute to $s(N)$.
Thus $\eta(N)$ is a measure of the optical efficiency of the system and $s(N)$ may be given
by:

$$160 \quad s(N) = d(N) m g \eta(N) = y(N) \eta(N) \quad (1)$$

In Eq. 1, the term $d(N)$ is given by the depth dose curve of the x-ray beam, m is the
mass per cell (required to convert dose to energy absorbed per cell), g is characteristic
of the scintillator and $\eta(N)$ must be calculated. We now present the two models for
determining $\eta(N)$.

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B. Monte Carlo (MC) Model

We have described this model previously⁶, and it is not further developed here, hence
a brief summary is presented here.

170 Optical photons were generated isotropically in the volume of each cell and
transported as vectors, with stochastic attenuation within the crystal volume and at
interfaces. The number of optical photons launched was scaled in proportion to the
volume of the scintillator. Each photon was transported through the scintillator with a
probability of being attenuated over path length, l , given by:

$$p_{vol}(l) = 1 - \exp(-l/l_{OAL}) \quad (2)$$

where l_{OAL} is the optical attenuation length for the scintillator material.

When a photon reached one of the five Lambertian faces it was absorbed with constant probability, p_{surf} . If not absorbed then the diffusely reflected output photon was generated with angular distribution⁶:

$$p_{lam}(\theta) = \sin(2\theta) \quad (3)$$

Unpolarized light was assumed, as the optical photons were expected to undergo a large number of reflections, and so, at the exit face, the probability of reflection was calculated as the average of the Fresnel intensity reflection coefficients for polarized light parallel and perpendicular to the plane of incidence. The sensor was modeled as a circle of radius 2 cm, concentric with the scintillator, at distance d_{sensor} and the number of optical photons reaching the sensor was scored.

The user inputs to this model were: refractive index (for Fresnel reflection), dose distribution ($d(N)$), l_{OAL} , p_{surf} , light yield/MeV (g), scintillator width and depth dimensions, and d_{sensor} .

C. Lambertian Light Guide (LLG) Model

Scintillators that are useful for imaging high energies are generally highly transparent to their characteristic light, with small light attenuation in their volume. In addition reflections from their side faces may help to channel the light towards a sensor. Thus they may be considered as being like a light guide and a scintillator with Lambertian sides may be considered to be a light guide with Lambertian faces.

200 Again we divide the light guide into cells (Fig. 1a). For such a system, light propagation depends on:

1. the mean solid angle of each cell subtended at the others and of the exit face subtended at each of the cells,
2. the angular distribution, which is isotropic initially (for optical photons created
205 in the volume by x-ray interaction) and Lambertian for reflections from each of the non-exit faces,
3. light loss in the volume and at the Lambertian faces, and
4. the refractive index of the scintillator and of the air outside the exit face.

210 Starting with isotropic light generation within each cell, an iterative matrix approach was used to model the transport of the optical photons. If ϕ_K is a vector describing the distribution of optical photons after the K 'th order transport, then it is related to ϕ_{K-1} by:

$$\phi_1 = S_n P_{n,m}^{initial} \phi_0 \quad (4a)$$

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$$\phi_K = S_n P_{n,m} \phi_{K-1} \quad (4b)$$

where ϕ_0 is the initial light distribution produced by x-ray interaction in the volume of the scintillator and $P_{n,m}$, $P_{n,m}^{initial}$ are matrices describing the probability of transport from cell m to cell n . $P_{n,m}^{initial}$ is different to $P_{n,m}$ as it describes the initial isotropic distribution of optical photons from x-ray absorption, whereas optical photons created
220 later in the transport process are the result of Lambertian scattering from faces of the scintillator. S_n is a matrix describing probability of not being absorbed in the faces of cell n . If the scintillator is divided into N_{cell} cells, then ϕ_K has one element for each cell, plus the entrance face and the sensor. As the exit face is specular, reflection from this may be modeled directly using the matrix $P_{n,m}$ as shown below:

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$$\phi = \begin{pmatrix} \text{Entrance surface} \\ \hline \text{Cell } N_{\text{cell}} \\ \vdots \\ \text{Cell } 1 \\ \hline \text{Sensor} \end{pmatrix} \quad (5)$$

If ϕ_0 is given unit intensity for cell N and zero for all other elements, then the value of the matrix element corresponding to the sensor position after a large number of iterations is the optical efficiency, i.e.:

$$\phi_{K \rightarrow \infty}(\text{Sensor}) = \eta(N) \quad (6)$$

230 In Eq. 5, cells are numbered with increasing distance from the sensor. A dashed line separates the entrance face from the volume of the scintillator and a solid line separates the sensor. S_n is a diagonal matrix:

$$S_n = \begin{pmatrix} (1 - p_{\text{surf}}) & & \\ \hline & I(1 - p_{\text{surf}}) & \\ & & 1 \end{pmatrix} \quad (7)$$

where I denotes the identity matrix. Each element of $P_{n,m}$ is a product of volume
235 attenuation, $V_{n,m}$, solid angle and angular distribution:

$$P_{n,m} = V_{n,m} \times \lambda_{n,m} \quad (8)$$

$$V_{n,m} = e^{-\bar{L}/L_{\text{OAL}}} \quad (9)$$

where $\bar{L}$ is the average path length from cell m to cell n (averaged over the surface area of both cells). $\lambda_{n,m}$ is the amount of light entering cell n from cell m minus that
240 escaping by passing through into the next cell from n (Fig. 1b):

$$\lambda_{n,m} = C_{n,m} - C_{n+1,m} \quad (10)$$

$C_{n,m}$ is the probability of optical photons scattered from the faces of cell m reaching the entrance of cell n . In the case of the initial isotropic distribution, this may be

calculated analytically from the expression for the solid angle in Cartesian
 245 coordinates:

$$4\pi C_{n,m}^{initial} = \Omega = \int_{-x_0}^{x_0} \int_{-y_0}^{y_0} \frac{z_{n,m} dx dy}{(x^2 + y^2 + z_{n,m}^2)^{3/2}} = \pi - 2 \sin^{-1} \left[1 - \frac{2x_0'^2 2y_0'^2}{(1+x_0'^2)(1+y_0'^2)} \right]$$

$$x_0' = \frac{x_0}{z_{n,m}} \quad (11)$$

$$y_0' = \frac{y_0}{z_{n,m}}$$

where the width and length of the scintillator are $2x_0$ and $2y_0$ and $z_{n,m}$ is the distance
 from the depth at which the light originates in cell m to the entrance of cell n . Two
 similar distributions were also needed: the probability of Lambertian reflection from
 250 the side face of cell m entering cell n and the probability for an end face (either
 entrance or exit):

$$4\pi C_{n,m}^{side} = \int_{-x_0}^{x_0} \int_{-y_0}^{y_0} \frac{4 y z_{n,m} dx dy}{(x^2 + y^2 + z_{n,m}^2)^2}$$

$$4\pi C_{n,m}^{end} = \int_{-x_0}^{x_0} \int_{-y_0}^{y_0} \frac{4 z_{n,m}^2 dx dy}{(x^2 + y^2 + z_{n,m}^2)^2} \quad (12)$$

These were calculated numerically using the trapezium rule. The dihedral symmetry
 of the rectangular x,y face meant that only one quadrant needed to be calculated. n_{trap}
 255 is the number of integration points in x and y (see Fig. 1c).

The probability of escape at the exit face of the scintillator following reflection from
 the side of cell m , f_m^{side} , was calculated using Fresnel's equations (again assuming
 unpolarized light) for each of the n_{trap}^2 points and averaged. The probability of
 260 escaping photons striking the detector sensor, d_m , was calculated as the solid angle
 subtended by the sensor at the exit face. Values of $C^{initial}$, C^{side} and C^{end} were averaged

over the central plane of the cell, the side face and the end face respectively. The number of points for averaging was n_{ave} in each dimension (see Fig. 1c).

265 Consider light propagating from cell m to n . It may either travel directly between the cells, in which case the probability depends on the distance between them $|m-n|$, so the two subscripts n,m in Eqs. 4-12 may be replaced by one: $m-n$ (for a scintillator with non-Lambertian sides, two subscripts might still be needed). Alternatively light from cell m may be reflected from the specular exit face (with a probability of escape

270 from this face) and go back to cell n . The distance the light travels between the cells for this mirror process is $m+n-1$ (the subscripts n,m in Eqs. 4-12 may be replaced by $m+n-1$). This process is illustrated in Fig. 1b, where the example of $m=4$, $n=2$ is shown, with the distance traveled 2 cells for the direct case and 5 for the mirror case.

Thus Eq. 10 may be split into two parts:

275 $P_{n,m} = P_{|n-m|}^{direct} + P_{m+n-1}^{mirror}$

$$P_{|n-m|}^{direct} = \left(\begin{array}{c|cccc|c} 0 & V_1^{ce} C_1^{side} & \dots & \dots & V_{N_{cell}}^{ce} C_{N_{cell}}^{side} & 0 \\ \hline V_1^{ce} \lambda_0^{side} & V_0^{cc} \lambda_0^{side} & V_1^{cc} \lambda_1^{side} & \ddots & V_{N_{cell}-1}^{cc} \lambda_{N_{cell}-1}^{side} & 0 \\ \vdots & V_1^{cc} \lambda_1^{side} & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & V_1^{cc} \lambda_1^{side} & \vdots \\ V_{N_{cell}}^{ce} \lambda_{N_{cell}-1}^{end} & V_{N_{cell}-1}^{cc} \lambda_{N_{cell}-1}^{side} & \ddots & V_1^{cc} \lambda_1^{side} & V_0^{cc} \lambda_0^{side} & 0 \\ \hline V_{N_{cell}}^{ee} C_{N_{cell}}^{end} f_{N_{cell}}^{end} d_{N_{cell}} & V_{N_{cell}}^{ce} C_{N_{cell}}^{side} f_{N_{cell}}^{side} d_{N_{cell}} & \dots & \dots & V_1^{ec} C_1^{side} f_1^{side} d_1 & 1 \end{array} \right)$$

$$P_{m+n-1}^{mirror} = \left(\begin{array}{c|cccc|c} V_{2N_{cell}}^{ce} C_{2N_{cell}}^{end} \alpha_{N_{cell}+1}^{f_{N_{cell}}^{end}} & V_{2N_{cell}}^{ce} C_{2N_{cell}}^{side} \alpha_{N_{cell}+1}^{f_{N_{cell}}^{side}} & \dots & \dots & V_{N_{cell}+1}^{ce} C_{N_{cell}+1}^{side} \alpha_{N_{cell}+1}^{f_1^{side}} & 0 \\ \hline V_{2N_{cell}}^{ce} \lambda_{2N_{cell}-1}^{end} \alpha_{N_{cell}}^{f_{N_{cell}}^{end}} & V_{2N_{cell}-1}^{cc} \lambda_{2N_{cell}-1}^{side} \alpha_{N_{cell}}^{f_{N_{cell}}^{side}} & V_{2N_{cell}-2}^{cc} \lambda_{2N_{cell}-2}^{side} \alpha_{N_{cell}-1}^{f_{N_{cell}-1}^{side}} & \ddots & V_{N_{cell}}^{cc} \lambda_{N_{cell}}^{side} \alpha_{N_{cell}}^{f_1^{side}} & 0 \\ \vdots & V_{2N_{cell}-2}^{cc} \lambda_{2N_{cell}-2}^{side} \alpha_{N_{cell}-1}^{f_{N_{cell}-1}^{side}} & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & V_2^{cc} \lambda_2^{side} \alpha_2^{f_2^{side}} & \vdots \\ V_{N_{cell}+1}^{ce} \lambda_{N_{cell}}^{end} \alpha_1^{f_{N_{cell}}^{end}} & V_{N_{cell}}^{cc} \lambda_{N_{cell}}^{side} \alpha_1^{f_{N_{cell}}^{side}} & \ddots & V_2^{cc} \lambda_2^{side} \alpha_1^{f_2^{side}} & V_1^{cc} \lambda_1^{side} \alpha_1^{f_1^{side}} & 0 \\ \hline 0 & 0 & \dots & \dots & 0 & 0 \end{array} \right)$$

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(13)

where the V terms were calculated using Eq. 9, taking into account whether the distance needed was between a cell and another (V^{cc}), a cell and an end face (V^{ce}) or between two end faces (V^{ee}). The subscripts of λ , C and V are $/m-n/$ in P^{direct} and $m+n-1$ in P^{mirror} . The right hand column is used to preserve the accumulated signal in the sensor after each iteration of Eq. 4. $\lambda_0 = 1 - 2C_1$. The terms α_{cell}^f in P^{mirror} denote the probability of light that reaches the exit face, being reflected and reaching a given cell. The sum of α over each column is $(1-f)$. See Fig. 1c. An analogous expression to Eq. 13 may be written for the initial isotropic distribution, with the first column elements all zero and the superscript *side* replaced with *initial*. The central region of P^{direct} has the Toeplitz structure characteristic of Markovian processes. Figure 2 shows example values of the C and f coefficients for from 1 to 20 cells.

Iterative Eq. 4 was used to calculate $\eta(N)$ as a function of starting cell in the scintillator. 300 iterations were used as this left a residual signal in the scintillator of order 10^{-7} .

D. Choice of parameters in LLG model

Most parameters in the LLG model have a physical basis and are identical to equivalent ones in the MC model. User variable parameters are the number of cells N_{cell} and the integration parameters n_{ave} and n_{trap} . We have chosen $N_{cell} = 10$ as the default as experience with the MC model showed that this gave reasonable results⁶. n_{ave} and N_{cell} are linked in that n_{ave} is the number of integration points along a cell side (Fig. 1c) and N_{cell} is the number of cells the scintillator is split into. Hence for a given scintillator length, the greater the value for N_{cell} , the closer spaced are the integration points for a given n_{ave} . Also attenuation in the volume of the scintillator is small and

hence the transport of optical photons is mainly determined by geometry, i.e. the shape of the scintillation crystal cells. This may be described in terms of the aspect ratio of the cell height to scintillator width. The greater the aspect ratio, the larger the value of n_{ave} needed to ensure adequate sampling of the sides. To determine the optimum value for n_{ave} , and for a given N_{cell} , the root mean square (RMS) difference between MC and LLG models (averaged over all cells) was determined for a range of cell aspect ratios.

The parameter n_{trap} is the number of integration points along the cell exit face. This is expected to be particularly important for the calculation of the signal in the sensor when the sensor is placed at a large distance (e.g. $d_{sensor} = 1000$ mm). In this case the sensor will present a small solid angle to the exit face and a large enough value of n_{trap} is needed to ensure sufficient sampling is carried out in the sensor.

320 **E. Signal Calculation for X-ray Spectra**

The decoupling of x-ray and optical photon calculations in the model means that various x-ray beams may be modeled without the need to recalculate optical photon transport, as the optical efficiency, $\eta(N)$, may be precalculated using either MC or LLG models. In addition the relationship between dose (and hence energy absorbed) and depth of a range of mono-energetic beams, $d_E(N)$, may be precalculated, where subscript E denotes the x-ray energy. For each energy, the average optical efficiency, $\bar{\eta}_E$, may be calculated:

$$\bar{\eta}_E = \frac{\sum_N \eta(N) d_E(N)}{\sum_N d_E(N)} \quad (14)$$

For a polychromatic beam, of fluence distribution ψ_E , the average optical efficiency,

330 $\bar{\eta}_{beam}$, may be calculated as:

$$\bar{\eta}_{beam} = \frac{\sum_E \bar{\eta}_E \Psi_E}{\sum_E \Psi_E} \quad (15)$$

The EGSnrc usercode DOSRZnrc^{31,32} was used to determine the dose $d_E(N)$, for a range of monochromatic x-ray energies, E . Data for polychromatic beams were
 335 generated by summing over the spectrum. For all DOSRZnrc calculations, 10^7 x-ray histories were modeled and a beam radius of 0.1 cm was used. The standard deviation on the dose calculated was typically 0.5% and no greater than 1.0%.

F. Optimization of Scintillator Thickness

340 For some applications, such as imaging in IGRT, it may be desirable to investigate optimization of the scintillator design. This may be achieved by varying the thickness of the scintillator. Increasing thickness will increase quantum efficiency, but may diminish optical efficiency. In the MC model, investigation of scintillator thickness dependence requires a new calculation for each case. In the LLG model, the
 345 coefficients may be calculated once for the longest scintillation crystal to be considered (the part of the process requiring the greatest CPU time) and a subset of the same coefficients reused to model shorter scintillators using fewer component cells. For instance, if we generate coefficients for 20 x 0.5 mm cells, giving a 10 mm length, these coefficients may also be used to estimate light yields from thicknesses
 350 that are integer multiples of 0.5 mm up to 10 mm.

G. Effects on Detective Quantum Efficiency

The conversion of x-rays into optical photons in the scintillator is a stochastic process and hence g , in Eq. 1, will vary about its mean value from x-ray photon to photon.

355 This variation is often assumed to have a Poissonian distribution and adds noise to the final signal^{31,32}. As we have shown in this paper, not all of the optical photons produced will be detected. If we denote s_{abs} as the number of optical photons detected per x-ray absorbed, then this will also approximately follow a Poissonian distribution. The signal to noise ratio (SNR) of the system is reduced by a factor:

$$360 \quad \frac{1}{(\text{SNR}_{\text{out}})^2} = \frac{1}{QE} \left(1 + \frac{1}{s_{abs}} \right) \frac{1}{(\text{SNR}_{\text{in}})^2} \quad (16)$$

where QE is the quantum efficiency and SNR_{in} and SNR_{out} are the input and output SNR, respectively. This process is often referred to as noisy gain. Variations in optical efficiency with scintillator dimensions and beam energy mean that the determination of Eq. 16 is not straightforward. Also, x-ray energy deposition in the scintillator will vary from x-ray photon to photon and this will constitute an extra source of noise. 365 This variation will be different for different x-ray energies. A polychromatic treatment beam will harden with depth in the scintillator and hence the noise associated with x-ray energy deposition may well change with depth, as does the light transport within the scintillator, which this work investigates. To illustrate the effects of differences 370 between light transport in scintillators we neglect the second of these two noise sources, i.e. the variations in the x-ray energy deposition process.

Quantum efficiency, QE , is given by:

$$QE = 1 - \exp(-\bar{\mu}t) \quad (17)$$

375 with t the thickness and $\bar{\mu}$ the average attenuation coefficient over the 6 MV spectrum. s_{abs} is given by:

$$s_{abs} = \frac{\sum_N d(N)m}{QE} g \bar{\eta}_{beam} \quad (18)$$

where the first term gives the energy absorbed per x-ray interaction (the QE term in the denominator is needed to convert from energy per x-ray incident to per x-ray absorbed). $\bar{\eta}_{beam}$ may be calculated using either MC or LLG models. Detective quantum efficiency^{33,34}, DQE , is:

$$DQE = \left(\frac{SNR_{out}}{SNR_{in}} \right)^2 = QE \left(1 + \frac{1}{s_{abs}} \right)^{-1} \quad (19)$$

H. Parameters Studied

385 The scintillator material was modeled as cesium iodide, CsI. The parameters used were taken from our previous work⁶. Density $\rho = 4.51 \text{ g/cm}^3$, refractive index = 1.8, light yield $g = 56000 \text{ photons/MeV}$, optical attenuation length $l_{OAL} = 1000 \text{ mm}$, surface attenuation, $p_{surf} = 0.07$.

390 The scintillation crystals were square in cross-section, two widths were modeled: 1.5 and 3 mm. These are indicative of scintillator dimensions discussed in the literature⁶. Crystal depths of 1, 5 and 10 mm were used. d_{sensor} was 1 mm and 1000 mm, both in air (to model the worst optical coupling case). 1 mm distance corresponds to a detector in, or close to, contact such as an amorphous silicon flat panel and 1000 mm distance corresponds to a camera, such as found in some electronic portal imaging devices. For this case, a lens radius of 20 mm was modeled, corresponding to an angular subtense of 1.15° .

For the first study, the results for the MC and LLG models were compared, with the
 400 MC model as the reference (since it was compared with experimental data⁶). The
 purpose of this was to validate the LLG model and find suitable values of n_{ave} and
 n_{trap} (see IID). The optimum values of n_{ave} and n_{trap} were determined to give RMS
 agreement with the MC model of 5% or better. N_{cell} was set to 10 and the RMS
 difference was determined as a function of the aspect ratio of cell height to scintillator
 405 width for d_{sensor} values of 1 mm and 1000 mm. In addition the dependence on n_{trap}
 was studied for the scintillator of 10 mm depth $\times$ 1.5 mm width $\times$ 1.5 mm length,
 with $n_{ave} = 21$ and $N_{cell} = 10$.

Once these parameters were chosen, results were analyzed cell by cell. This was done
 410 for 10 cells and for both widths and all three depths. In cases of large discrepancies
 between LLG and MC, the scintillator was split into more cells. In the second study,
 the effects of separating x-ray absorption and light transport were investigated for
 signal calculation for x-ray spectra. This was done for a polychromatic 6 MV
 spectrum²². A third study investigated the optimization of crystal thickness. This was
 415 done using coefficients for 20 and 30 cells in the LLG model for $d_{sensor} = 1$ and 1000
 mm, respectively. 10 cells were used for each thickness in the MC model. Finally the
 effects of optical photon collection on DQE were studied for the two values of d_{sensor} .

III. Results

420 A. Comparison of Monte Carlo and Lambertian Light Guide Models

Figure 3a shows the RMS difference between LLG and MC models as a function of
 scintillator aspect ratio for each of the three depths, and two widths of scintillator

studied. Data are shown for $n_{trap}=100$ and $n_{ave}=21$ for $d_{sensor} = 1$ mm, and for $n_{trap}=800$ and $n_{ave}=21$ for $d_{sensor} = 1000$ mm. Fig. 3b shows the RMS difference as a function of n_{trap} for $n_{ave}=21$ and $d_{sensor} = 1000$ mm. Two trends are evident. In fig. 3b, RMS difference decreases rapidly with n_{trap} until values of 400 to 800, and then sharply levels off. Data for $d_{sensor} = 1$ mm (not presented) shows a much weaker dependence. This trend is a consequence of the need to have sufficient sampling points to describe optical light collection in a sensor of radius 20 mm placed at a distance of 1000 mm, i.e. in Fig. 1c, if the sensor at the bottom subtends a very small solid angle, then n_{trap} needs to be very large such that sufficient samples contribute to the signal in the sensor. For $d_{sensor} = 1$ mm, this has less effect and the sampling along the side of the cell is more important as shown in Fig. 3a, where the data for $d_{sensor} = 1000$ mm (open squares) is essentially flat and that for $d_{sensor} = 1$ mm (solid circles) shows a rise with increasing aspect ratio. The arrows show the effect of increasing the number of cells if aspect ratio is large. The tails of the arrows show results for 10 mm depth $\times$ 1.5 mm width $\times$ 1.5 mm length divided into 10 cells of aspect ratio 0.67 and the heads of the arrows the results of choosing 20 cells, giving an aspect ratio of 0.33. The results for $d_{sensor} = 1$ mm are improved, whereas those for $d_{sensor} = 1000$ mm are changed little. Thus we conclude the parameter value $n_{ave} = 21$ is adequate for both values for d_{sensor} , for small d_{sensor} a smaller value of n_{trap} may be used (i.e. 100) and for large d_{sensor} , n_{trap} must be larger, with a value of up to 800 for very large d_{sensor} . In the case of very long thin crystals large n_{ave} or more cells are needed. This is necessary when the aspect ratio is in excess of 0.33.

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Figure 4a shows light collection efficiency, $\eta(N)$, as a function of cell number where light originated, N , for all crystal size combinations and $d_{sensor} = 1$ mm from the exit

face. $N_{cell}=10$. Cells are numbered from 1 adjacent to the exit face to 10 adjacent to the x-ray entrance face as in Fig. 1a. The lines are labeled “depth $\times$ width $\times$ length” (in millimeters). MC results are shown by cross symbols joined by solid lines. For all MC calculations the number of histories was $10^5/\text{mm}^3$. This gave a statistical error of under 1%. The LLG results are shown by open symbols joined by dashed lines and closely overlap the MC results. Results were generated using $n_{trap}=100$ and $n_{ave}=21$. Figure 4b shows calculations for $d_{sensor} = 1000$ mm. The lower light collection efficiency for this case meant more histories, 10^7 , were needed for the MC (for 1% error). For the LLG model, $n_{trap}=800$ and $n_{ave}=21$. The larger value of n_{trap} was used to ensure the numerical integration was amply sampled to cover the sensor as discussed above.

Figures 5a and 5b shows the percentage difference between MC and LLG results in Fig. 4 for $d_{sensor} = 1$ and 1000 mm, respectively. Results are shown as $(LLG-MC)/MC \times 100$. All are within 5% for 5a, except the $10 \times 1.5 \times 1.5$ case. A smaller deviation was obtained with $N_{cell}=20$ (as discussed above). The results of adjacent cells were averaged to produce data at the same points as the MC. For 5b, the errors between MC and LLG are smaller than 10% for the majority of points. Table 1 shows statistics for the comparison between the two models, with MC as the gold standard. RMS agreement (between the two methods) is within 5% in all cases and of order 1% for the $d_{sensor} = 1$ mm situation.

B. Signal Calculation for X-ray Spectra

Modeling a polychromatic x-ray spectrum is illustrated in figure 6. Fig 6a shows normalized dose (and hence energy absorbed) per cell as a function of x-ray energy

and depth in the crystal for a $10 \times 3 \times 3 \text{ mm}^3$ scintillator, determined using DOSRZnrc as described in section IIE. Fig. 6b shows the result of multiplying the data in 6a by the optical efficiencies from the LLG model in Fig. 4, as given by Eq. 14. Fig. 6c shows the result of a weighted summation of 6b over the 6 MV spectrum for a crystal cross-sectional area of $3 \times 3 \text{ mm}^2$ and depths of 1, 5 and 10 mm, and for $d_{\text{sensor}} = 1$ and 1000 mm, as in Eq. 15.

C. Optimization of Scintillator Thickness

Figure 7a shows $\eta(N)$ as a function of cell position for a range of scintillation crystal thicknesses and with $d_{\text{sensor}} = 1 \text{ mm}$. For the LLG model, each cell has cross-sectional area $1.5 \times 1.5 \text{ mm}^2$ and depth 0.5 mm. Data for 4 to 20 cells are shown, giving thicknesses of 2 mm to 10 mm in steps of 0.5 mm. Data are shown as lines, alternating between solid and dashed to aid distinction between them. MC model results are also shown for each thickness by circles, alternating between closed and open. Here data were generated for 10 cells for all thicknesses. The purpose of this choice of cell number was that the MC data could be a reference against which to evaluate the use of the LLG model for optimization in this way. Hence the effects of varying the number of cells were removed by keeping N_{cell} constant in the MC case. Fig. 7b shows $\eta(N)$ as a function of cell position for $d_{\text{sensor}} = 1000 \text{ mm}$. 20 cells were used for the LLG model. MC calculations for integer thickness in mm, 10 cells and 10^7 histories/ mm^3 are shown by solid circles.

495 **D. Effects on Detective Quantum Efficiency**

Figures 8a and 8b show the use of the LLG model data in Fig. 7 to calculate some properties of the imaging system for different scintillator thicknesses, for the 6 MV beam. Data shown are $\bar{\eta}_{beam}$, S , S_{abs} , QE and DQE.

500 **E. Computer Timings**

All calculations were carried out on an IBM blade computer with two 2.8 GHz Xeon CPUs.

In the LLG model, by far the largest component of CPU time is required by the
505 numerical integrations in Eq. 12. Once these coefficients are generated, the CPU time required to carry out the iterations in Eq. 4 is less than 1s. For the single depth calculations in Figs. 4a and 5a, the MC model required 8 minutes for each crystal, whereas the LLG model required 16 minutes for $N_{cell} = 10$ and 31 minutes for $N_{cell} = 20$ (' $10 \times 1.5 \times 1.5$ ' data in Fig 4a). The data for $d_{sensor} = 1000$ mm in Figs. 4b and 5b
510 required 16 hours for both optical photon transport models. This extra time is needed because of the greater value for n_{ave} needed in the LLG model and the greater number of histories needed in the MC model. The data in Fig. 7 for calculating light yield as a function of scintillator thickness required 45 and 91 min in 7a and 63 and 95 hours in 7b for LLG and MC models, respectively.

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IV. Discussion

The results in Figs. 4 and 7 show that in the context of the assumptions made and systems modeled in this study, the average optical efficiency decreases with increased scintillator thickness. This is because as thickness increases there is greater chance of

520 absorption in the side faces. For long thin scintillators, there is a significant variation in signal with depth. For the sensor close to the exit face, the signal increases as the optical photons are created closer to the exit, mainly due to the lower probability of absorption in the side faces. For a small area sensor placed a long distance away, the signal is formed of optical photons leaving the scintillator traveling almost perpendicular to the exit face (for $d_{sensor} = 1000$ mm and a 20 mm radius lens, the angular subtense of the lens is 1.15° and hence the angle of incidence must be below 0.57°). The Lambertian side and entrance faces produce independent scattering events which help to produce optical photons with the necessary trajectory to exit the scintillator and reach the lens. Thus a channeling effect is produced. Optical photons 530 launched far from the exit face have a greater probability of reaching and scattering at the side and entrance faces, and hence a greater probability of having the necessary trajectory to escape and reach the sensor. Thus for Figs. 4b and 7b the opposite pattern is seen to Figs. 4a and 7a and the signal decreases for optical photons launched close to the exit face. The data for 10x3x3 and 5x1.5x1.5, which have the same shape but 535 different scale, almost overlap perfectly. This is because the volume attenuation is negligible for this size, helping to justify the use of a light guide model.

Fig. 5 shows that for similar CPU times to within a factor of two, agreement between MC and LLG of better than 5% may be achieved for a sensor close to the exit face of 540 the scintillator. A trend for the error in the LLG result to go from negative to positive as cell number increases is more strongly evident for $d_{sensor} = 1$ mm. For $d_{sensor} = 1000$ mm errors are larger, but still better than 10% for the majority of cases. The reason for these larger errors is the fact that the sensor subtends such a small solid angle at the exit face: for a 20 mm diameter sensor at 1000 mm, the angular subtense is 1.15° ,

545 giving a solid angle of 3×10^{-4} steradians. Hence of the n_{trap} integration points used to calculate the probability of exiting the crystal (see Fig. 1c), only a small fraction pass through the sensor and contribute to the calculation of the signal in the sensor, hence its limited accuracy compared to the case when the sensor is close to the exit of the crystal.

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The decoupling of the x-ray and optical photon transport is illustrated in Fig. 6 and allows calculation of the detector signal without remodeling the optical component for each x-ray beam. This requires the light yield per unit energy absorbed to be linear and its statistics to scale with photon number³⁴. This work and the other literature
555 modeling signals from these systems assume the relationship between incident x-ray energy and signal in the sensor is linear. The literature on this issue is limited, but suggests there is a deviation from linearity for low energies, particularly close to the K and L edges³⁵, with an over-response of 10-15%. These data however were acquired with gamma sources using the Compton coincidence technique, hence under much
560 lower dose rates than encountered in radiotherapy. Variations in light yield with x-ray energy could be folded into the spectral model presented in IID and fig. 6.

The results of Fig. 7 show that the LLG model may be used for detector thickness optimization with reasonable accuracy. For $d_{sensor} = 1$ mm, good agreement between
565 LLG and MC is seen above 2.5 mm thickness (5 cells for LLG). The cross symbols, close to the 2 mm data, in Fig. 7a show the LLG results for 2 mm thickness and 10 cells. Agreement with MC is now good suggesting that the discrepancy between MC and LLG for 2 mm thickness is due to the small number of cells used in the LLG calculation. Fig. 7b shows a similar level of agreement for all thicknesses studied.

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The LLG model has been used to test if a light guide approach may be used to describe such a scintillator system as an alternative to the Monte Carlo. The good agreement with the MC model would suggest there is a sound physical basis for this alternative approach. The purpose of developing the new approach was partly to
575 provide physical insight, e.g. the macroscopic nature of the LLG model emphasizes the importance of basic geometric considerations in determining the light yield in the sensor.

The similar timings for the two optical photon models and the 5% RMS error for the
580 LLG model in Fig. 5 would suggest that there may be no particular advantage in using the LLG model for calculations for a single scintillator. The close agreement seen in Fig. 7 between the two models and the strong trends in light output seen as a function of distance from exit surface and scintillator thickness would suggest the LLG model could be used to generate light output as a function of cell thickness with savings in
585 CPU time of 45 min and 32 hours for $d_{sensor} = 1$ mm and 1000 mm, respectively.

The CPU time required by the LLG is dominated by the numerical integrations in Eq. 12. Good analytical approximations to these expressions, along the lines of Eq. 11 would speed up this model considerable and yield significant benefit over the MC
590 model.

An issue with the LLG model is the need to find values of parameters. However, this study has covered a range of scintillator thicknesses from 1 to 10 mm and two extremes of sensor positioning and found that $n_{ave}=21$, a choice of cell number to keep

595 the aspect ratio no greater than 0.33, with $n_{trap}=100$ for a close sensor and 800 for a very distant sensor gives 5mm RMS accuracy with respect to the MC model. These parameters are expected to be suitable for most situations modeled in medical imaging applications.

600 Analysis of the data presented in fig. 8a showed that the ratio of signal for a 10 mm scintillator to that for a 2 mm scintillator (open squares joined by dotted line), $S_{10/2}$, was 1.98 whereas the ratio of quantum efficiency (solid squares joined by solid line), $QE_{10/2}$, was 4.62, indicating a decrease in percentage light signal as scintillator thickness is increased. For Fig. 8b, the values show a similar behavior, with $S_{10/2} =$
605 3.00. The results in Fig. 8a also show that, as expected, if most of the exiting light is collected (i.e. s_{abs} is large), then the effect of the noisy gain is small. In other words, DQE is equal to QE in Eq. 19. In 8b, the effects of low optical photon collection efficiency produce a significant effect on DQE, as shown by the separation of the QE and DQE lines. The simplifying assumptions made in generating Fig. 8 should be
610 remembered however, i.e. that the variation in energy deposited per x-ray may be neglected. The results are meant to be illustrative of the model.

This work has considered one example scintillator, CsI, and the Lambertian case. In our previous work using the MC model⁶ we have also considered specular scintillators
615 and bismuth germanate, BGO, and zinc tungstate, $ZnWO_4$, in addition to CsI, but showed CsI produced the greatest light output. The analytical model could easily be used for single crystal scintillators other than CsI using the appropriate parameters for refractive index, l_{OAL} , p_{surf} , g etc. For specular crystal faces a more conventional light guide model could be used, with reflective faces. However our previous studies

620 showed that the light yield for Lambertian faces was typically three times higher than for specular faces⁶, making the Lambertian case the one of most interest. That study also presented measurements of light output as a function of scintillator type and surface finish.

625 Several authors have studied the dose response of imaging systems used at high x-ray energy. These studies have generally considered ionizing radiation transport only and/or phosphor screens, containing polycrystalline gadolinium oxysulfide. Jaffray et al.³⁶ calculated absorbed energy distributions for a range of gadolinium oxysulfide thicknesses and energies using MC. Other authors have generated MC based
630 dosimetric models of complete EPIDs^{37,38}. Radcliffe et al.³⁹ presented a MC model of the light output from gadolinium oxysulfide screens. This model described optical transport assuming the screen to be a weakly absorbing medium, with scattering due to Fresnel reflection and refraction at the boundaries between the binder and the phosphor grains. Bissonnette et al.⁴⁰ used the average optical photon yield from
635 Radcliffe et al. in a model of video based EPIDs. This was further used to develop a model to determine optimal phosphor thickness⁴¹. The models and results presented here, for single crystal scintillators, could readily be incorporated into such a model to describe the optical photon yield from an array of such crystals.

640 **V. Conclusions**

Two models for calculating the light output from scintillators crystals have been compared. One is a Monte Carlo simulation of optical photon transport, previously presented and the other a description of a light guide with Lambertian faces. The Lambertian light guide models generally agree to within 5% with the Monte Carlo,

645 which was seen as a gold standard. Results show a variation in light output with
position of dose deposition and with scintillator length of typically a factor of two in
each case. Both models may be used to determine the variation in detector signal as a
function of detector thickness. Thus they are suited to detector optimization.

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Table Caption

760

Table 1: Values of difference in $\eta(N)$ between LLG and MC models for the six scintillator dimensions studied and for the two values of d_{sensor} . ‘max’ denotes the maximum absolute error value and ‘RMS’ denotes root mean square error.

765 **Table 1**

Cell Dimensions (mm ³)	d _{sensor} = 1 mm		d _{sensor} = 1000 mm	
	max	RMS	max	RMS
	(%)	(%)	(%)	(%)
1x3x3	0.74	0.31	9.94	4.79
1x1.5x1.5	0.73	0.33	13.15	4.50
5x3x3	0.32	0.21	10.56	3.78
5x1.5x1.5	1.75	1.01	5.51	4.16
10x3x3	1.47	0.89	6.07	3.93
10x1.5x1.5	7.21	4.40	7.68	4.39
10x1.5x1.5 (20 cells)	3.36	2.03	6.01	3.70

Figure Captions

770 **Figure 1:** Illustration of the multicell model. a) 3D representation of x-rays incident on entrance face of scintillator from above, showing cell labeling scheme and propagation of optical photons to the sensor. b) illustration of calculation of transport from point P in cell m to surfaces points in cell n in the LLG model. The number of photons interacting in cell n is equal to the number entering the cell, minus those
775 passing through to the cell beyond (shown by the 4 arrows for “Direct”). Left side shows “Direct” component from m to n . “Mirror” shows component from reflection at exit face. c) illustration of integration parameters n_{ave} (number of positions of P along each face of cell m) and n_{trap} (number of points used in trapezium integration) in the LLG model. Also shown is $\alpha_n^{f_m^{side}}$, probability of optical photon starting at the side
780 face of m , reflecting from the exit face and reaching n .

Figure 2: Values of the coefficients $C^{initial}$, C^{side} , C^{end} , $f^{initial}$, f^{side} , f^{end} in the LLG model as a function of cell number, for 20 component cells of width 1.5 mm, length 1.5 mm and depth 0.5 mm. The x axis is $/n-m/$. Points are defined for integer values, with the lines to aid the eye.

785 **Figure 3:** Illustration of the dependency of the model parameters, N_{cell} , n_{ave} and n_{trap} on the RMS error of the LLG model results compared to the MC model. a) shows results as a function of cell aspect ratio with $n_{ave} = 21$, and $n_{trap} = 100$ and 800 for d_{sensor} values of 1 mm (solid circles) and 1000 mm (open squares) respectively. Data are shown for $N_{cell} = 10$, except the larger symbols at the heads of the arrows, for
790 which $N_{cell} = 20$. The arrows are further discussed in the text. b) shows results for $n_{ave} = 21$ and $d_{sensor} = 1000$ mm as a function of n_{trap} .

Figure 4: Optical efficiency, $\eta(N)$, as a function of cell number where light originates for six CsI scintillator sizes. Monte Carlo model results are shown as

crosses joined by solid lines, to aid the eye, and Lambertian Light Guide model results
795 as open symbols joined by dashed lines. a) $d_{sensor} = 1$ mm. b) $d_{sensor} = 1000$ mm.

Figure 5: Percentage difference between Monte Carlo and Lambertian Light Guide models for a) $d_{sensor} = 1$ mm. b) $d_{sensor} = 1000$ mm. Results by cell number and the average over all cells. In a) “10x1.5x1.5 (20 cells)” denotes calculation using 20 cells for LLG and averaging to yield results for 10 cell. The solid lines at $\pm 1\%$ show
800 the standard deviation of the MC calculations.

Figure 6: a) DOSRZnrc calculations of dose per cell as a function of x-ray energy in MeV, E , and depth for a 10x3x3 mm³ CsI scintillator, split into 10 cells. Results are normalized for each energy so that the sum under each curve is 1. b) optical efficiency as a function of x-ray energy, summed over all cells, $\bar{\eta}_E$,
805 determined using LLG model. Solid symbols show results for $d_{sensor} = 1$ mm (left hand y axis) and open symbols for $d_{sensor} = 1000$ mm (right hand y axis). The lines are to aid the eye. c) results of a weighted sum of 6b over an example 6 MV spectrum, $\bar{\eta}_{beam}$, for CsI scintillators of 3x3 mm² cross-section and 1, 5 and 10 mm depth.

Figure 7: Optical efficiency, $\eta(N)$, as a function of distance from exit face for a
810 series of CsI scintillator thicknesses from 2 mm to 10 mm and 1.5x1.5 mm² cross section. a) $d_{sensor} = 1$ mm. b) $d_{sensor} = 1000$ mm. LLG model results are shown for constant cell thickness of 0.5 mm, by solid (even cell number) and dashed (odd cell number) lines. MC model results are shown for 10 cells, by solid (a and b) and open circles (a only) corresponding to solid and dashed line LLG results respectively. The
815 crossed points at 2 mm thickness in a) are the results of the LLG model for 10 cells and this thickness.

Figure 8: Example use of LLG model to calculate $\bar{\eta}_{beam}$, QE , DQE , s_{abs} , and s as a function of CsI scintillator thickness for a 6 MV beam spectrum. Scintillator cross section was $1.5 \times 1.5 \text{ mm}^2$. a) $d_{sensor} = 1 \text{ mm}$. b) $d_{sensor} = 1000 \text{ mm}$.

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