Photon diffusion in a homogeneous medium bounded externally or internally by an infinitely long circular cylindrical applicator. II. Quantitative examinations of the steady-state theory

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This is Part II of the work that examines photon diffusion in a homogenous medium enclosed by a concave circular cylindrical applicator or enclosing a convex circular cylindrical applicator. Part I of this work [J. Opt. Soc. Am. A 27, 648 (2010)] analytically examined the steady-state photon diffusion between a source and a detector for two specific cases: (1) the detector is placed only azimuthally with respect to the source, and (2) the detector is placed only longitudinally with respect to the source, in the infinitely long concave and convex applicator geometries. For the first case, it was predicted that the decay rate of photon fluence would become smaller in the concave geometry and greater in the convex geometry than that in the semi-infinite geometry for the same source–detector distance. For the second case, it was projected that the decay rate of photon fluence would be greater in the concave geometry and smaller in the convex geometry than that in the semi-infinite geometry for the same source–detector distance. This Part II of the work quantitatively examines these predictions from Part I through several approaches, including (a) the finite-element method, (b) the Monte Carlo simulation, and (c) experimental measurement. Despite that the quantitative examinations have to be conducted for finite cylinder applicators with large length-to-radius ratio to approximate the infinite-length condition modeled in Part I, the results obtained by these quantitative methods for two concave and three convex applicator dimensions validated the qualitative trend predicted by Part I and verified the quantitative accuracy of the analytic treatment of Part I in the diffusion regime of the measurement, at a given set of absorption and reduced scattering coefficients of the medium. © 2011 Optical Society of America

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1. INTRODUCTION

This is a continuation of the work that examines the photon diffusion in a homogenous medium that is either enclosed by or enclosing an infinitely long circular cylindrical applicator. The geometry of imaging a medium enclosed by an infinitely long circular cylindrical applicator resembles approximately that of imaging externally accessible tissue, such as breast or arm, using a ring-shaped applicator and is referred to as a concave geometry in this work. The geometry of imaging a medium enclosing a circular cylindrical applicator resembles closely that of imaging internally accessible tissue, such as prostate or rectum, using an endorectal applicator, and is referred to as a convex geometry in this work. In Part I [1] of this work, the solutions to the steady-state photon diffusion associated with concave and convex geometries were derived by employing the extrapolated boundary condition [2,3] and expressed in closed forms using the modified Bessel functions. The validity of the approach in [1], which has to our knowledge for the first time unified the analytic treatments of photon diffusion in both concave and convex geometries, was examined qualitatively for the case wherein the radial dimension of the tissue–applicator interface would reach infinity. As is expected, the decay rate of photon fluence for the case of applicator radius approaching infinity was found to asymptotically reach that for a planar interface case or the semi-infinite geometry. The analytic approach was then applied to the concave and convex geometries with the radial dimensions of the tissue–applicator interfaces comparable to those found in practical applications. For these practical geometries, the work in [1] further examined two specific configurations: (1) the source and the detector have the same longitudinal coordinate and are placed along the azimuth direction on the boundary, and (2) the source and the detector have the same azimuth angle and are placed along the longitudinal direction on the boundary. For case (1), which is called “case-azi” in this work, it was predicted that the decay rate of photon fluence would become smaller in the concave geometry and greater in the convex geometry than that in a semi-infinite geometry for the same source–detector distance. For case (2), which is called “case-longi” in this work, it was projected that the decay rate of photon fluence would be greater in the concave geometry and smaller in the convex geometry than that in a semi-infinite geometry for the same source–detector distance.

This Part II of the work examines the predictions given in Part I for steady-state photon diffusion in the case-azi and
case-longi configurations within the concave and convex geometries by the following quantitative methods: (a) the finite-element method (FEM), (b) the Monte Carlo (MC) simulation, and (c) experimental measurement. The predictions for case-azi and case-longi configurations in Part I, which were based upon solving the equation of photon diffusion analytically in the studied geometries, is to be first examined by solving the same equation of photon diffusion numerically in the same geometries using the widely validated FEM solver. It is expected that the FEM-based results will support the analytic solution that has been proposed, but as both the FEM and analytical solutions are based upon the model of photon diffusion, the expected model-data match between these two does not necessarily substantiate the validity of the analytic approach. The ultimate verification of any analytic approach of photon propagation requires examining it against experimental measurement or the gold standard numerical method of MC. Among the three quantitative methods of the FEM, the MC, and experimental measurement employed in this work, the experimental examination apparently has the least flexibility in the study design; therefore, it becomes rational to conduct the FEM and MC examinations by employing as many available parameters as possible for the experimental measurements. It is noted that the infinitely long cylindrical applicator modeled in Part I cannot be reproduced in any of the three methods of the FEM, the MC, and experimental examination, but it can be approximated by one cylindrical applicator whose longitudinal dimension is much greater than its radial dimension, e.g., with a large length-to-radius ratio.

The rest of this Part II work is structured into the following sections. Section 2 reprints the analytic results derived in Part I that are relevant to the predictions for case-azi and case-longi configurations. Section 3 details the configurations of the FEM, MC, and the experimental examinations. Section 4 evaluates the effects of the measurement errors associated with the positioning of the source and detector due to the limitations of the experimental study, and discusses the rationale of minimizing the error-induced data-model deviation when the experimental measurements are grouped with the FEM and the MC for examining the analytic predictions. Section 5 examines the analytic predictions of case-azi and case-longi configurations in two concave and three convex applicator dimensions against the FEM, MC, and experimental results, for a given set of medium optical properties.

2. RELEVANT ANALYTIC RESULTS DERIVED IN PART I

The following notations have been used in [1]: \( \vec{r}_0 = (R_0, \varphi, z') \) is the position of the source, \( \vec{r} = (R_0, \varphi, z) \) is the position of the field or the detector, \( S \) is the intensity of the source, \( \Psi \) is the photon fluence rate at the field/detector position, \( \mu_a \) is the absorption coefficient, \( \mu'_s \) is the reduced or transport scattering coefficient, \( D = [3(\mu_a + \mu'_s)]^{-1} \) is the diffusion coefficient, \( R_s = 1/\mu'_s \) is the mean path length for the photon to lose its history of incident direction and is used for modeling the directional source as an isotropic source placed into the medium, \( R_0 = 2AD \) is the distance from the extrapolated boundary to the physical boundary wherein \( A \) is a parameter determined by the refractive index mismatch across the tissue-applicator interface.

The steady-state photon fluence rate \( \Psi \) associated with a concave geometry of radius \( R_0 \) is

\[
\Psi = \frac{S}{2\pi^2 D} \int_0^\infty dk \left\{ \cos[k(z - z')] \times \sum_{m=0}^\infty \varepsilon_m I_m[k_{\text{eff}}(R_0 - R_s)]K_m(k_{\text{eff}}R_0) \right.
\]

\[
\left. - \left( 1 - \frac{I_m(k_{\text{eff}}R_0) K_m(k_{\text{eff}}R_0 + R_s)}{K_m(k_{\text{eff}}R_0) I_m[k_{\text{eff}}(R_0 + R_s)]} \right) \cos[m(\varphi - \varphi')] \right\},
\]

\[ (2.1c) \]

where \( I_m \) and \( K_m \) are the modified Bessel functions of the first and second kind at order \( m \), respectively. Similarly, the steady-state photon fluence rate \( \Psi \) associated with a convex geometry of radius \( R_0 \) is

\[
\Psi = \frac{S}{2\pi^2 D} \int_0^\infty dk \left\{ \cos[k(z - z')] \sum_{m=0}^\infty \varepsilon_m I_m(k_{\text{eff}}R_0) \times K_m[k_{\text{eff}}(R_0 + R_s)] \right. 
\]

\[
\left. \left( 1 - \frac{K_m(k_{\text{eff}}R_0) I_m[k_{\text{eff}}(R_0 - R_s)]}{I_m(k_{\text{eff}}R_0) K_m[k_{\text{eff}}(R_0 - R_s)]} \right) \cos[m(\varphi - \varphi')] \right\},
\]

\[ (2.1v) \]

For equations in (2.1), if the source and the detector locate at the same azimuth plane, e.g., in case-azi configuration, we have

\[
\Psi = \frac{S}{2\pi^2 D} \int_0^\infty dk \left\{ \sum_{m=0}^\infty \varepsilon_m I_m(k_{\text{eff}}(R_0 - R_s))K_m(k_{\text{eff}}R_0) \right. 
\]

\[
\left. - \frac{I_m(k_{\text{eff}}R_0) K_m[k_{\text{eff}}(R_0 + R_s)]}{K_m(k_{\text{eff}}R_0) I_m[k_{\text{eff}}(R_0 + R_s)]} \cos[m(\varphi - \varphi')] \right\},
\]

\[ (2.2c) \]

and if the source and the detector locate longitudinally with the same azimuth angle, e.g., in case-longi configuration, we have

\[
\Psi = \frac{S}{2\pi^2 D} \int_0^\infty dk \left\{ \cos[k(z - z')] \sum_{m=0}^\infty \varepsilon_m I_m[k_{\text{eff}}(R_0 - R_s)] \right. 
\]

\[
\left. - \frac{K_m(k_{\text{eff}}R_0) I_m[k_{\text{eff}}(R_0 - R_s)]}{I_m(k_{\text{eff}}R_0) K_m[k_{\text{eff}}(R_0 - R_s)]} \cos[m(\varphi - \varphi')] \right\},
\]

\[ (2.2v) \]
\[
\Psi = \frac{S}{2\pi D} \int_0^\infty dk \left\{ \cos[k(z-z')] \right\} \sum_{m=0}^\infty \epsilon_m I_m(k_{\text{eff}}R_0)K_m(k_{\text{eff}}R_0) \\
+ R_0) \left\{ 1 - K_m(k_{\text{eff}}R_0) I_m(k_{\text{eff}}(R_0 - R_0)) \right\} \\
\right\}. \\
(2.3\text{conV})
\]

3. CONFIGURATIONS OF THE QUANTITATIVE EXAMINATIONS

A. Configuration of the FEM Solver to the Equation of Photon Diffusion

The FEM-based computation [4,5] of photon diffusion is based on our work [6] of solving the equation of steady-state photon diffusion under a Rtyoe boundary condition using NIRFAST [7]. It is noted that the source term in the FEM is often defined as a distributed, Gaussian source, matching the intensity profile at the tip of the optical fiber, and the source may therefore be defined over more than one element [7]. The source term in the FEM is thus different from the basis of Green’s function in analytic treatt. This difference is expected to cause a mismatch between the FEM and analytical results as the source–detector distance becomes comparable to the spatial dimension of the Gaussian source even though both methods are based on the same model of photon propagation. The finite-element meshes for the case-azi and case-longi configurations of the concave geometry are shown in Figs. 1(a) and 1(b), respectively. Two sets of the concave geometry are considered: one has a radius of 0.95 cm and a length of 40 cm, and the other has a radius of 2.53 cm and a length of 40 cm. The radii of the two concave geometry sets are chosen the same as those used in the experiments, but the length-to-radius ratios of the two geometry sets are 2.62 times those employed in the experimental study as that in the concave geometry. The discretized domain of the convex geometry is illustrated in Fig. 1(d), which shows only the case-azi configuration and does not visualize the meshes at the outer surfaces for the purpose of clarification. The domain of FEM modeling with an inner radius of 1.27 cm is discretized into a mesh of 90,856 tetrahedral elements and 17,545 nodes. The domains of FEM modeling with inner radii of 2.31 cm and 5.07 cm are discretized into meshes of the same density as that in the radius of 1.27 cm. The value of A is experimentally determined (detailed in Subsection 3.D) as being 1.86 for the interface between the tissue/medium and the applicator.

B. Configuration of the Monte Carlo Simulation

The MC model was adapted from a program previously developed for simulating photon migration in cylindrical blood vessels [8]. The concave and convex geometries for MC simulation are illustrated in Fig. 2, with Figs. 2(a) and 2(c) for the case-azi configurations, and Figs. 2(b) and 2(d) for the case-longi configurations. For both case-azi and case-longi configurations, two sets of the concave applicator dimensions are considered: one has a radius of 0.95 cm and a length of 40 cm, and the other has a radius of 2.53 cm and a length of 40 cm; three sets of the convex applicator dimensions are considered: all have a longitudinal dimension of 40 cm and an outer radius of 15 cm, and the inner radii are 1.27 cm, 2.41 cm, and 5.07 cm. The radii of the three convex geometry sets are chosen the same as those found in the experiments, but the length-to-radius ratios of the three geometry sets are also 2.62 times those employed in the experimental study as that in the concave geometry. The discretized domain of the convex geometry is illustrated in Fig. 1(d), which shows only the case-azi configuration and does not visualize the meshes at the outer surfaces for the purpose of clarification. The domain of FEM modeling with an inner radius of 1.27 cm is discretized into a mesh of 90,856 tetrahedral elements and 17,545 nodes. The domains of FEM modeling with inner radii of 2.31 cm and 5.07 cm are discretized into meshes of the same density as that in the radius of 1.27 cm. The value of A is experimentally determined (detailed in Subsection 3.D) as being 1.86 for the interface between the tissue/medium and the applicator.
The experimentally determined value of $A = 1.86$ on the tissue-applicator interface is implemented in the MC as a 30% probability of photon re-entering the modeled tissue domain after reaching the applicator boundary. The number of incident photons ranged from $5 \times 10^7$ for convex geometry with a small radius to $2 \times 10^6$ for the concave geometry. All recordings had a smaller than 10% error (the ratio of the standard deviation to the mean).

C. Configuration of the Experimental Study
1. Dimensions of the Applicators in Concave and Convex Geometries
Five pieces of cylindrical applicators, shown schematically in Fig. 3(a) and photographed in Fig. 3(b), were fabricated from presorted 6 in. long (15.24 cm in length, compared to the 40 cm long imaging domain used for the FEM and the MC simulation) raw black acetal materials. These cylindrical pieces could be used for both concave and convex imaging geometries; however, due to the difficulty of fabricating both the external and internal surfaces of the same cylindrical applicator under identical machining processes to make the boundary conditions consistent, each piece was used for either the concave or convex imaging geometry, but not for both. Two applicator pieces with inner radii of 0.95 cm and 2.53 cm were used as the concave imaging geometry whereat the measurement was made along the inner surface [the dashed line on the two pieces at the lower row of Fig. 3(a)] enclosing the tissue medium, and three applicator pieces with outer radii of 1.27 cm, 2.41 cm, and 5.07 cm were used as the convex imaging geometry whereat the measurement was made along the outer surface [the solid line on the three pieces at the upper row of Fig. 3(a)] enclosed by the tissue medium. Therefore, for each group of case-azi or case-longi measurements, the results contained two sets from the concave geometries with different radii and three sets from the convex geometries with different radii.

2. Configuration of the Measurement Assembly Using the Cylindrical Applicator
The analytic treatments in [1] utilized a well-known important approach of modeling a directional illumination (from a fiber) as an isotropic source placed into the medium at a distance of $1/\mu_s$ from the directional incident point. The FEM solver adopted this approach of modeling a fiber illumination by simply placing an equivalent isotropic source at the $1/\mu_s$ distance into the medium. In the MC simulation, since the incident photon is strictly forward launched (pencil beam), the condition of an equivalent isotropic source at the $1/\mu_s$ distance is also satisfied. In the experimental study, placing the facet of an illumination fiber evenly on the applicator–tissue interface can mimic the condition of an equivalent isotropic source; however, the accuracy of the setup was limited by the variable practicability among the different applicator pieces employed and would not be as desirable as those in the FEM and MC studies. The examination of the analytic predictions for case-azi and case-longi configurations also was in need of continuously translating either the source or the detector fiber azimuthally or longitudinally, which further discouraged the experimental implementation that involved inserting a fiber in the wall of the applicator piece unless it was the only feasible choice. It has been argued that the measurement of a diffuse photon is insensitive to the orientation of the detector fiber [9]; nevertheless, using an isotropic detector shall provide measurement of the photon diffusion that is minimally affected by the orientation of the detector fiber. In light of all these restrictions, the experimental design physically placed a fiber with an isotropic diffuser tip as the source in the medium at a distance of $1/\mu_s$ from the tissue–applicator boundary, instead of inserting a regular fiber through the applicator wall, and used a fiber with isotropic sensing tip as the detector.

A diffuser (Medlight SD200) with a spherical tip of 2 mm in diameter was used as the isotropic source, and an isotropic probe (Medlight IP159) with a spherical tip of 1.59 cm in diameter was used for detection of the diffuse photon. The 785 nm light from a laser diode (Thorlabs, model HL7851G) operating at constant power mode was fiber-coupled to the spherical diffuser. The isotropic detector probe was coupled to a spectrometer (Princeton Instruments, SpectraPro 2300i, not necessary for the measurement but kept for system integrity and convenience of use) for readout of the detected photon intensity by a 16 bit CCD camera (Photometrics Cascade 512F).

The source and the detector fibers were fixed individually in stainless tubes [except for the detection fiber shown in the configuration in Fig. 6(a) only], which were then fixated to the positioning structure. The stainless tube for housing the source fiber had a diameter of 4.76 mm (3/16 in.) and the one for fixing the detector fiber had a diameter of 3.18 mm (1/8 in.). Figure 4 is an exemplary photograph of the complete setup for measurement of the case-azi configuration in the convex geometry, wherein the source and detector fibers were placed azimuthally and outside of the cylindrical
applicator at the same longitudinal coordinate. The entire positioning assembly as shown on the breadboard was then immersed in a large tank filled with bulk Intralipid solution as the homogenous medium.

3. Control of the Source-Detector Distance for Measurement in the Case-Azi Configuration

For the case-azi configuration in concave geometry as shown in Fig. 5(a), the isotropic detector was fixed at the inner surface of the cylindrical applicator, and the isotropic source was placed at a distance of $1/\mu_s'$ inward from the inner surface. The isotropic source rotated isozimuthally with respect to the isotropic detector and the center of the applicator curvature. The Intralipid solution filled the inside of the cylindrical applicator. For the case-azi configuration in convex geometry as shown in Fig. 5(b), both the isotropic source and detector were placed at the outer surface of the cylinder applicator, with the source placed at a distance of $1/\mu_s'$ outward from the outer surface. The isotropic source rotated isozimuthally with respect to the isotropic detector and the center of the applicator curvature. The Intralipid solution filled up the tank that housed the cylinder applicator. The azimuth plane that contains the source and the detector was halfway along the longitudinal working range of the cylinder applicator to minimize the effect of the finite length of the applicator. The chord distance $d$ between the positions of the modeled directional source and the detector on the applicator surface was calculated by $d = 2R\sin(\theta/2)$, where the angle $\theta$ between the azimuth coordinates of the source and the detector was directly read out from the rotational stage controlling the source position.

4. Control of the Source-Detector Distance for Measurement in the Case-Longi Configuration

For the case-longi configuration in concave geometry, as shown in Fig. 6(a), the isotropic detector fiber without the stainless tube passed through the wall of the cylindrical applicator and was fixed at the inner surface of the applicator. The isotropic source was placed at a distance of $1/\mu_s'$ inward from the inner surface of the applicator and translated longitudinally. The Intralipid solution filled the inside of the cylindrical applicator. For the case-longi configuration in convex geometry, as shown in Fig. 6(b), the cylindrical applicator was placed horizontally. The isotropic detector housed by the stainless tube was placed on the outer surface of the applicator. The isotropic source was placed at a distance of $1/\mu_s'$ outward from the outer surface and translated longitudinally with respect to the isotropic detector. The Intralipid solution filled the tank that housed the cylindrical applicator and most parts of the fiber-holding stainless tubes.

In the experimental study, all measurements were based on a bulk Intralipid solution of 0.5% concentration. This concentration of Intralipid solution gave $\mu_s' = 5\text{ cm}^{-1}$ at 785 nm [10], with which $1/\mu_s' = 2\text{ mm}$, so there was sufficient space to place the 1-mm radius spherical diffuse source away from the applicator surface, and the scattering-dominant condition was also satisfied as $\mu_s = 0.025\text{ cm}^{-1}$ [11]. Using a single concentration of the Intralipid solution undoubtedly limited the experimental examinations to a single set of $\mu_s$ and $\mu_s'$ of the medium properties; however, if the analytical treatment had been incorrect, none of the predictions made could have matched with the experimental results.

D. Experimental Determination of the A Value

In the experimental examinations, all of the parameters appearing in Eqs. (2.2conC), (2.2conV), (2.3conC), and (2.3conV) were known, except for the $A$ value appearing in $R_0 = 2AD$. $A$ is determined by the refractive index mismatch between an applicator material and the diffuse medium, usually based on the assumption of a tissue–air interface, even though that does not accurately represent the tissue–applicator interface. In this study, the $A$ value must be experimentally determined in order to assure the accuracy of model-data examination.

The determination of the $A$ value involved two steps. In the first step, the same set of isotropic diffuser source and detector as that used for the studies in Subsection 3.C were immersed in the same 0.5% Intralipid solution to form an infinite-medium geometry. The measurement of photon diffusion in this infinite-medium geometry was specified by the well-known formula [1] of

$$\ln(\Psi \cdot d) = -\frac{\mu_\text{imag}}{D} + \ln \left(\frac{S}{4\pi D}\right),$$

where $d$ is the source–detector distance. The source term $S/4\pi D$ or the intercept term $\ln(S/4\pi D)$ was found by fitting the experimental data to the linear relationship between $\ln(\Psi \cdot d)$ and $d$. In the second step, a semi-infinite geometry was constructed using a large plate of black acetal, which was materially the same as that used for the studies in Subsection 3.C. The measurement of photon diffusion in this semi-infinite-medium geometry was specified by the formulas [1,12] of

$$\Psi = \frac{S}{4\pi D_{\text{real}}} e^{-k_{\text{real}}l_{\text{real}}} - \frac{S}{4\pi D_{\text{imag}}} e^{-k_{\text{imag}}l_{\text{imag}}},$$
where
\[
\begin{align*}
I_{\text{real}} &= \sqrt{d^2 + R_a^2}, \quad R_a = 1/\mu_s, \\
I_{\text{imag}} &= \sqrt{d^2 + (2R_b + R_a)^2}, \quad R_b = 2AD.
\end{align*}
\] (3.3)

By substituting the value of $S/4\pi D$ obtained from (3.1) into (3.2) and fitting the experimental data $\Psi$ to different $A$ values, the $A$ value was determined as 1.86 after averaging four sets of measurements ($A = 1.897, 1.806, 1.905, 1.814$).

4. ANALYSIS OF THE MEASUREMENT ERROR ASSOCIATED WITH INACCURATE POSITIONING OF THE SOURCE AND DETECTOR

4.1 Effect of the Radial Positioning Errors of the Source and the Detector

In the analytic solutions, both the source and the detector are assumed as infinitesimally small, whereas the isotropic source and detector used in the experiments had finite sizes, specifically spherical tips with diameters of 2 mm and 1.59 mm, respectively. In all the experimental setups except the one shown in Fig. 6(a), the source and detector fibers were first fixed in stainless tubes, which were then fixed onto the positioning stages. Thus, the detector might not have been located precisely on the surface of the applicator, and the source might not have been positioned precisely $1/\mu_s$ from the surface of the applicator. To model how much the measurement could be affected due to the positioning error, Eqs. (2.1conC) and (2.1conV) are rewritten to

\[\Psi = \frac{S}{2\pi^2D} \int_0^\infty dk \left\{ \cos[k(z - z')] \sum_{m=0}^{\infty} e_m I_m(k_{\text{eff}r_c}) K_m(k_{\text{eff}r_c}) \cdot \left( 1 - \frac{I_m(k_{\text{eff}r_c}) K_m[k_{\text{eff}}(R_0 + R_b)]}{I_m[k_{\text{eff}}(R_0 + R_b)]} \right) \cos[m(\varphi - \varphi') \right\},\] (4.1conC)

\[\Psi = \frac{S}{2\pi^2D} \int_0^\infty dk \left\{ \cos[k(z - z')] \sum_{m=0}^{\infty} e_m I_m(k_{\text{eff}r_c}) K_m(k_{\text{eff}r_c}) \cdot \left( 1 - \frac{K_m(k_{\text{eff}r_c}) I_m[k_{\text{eff}}(R_0 - R_b)]}{K_m[k_{\text{eff}}(R_0 - R_b)]} \right) \cos[m(\varphi - \varphi') \right\},\] (4.1conV)

where $r_c$ and $r_r$ indicate the smaller and larger radial coordinates of the source and the detector. For the concave geometry, $r_c = R_0 - R_a$ and $r_r = R_0$, for the convex geometry, $r_c = R_0$ and $r_r = R_0 + R_b$ [1]. When there is positioning error for the source or the detector in the azimuth plane, the $r_c$ and $r_r$ for the concave geometry and convex geometry can be expressed, respectively, as

\[r_c = R_0 - R_a - \xi_{\text{source}}, \quad r_r = R_0 - \xi_{\text{detector}}, \] (4.2conC)

\[r_c = R_0 + \xi_{\text{detector}}, \quad r_r = R_0 + R_a + \xi_{\text{source}} \] (4.2conV)

where $\xi_{\text{subscript}}$ denotes the shift of the position of the subscript from the intended location in the azimuth plane. The details of $r_c$ and $r_r$ in the azimuth plane are shown in Figs. 7(a) and 7(b) for concave and convex geometry, respectively. By using the notations $r_c$ and $r_r$ defined in (4.2), Eqs. (2.2conC) and (2.2conV) for the case-azi configuration can be converted to

\[\Psi = \frac{S}{2\pi^2D} \int_0^\infty dk \left\{ \sum_{m=0}^{\infty} e_m I_m(k_{\text{eff}r_c}) K_m(k_{\text{eff}r_c}) \left( 1 - \frac{I_m(k_{\text{eff}r_c}) K_m[k_{\text{eff}}(R_0 + R_b)]}{I_m[k_{\text{eff}}(R_0 + R_b)]} \right) \cos[m(\varphi - \varphi')] \right\},\] (4.3conC)

\[\Psi = \frac{S}{2\pi^2D} \int_0^\infty dk \left\{ \sum_{m=0}^{\infty} e_m I_m(k_{\text{eff}r_c}) K_m(k_{\text{eff}r_c}) \left( 1 - \frac{K_m(k_{\text{eff}r_c}) I_m[k_{\text{eff}}(R_0 + R_b)]}{K_m[k_{\text{eff}}(R_0 + R_b)]} \right) \cos[m(\varphi - \varphi')] \right\},\] (4.3conV)

and Eqs. (2.3conC) and (2.3conV) for the case-longi configuration can be converted to

\[\Psi = \frac{S}{2\pi^2D} \int_0^\infty dk \left\{ \cos[k(z - z')] \right\} \times \sum_{m=0}^{\infty} e_m I_m(k_{\text{eff}r_c}) K_m(k_{\text{eff}r_c}) \left( 1 - \frac{I_m(k_{\text{eff}r_c}) K_m[k_{\text{eff}}(R_0 + R_b)]}{I_m[k_{\text{eff}}(R_0 + R_b)]} \right),\] (4.4conC)

\[\Psi = \frac{S}{2\pi^2D} \int_0^\infty dk \left\{ \cos[k(z - z')] \right\} \times \sum_{m=0}^{\infty} e_m I_m(k_{\text{eff}r_c}) K_m(k_{\text{eff}r_c}) \left( 1 - \frac{K_m(k_{\text{eff}r_c}) I_m[k_{\text{eff}}(R_0 - R_b)]}{K_m[k_{\text{eff}}(R_0 - R_b)]} \right),\] (4.4conV)

Equations (4.3conC), (4.3conV), (4.4conC), and (4.4conV) were numerically implemented by letting $\xi_{\text{detector}}$ change from 0 to 1 mm and $\xi_{\text{source}}$ change from -0.5 mm to 0.5 mm, to assess the effect of the positioning errors of the source and the detector in the azimuth plane within 1 mm, based on the set of parameters, including $\mu_s = 0.025$ cm$^{-1}$, $\mu_s' = 5$ cm$^{-1}$, $A = 1.86$, and $S = 1$. The concave geometry dimensions being evaluated had the radii of 0.95 cm and 2.53 cm, and the convex geometry dimensions being evaluated had the radii of 1.27 cm, 2.41 cm and 5.07 cm, as those studies in Section 3. The results for the case-azi configuration are shown in Fig. 8. Figure 8(a) presents the results for the source fixed but the detector shifted...
radially on the same azimuth plane by 0 mm, 0.5 mm, and 1 mm. Figure 8(b) presents the results for the detector fixed but the source shifted radially on the same azimuth plane by −0.5 mm, 0 mm, and 0.5 mm. For the evaluations in Fig. 8, the longitudinal positioning of the source and the detector has been assumed accurate. It is indicated from Figs. 8(a) and 8(b) that, for source–detector distances greater than approximately five times the transport mean free path length (≥5/μs = 1 cm in this case), the 1 mm radial positioning error of the source and the detector in the azimuth plane would have negligible effect upon the measurement of photon fluence. The results for the case-azi configuration are shown in Fig. 9. Figure 9(a) is for the source fixed but the detector shifted radially on the same azimuth plane by 0 mm, 0.5 mm, and 1 mm. Figure 9(b) is for the detector fixed but the source shifted radially on the same azimuth plane by −0.5 mm, 0 mm, and 0.5 mm. For the evaluations in Fig. 9, the longitudinal positioning of the source and the detector has been assumed accurate. Figures 9(a) and 9(b) again indicate that the 1 mm radial positioning error of the source and the detector has negligible effect to the measurements of photon fluence when the source-detector distance is greater than approximately five transport mean free path lengths (≥5/μs). Based on Figs. 8 and 9, it was expected that the experimental measurement in the diffusion regime of the given setup should be insensitive to small inaccuracy of the radial positions of the source and the detector.

B. Effect of the Initial Error of the Source–Detector Distance

In the analytical evaluation, the source–detector distance is precisely determined. In the experimental measurement, either the source or the detector was fixed, and the other was translated continuously starting from an initial value of source–detector distance that was subjected to an error. The effect due to the error of this initial measurement of source–detector distance is investigated in Figs. 10(a) and 10(b). The evaluations are similar to those in Figs. 8 and 9, with the changes being made from varying the radial position of the source or the detector to instead increasing or decreasing the initial source–detector distances, respectively, by 0 mm, 0.5 mm, and 1 mm. The curves shown in Figs. 10(a) and 10(b) have been shifted vertically with respect to the one with the defined initial distance to give more direct comparisons. It is indicated from Fig. 10 that, for both the case-azi and case-longi configurations, the effect of the error of the initial source–detector distance resembles changing the radius of the cylindrical applicator as demonstrated in Fig. 8 for the case-azi and Fig. 11 for the case-longi configurations in Part I of this work [1]. This agrees with the expectation that the measurement of the
photon fluence decay will be sensitive to the initial source–detector distance, but it also implies that experimental measurements with an uncertainty of the initial source–detector distance is justifiable using analytical predictions by slightly varying the radius parameter in the computation.

5. RESULTS OF QUANTITATIVE EXAMINATION

This section compares the analytic predictions made for the case-azi and case-longi configurations with respect to the results obtained from the FEM, the MC, and the experimental examinations. The differences in the source intensity settings in all of these quantitative measurements were compensated by a vertical shift for each of them in Fig. 11 in order to compare with the analytic predictions. The results for the case-azi configuration are given in Fig. 11(a). The shortest source–detector distance implemented in the analytic predictions, the FEM, and the MC simulations were seen as at or below 0.1 cm, but that in the experimental examinations had been at approximately 1 cm. This was due to the consideration of maximizing the measurement consistency, because each set of data corresponding to the available range of source–detector distance was acquired by setting the source power and CCD gain as fixed, rather than as variable to only accommodate a larger dynamic range. As indicated previously, the measurement of the initial source–detector distance was subjected to an error due to the spherical diffuser tips as well as other experimental limitations, but the error was controlled to be within 0.9 mm for the case-azi and 0.5 mm for the case-longi configurations.

The decay rate of photon fluence for the case-azi configuration made by analytic predictions was compared with those by the FEM, the MC, and the experimental examinations in Fig. 11(a). The data are plotted for $\ln(\psi d^2)$ as a function of $d$ to verify the different trends of photon fluence decay expected for the concave and convex geometries, with respect to that for a semi-infinite medium, which is largely linear over the entire range of source–detector distance. It was predicted analytically that the decay rate of photon fluence of the case-azi configuration in concave geometry would be smaller than that in the semi-infinite medium, which was expected as the decreasing magnitude of the curve’s slope toward longer source–detector distance, e.g., the curve becoming upward bended. It had also been predicted analytically that the decay rate of photon fluence of the case-azi configuration in convex geometry would be greater than that in the semi-infinite medium, which was expected as the increasing magnitude of the curve’s slope toward longer source–detector distance, e.g., the curve becoming downward bended. For the case-azi...
configurations of concave geometry and convex geometry that have the same radius parameter, it has also been predicted that the deviation of the upward-bending curve of concave geometry from the semi-infinite line (e.g., the magnitude of the slope difference between them) is smaller than that of the downward-bending curve of convex geometry from the semi-infinite line. The comparison for the decay rate of photon fluence for the case-longi configuration is shown in Fig. 11(b). Contrary to that in the case-azi configuration, in the concave geometry, the decay rate of photon fluence is larger than that in the semi-infinite medium, and in the convex geometry, the decay rate of photon fluence is smaller than that in the semi-infinite medium. However, for both the concave and convex geometries, the slope of the curve in either concave or convex geometry tends to be largely constant, with the slope of concave geometry greater in magnitude than that of semi-infinite medium and the slope of convex geometry smaller in magnitude than that of semi-infinite medium.

It was observed that the analytical, the FEM, the MC, and the experimental measurements agree with each other qualitatively, in terms of the pattern of deviation from the semi-infinite geometry, for the entire range of source–detector distances investigated for both case-azi and case-longi configurations. For source–detector distances greater than approximately five times of the transport mean free path, the results from the four methods agree quantitatively with each other.

6. DISCUSSION
Numerous studies have demonstrated that the assumption of a spherically isotropic source in the diffusion model accurately reflects experimental data when the source is centered one transport scattering distance within the medium from the boundary. This type of equivalent representation of a directional source by an inwardly displaced isotropic source can well quantify the fluence rate at distances greater than 3–5 transport scattering lengths from the source [15]. The agreement shown in this work among the four methods, for a considerable range of source–detector separations as long as they are greater than approximately five transport scattering lengths, is again supportive of the diffusion treatment of directional source using a spherically isotropic source placed one transport scattering distance into the medium, even for concave or convex geometries with a considerably small radius.

At the subdiffusion regime, a disagreement is expected between diffusion model and experimental result, which in this work has been carried out by the MC simulation, as physical measurement for the given geometries became impractical at source–detector distances shorter than approximately five transport scattering lengths. Between the diffusion-based analytical quantification and the FEM simulation for the subdiffusion regime, however, the analytical result is slightly closer to the MC results than the FEM simulation is. This is largely due to the fact that, for the given spatial dimension, the spatial impulse source employed in the analytical solution is physically analogous to the launching of strictly forward-directional photons at a single point in the MC simulation, whereas the size effect of the spatially distributed Gaussian source profile implemented in the FEM is manifested at shorter distances from the source. Besides, our treatment of boundary effect, e.g., the probability of a boundary-reaching photon returning to the medium, in the MC simulation was based on the experimental measurements by use of extrapolated boundary condition as in the analytical model, whereas a Robin-type boundary condition was used by the FEM. The subtle difference in the boundary conditions could have been amplified at the subdiffusion regime.

The analytic model investigated in [1] and utilized in this work assumes that the cylindrical applicator is infinitely long, whereas the one tested in our experiments has finite length. For the case-azi configurations shown in Fig. 11(a), all experimental measurements have been confined in an azimuth plane that is several centimeters away from the edge of the applicator. The results in Fig. 11(a) show no noticeable edge effect, which is specified as the degree of the model-data mismatch being proportional to the radius of the applicator. For the case-longi configuration shown in Fig. 11(b), either the source or detector has been translated 4 cm from the middle of the applicator toward the edge, and the edge effect may be perceived as a slightly larger deviation of the experimental data from the analytical predictions for a larger applicator radius that gives smaller length-to-radius ratio. The effect of the finite length of the applicator may be accounted for by considering the effects of two additional image sources of the physical source, with respect to the two longitudinal boundary facets, or modeled rigorously by deriving the Green’s function specific to the geometry of a finite cylindrical applicator. In fact, Liemert and Kienle[14] have had extensive analysis of photon diffusion in finite concave cylindrical applicator geometry for time-domain and frequency-domain measurements. Their derivation of the Green’s function for the time-domain or frequency-domain photon diffusion in the finite concave geometry used the cosine transform and Hankel transform, which can be readily extended to finite convex applicator geometry to understand time-domain or frequency-domain photon diffusion in a geometry similar to that investigated in our experiments. Our analytic approach in [1] has been for the steady-state photon diffusion only by expanding the Green’s function in Fourier series and Fourier transform; however, our approach provides the first insights for the models of photon diffusion in both concave and convex geometries. The analytic treatment in [1] involved a real k in the solution of steady-state photon diffusion. By implementing a complex k in the analytic process, the approach may be extended to frequency-domain analysis for both concave and convex geometries, but for time-domain analysis, the method of Liemert and Kienle [14] may be the method to follow. The approaches by Liemert and Kienle [14] and that demonstrated in [1] are complimentary and when combined may render analytic solutions to more geometries and measurement conditions.

Our unified modeling of both concave and convex geometries has given us the opportunity of observing some previously less-known patterns of photon diffusion associated with a cylindrical applicator. Figure 11 verified that, for the specific case of having the source and detector located azimuthally on the same axial plane, the decay rate of photon fluence is smaller in the concave geometry and greater in the convex geometry than that in the semi-infinite geometry for the same source–detector distance. For the specific case of having the source and detector located longitudinally with the same azimuth angle, the decay rate of photon fluence is greater in the concave geometry and smaller in the convex geometry than that in the semi-infinite geometry for the same source–detector...
distance. These interesting findings imply the existence of a potentially spiral direction on the surface of both the concave cylindrical applicator and the convex cylindrical applicator, along which the decay rate of photon fluence could be equivalent to that in a planar surface or a semi-infinite geometry. This interesting phenomenon of photon diffusion that may associate with a cylindrical applicator is predicted as “spiral-planar equivalence.” If the existence of such a planar-equivalent spiral direction inside or outside a cylindrical applicator is verified, for certain transluminal sensing or imaging applications, the semi-infinite geometry may be implemented for greatly simplified modeling and rapid recovery of tissue optical properties. Work is ongoing to investigate the validity of the hypothesis of a spiral-planar equivalence phenomenon.

7. CONCLUSION

Part I of this work analytically examined the steady-state photon diffusion along the azimuth direction or the case-azi configuration and the longitudinal direction or case-longi configuration, in the infinitely long concave and convex applicator geometries. This Part II of the work quantitatively examined the predictions of Part I for the case-azi configuration that the decay rate of photon fluence would become smaller in the concave geometry and greater in the convex geometry than that in the semi-infinite geometry for the same source–detector distance. This Part II work also examined predictions of Part I for the case-longi configuration, which suggested that the decay rate of photon fluence would be greater in the concave geometry and smaller in the convex geometry than that in the semi-infinite geometry for the same source–detector distance. The results of three quantitative examination approaches, including (a) the FEM, (b) the MC simulation, and (c) experimental measurement on finite cylindrical-applicator geometries with large a length-to-radius ratio, validated the qualitative trend predicted by Part I and verified the quantitative accuracy of the analytic treatment of Part I in the diffusion regime of the measurement, at a given set of absorption and reduced scattering coefficients of the medium.

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