Photon diffusion in a homogeneous medium bounded externally or internally by an infinitely long circular cylindrical applicator. III. Synthetic study of continuous-wave photon fluence rate along unique spiral paths

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This is Part III of the work that examines photon diffusion in a scattering-dominant medium enclosed by a “concave” circular cylindrical applicator or enclosing a “convex” circular cylindrical applicator. In Part II of this work Zhang et al. [J. Opt. Soc. Am. A 28, 66 (2011)] predicted that, on the tissue-applicator interface of either “concave” or “convex” geometry, there exists a unique set of spiral paths, along which the steady-state photon fluence rate decays at a rate equal to that along a straight line on a planar semi-infinite interface, for the same line-of-sight source–detector distance. This phenomenon of steady-state photon diffusion is referred to as “straight-line-resembling-spiral paths” (abbreviated as “spiral paths”). This Part III study develops analytic approaches to the spiral paths associated with geometry of a large radial dimension and presents spiral paths found numerically for geometry of a small radial dimension. This Part III study also examines whether the spiral paths associated with a homogeneous medium are a good approximation for the medium containing heterogeneity. The heterogeneity is limited to an anomaly that is aligned azimuthally with the spiral paths and has either positive or negative contrast of the absorption or scattering coefficient over the background medium. For a weak-contrast anomaly the perturbation by it to the photon fluence rate along the spiral paths is found by applying a well-established perturbation of the absorption or scattering coefficient over the background medium. For a strong-contrast anomaly the change by it to the photon fluence rate along the spiral paths is computed using the finite-element method. For the investigated heterogeneous-medium cases the photon fluence rate along the homogeneous-medium associated spiral paths is macroscopically indistinguishable from, and microscopically close to, that along a straight line on a planar semi-infinite interface. © 2012 Optical Society of America

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1. INTRODUCTION

The diffusion process is used to describe many types of particles or energy transfer in scattering media, including photon propagation in biological tissue [1], charge-carrier conveyance in semiconducting material [2], and neutron navigation in a nuclear reactor [3]. The diffusion model also applies to observances such as harmonic mass-transport [4], modulated eddy current [5], thermal waves [6], and the still-controversial viscosity waves [7]. Accurate and accessible quantitation of diffusion is fundamental to probing the properties of associated media and predicting processes [8].

Characterization of the diffusion in a medium nondestructively is often done through surface measurements, in which the particle or energy for transport is launched into the medium, and then the measured diffuse fluence rate is compared against a model-predicted value. Numerical computation based on accurate analytic modeling of diffusion in a nondestructive probing configuration is nontrivial even for a homogeneous medium within a seemingly regular boundary. For the instances of interrogating biological tissue, one could easily find rigorous analytic models of photon diffusion in a homogeneous medium bounded by various shapes of applicator-tissue interface [9]. However, direct numerical implementation of these analytic entities for characterizing the diffusion is daunting; therefore alternative numerical approaches, including the Monte Carlo (MC) method [10], the finite-element method (FEM) [11], and the finite difference method [12], have been used.

In regard to photon diffusion for noninvasive biological imaging applications, arguably the simplest geometry approximated is that of an infinite planar volume of tissue interfaced with an infinite planar applicator—such is a “semi-infinite” geometry [13], of which the photon fluence rate between a source-detector pair on the interface is determined “straight-forwardly” by the line-of-sight distance between the positions of a source and a detector [14] for a given set of associated optical properties. In practice, however, the imaging configurations commonly encountered could be idealized by either a “concave” geometry, wherein the photon probes the regime inner to a cylindrical tissue-applicator interface, or a “convex” geometry, wherein the photon probes the regime outside a cylindrical tissue-applicator interface. These three geometries of approximating the tissue-applicator interface are illustrated in Fig. 1(A). The photon fluence rate associated with any source-detector paths along the interface in either concave or convex geometry likely will differ from the fluence rate along a “straight” line on a semi-infinite interface for the same line-of-sight source–detector distance; however, analytic treatments
for both concave and convex geometries that can be conveniently translated to quantitative evaluations had been, to our knowledge, absent.

In Part I of this study [15] we introduced an analytic approach to steady-state photon diffusion in both concave and convex geometries of an infinitely long cylinder applicator. The analytic results to both concave and convex geometries are similar in the format, with the actual geometry accounted for by the differences in three aspects, including the sequence of the kinds of the modified Bessel functions in a term, the sequence of the terms with and without those modified Bessel functions, and the arguments of the modified Bessel functions containing the radial coordinates of the extrapolated boundary and the equivalent isotropic source.

For both concave and convex geometries, there are apparently two specific configurations for evaluating the photon fluence rate on the tissue-applicator interface: (1) a case-azi configuration as shown in Fig. 1(B), wherein the position of the photon launching into the tissue and the position of the detector are at the same azimuthal plane; (2) a case-longi configuration as shown in Fig. 1(C), wherein the position of the photon launching into the tissue and the position of the detector are at the same longitudinal plane. It is straightforward to appreciate that, as the radial dimension of either the concave or the convex geometry reaches infinity, both case-azi and case-longi configurations will become the case of a straight line on a semi-infinite interface.

For either the concave or the convex geometry of the radius at the order of centimeters, the photon fluence rates associated with both case-azi and case-longi configurations have been investigated, with respect to the fluence rate along a straight line on a semi-infinite interface, in Part II of this study [16]. The analytic solution to the photon diffusion equation for the idealized concave and convex geometries being demonstrated in Part I was first numerically evaluated and then validated against the FEM solution to the same photon diffusion equation, MC simulation, and experimental measurements, all made in geometries identical to the two idealized ones except with a finite length of the cylinder. For the concave geometry it is found that the photon fluence for the case-azi configuration decays slower than the photon fluence along a straight line on a semi-infinite interface, and the photon fluence for the case-longi configuration decays faster than the photon fluence along a straight line on a semi-infinite interface, for the same line-of-sight source–detector distance. Conversely, for the convex geometry it is found that the photon fluence for the case-azi configuration decays faster than the photon fluence along a straight line on a semi-infinite interface, and the photon fluence for the case-longi configuration decays slower than the photon fluence along a straight line on a semi-infinite interface, for the same line-of-sight source–detector distance. These findings suggest that on either a concave or a convex interface there exists a set of directions that are oblique to the azimuthal and longitudinal directions (thereby spirally shaped), along which the photon fluence decays at a rate equal to that along a straight line on a semi-infinite interface, for the same line-of-sight source–detector distance. Such a phenomenon, referred to as “straight-line-resembling-spiral paths” of the photon fluence rate associated with concave or convex geometry, was first rationalized in Part II of this study [16].

Note that the straight-line-resembling-spiral paths should not be exclusive to photon diffusion. As long as the energy or particle transfer undergoes diffusion loss in the medium, and the medium-applicator interface imposes “lossy” boundary conditions, the straight-line-resembling-spiral paths likely would occur for cylindrical interfacing cases.

Recently the straight-line-resembling-spiral paths of photon fluence rate (hereafter abbreviated as “spiral paths”) associated with concave or convex geometries were demonstrated for homogeneous-medium conditions in [17]. In [17] the existence of such spiral paths was shown through analytic treatments for concave and convex geometries of large radii that rendered favorable analytic approximations, and through numerical methods for concave and convex geometries of smaller practical dimensions. A rigorous accounting of the approximation leading to the analytic representation of the shown spiral paths for concave or convex geometries of large radii, which was not included in [17] owing to the length limit, could shed light on the pattern of spiral paths found numerically for concave or convex geometry of smaller practical radii. As the spiral paths have been shown to exist in concave or convex geometries with homogeneous-medium conditions, it would also be interesting to question whether the spiral paths found for the homogeneous medium would hold for the same geometry if the medium contains heterogeneity. Such issues are among the topics of Part III of this study.

Part III of the study consists of the following sections: Section 2 details the approach leading to the analytic representation of the spiral paths for concave and convex geometries of large radius with homogeneous-medium conditions. Section 3 summarizes the numerical approach used in [17] to find the spiral paths for concave and convex geometries of smaller radius with homogeneous-medium conditions. Section 4 employs the Born approximation to analyze the perturbation introduced to the photon fluence rate by a single heterogeneity with contrast in absorption ($\mu_s$) and reduced scattering ($\mu_t$). A mistake seen in analytic descriptions of some previous works regarding the sign associated with a scattering perturbation term is identified. Section 5 implements numerically the analytic results from Section 4 to
the case of single heterogeneity with weak perturbation strength, to examine the photon fluence rate along the spiral paths identified for the otherwise homogeneous medium. Section 6 quantifies the effect of single heterogeneity of strong perturbation strength on the photon fluence rate along the spiral paths identified for the otherwise homogeneous medium, by the use of FEM. Both Secs. 5 and 6 limit the evaluations to the case of single heterogeneity aligned azimuthally with the spiral paths; however, four cases of the contrast of the heterogeneity are considered: (1) positive absorption contrast, (2) negative absorption contrast, (3) positive reduced-scattering contrast, and (4) negative reduced-scattering contrast. Section 7 discusses the dependence of the spiral paths upon the optical properties of the homogeneous medium as well as the radial dimension of the concave or convex geometry.

2. SPIRAL PATHS ASSOCIATED WITH CONCAVE AND CONVEX GEOMETRIES OF LARGE RADI

This section derives the analytic representation of the spiral paths for concave and convex geometries of a large radial dimension. We assume that the radial dimension is substantially greater than the source-detector distance, which is also much greater than the scattering path length. These assumptions are necessary to simplify the photon fluence to a form from which the analytic profile of the spiral paths could be reached.

The general case of a source and a detector located on the tissue-applicator interface is illustrated in Figs. 2(A) and 2(B), for concave and convex geometries, respectively. The tissue enclosed by the interface in the concave geometry or enclosing the interface in the convex geometry has an absorption coefficient \( \mu_a \), a reduced-scattering coefficient \( \mu_s' \), a diffusion coefficient \( D \), and an effective attenuation coefficient \( k_0 = \sqrt{\mu_a/D} \). The radius of the infinitely long circular cylindrical interface is \( R_0 \); therefore, by cylindrical coordinates, the source with an intensity of \( S \) locates at \((R_0, 0, 0)\) and the detector locates at \((R_0, \phi, z)\). The line-of-sight distance between the source \((R_0, 0, 0)\) and the detector \((R_0, \phi, z)\) is denoted by \( d \). The projection of \( d \) to the azimuthal plane or the projection of \( d \) perpendicular to the longitudinal axis of the cylindrical interface is denoted as \( d_\perp = d \cdot \cos \alpha \), where \( \alpha \) is the angle between \( d \) and \( d_\perp \). The position of the detector with respect to the source can then be represented by \((a, d_\perp)\). If keeping the source fixed at \((R_0, 0, 0)\) and increasing the radius \( R_0 \), the detector will eventually reach a plane that is tangential to the shown cylindrical interface and intersects with the interface at the longitudinal line crossing the source \((R_0, 0, 0)\). Such a plane forms the semi-infinite geometry limit of the concave or convex geometry [15].

A. Analytic Representation of the Spiral Paths Associated with Concave Geometry of Large Radii

Consider the concave geometry shown in Fig. 2(A). The source illuminating into the tissue at \((R_0, 0, 0)\) can be represented by an isotropic source at \((R_0 - R_a, 0, 0)\), where \( R_a = 1/\mu_a \). An extrapolated boundary in the imaginary “semi-infinite geometry” will be placed at \( R_b = 2AD \), where \( A \) is a parameter determined by the refractive index mismatch across the tissue-applicator interface, outward from the source \((R_0, 0, 0)\). For the equivalent isotropic source at \((R_0 - R_a, 0, 0)\), its image source with respect to the extrapolated boundary of the imaginary “semi-infinite geometry” locates at \((R_0 + R_a + 2R_b, 0, 0)\).

Denote \( l_r \) as the distance from the detector \((R_0, \phi, z)\) to the equivalent “real” isotropic source at \((R_0 - R_a, 0, 0)\), and \( l_i \) as the distance from the detector \((R_0, \phi, z)\) to the “image” source \((R_0 + R_a + 2R_b, 0, 0)\) associated with the imaginary semi-infinite geometry. For \( R_0 \gg d \gg R_a, R_b \), the photon fluence rate at the detector position can be expressed by [15]

\[
\Psi = \frac{S}{4\pi D} \left( e^{k_0 l_i} - e^{k_0 l_r} \right) \frac{R_0 + R_a + 2R_b}{R_0 - R_a},
\]

(1)

and we have

\[
l_r = d \sqrt{1 + \frac{R_a^2}{d^2} \left( \frac{R_a}{\cos \alpha} \right)^2}.
\]

(2)

Fig. 2. (Color online) Notations and physical entities of concave or convex geometry for analytic evaluation of photon fluence rate associated with larger radius. (A) The tissue is at the concave side of the circular cylindrical tissue-applicator interface, so the equivalent isotropic source of the physical source that illuminates into the medium is located closer to the center axis than the physical source is. (B) The tissue is at the convex side of the circular cylindrical tissue-applicator interface, so the equivalent isotropic source of the physical source that illuminates into the medium is located farther from the center axis than the physical source is.
\[ l_i = d \sqrt{1 + \left( \frac{(R_s + 2R_b)^2}{d^2} + \frac{R_s + 2R_b}{R_0} (\cos \alpha)^2 \right)}. \] (3)

Since
\[ \sqrt{\frac{R_0 + R_s + 2R_b}{R_0 - R_s}} = \left( 1 + \frac{2R_s + 2R_b}{R_0 - R_s} \right)^{1/2} = 1 + \frac{R_s + R_b}{R_0 - R_s} \] (4)

and for \( d \gg R_s, R_b \) one has \( k_0d \gg 1 \), so Taylor-series expansion gives
\[ \frac{e^{-k_0d}}{d^{\sqrt{1 + \Delta}}} = \frac{e^{-k_0d}}{d} \left[ 1 - \frac{1}{2} \left( k_0d + 1 \right) \Delta \right] = \frac{e^{-k_0d}}{d} \left[ 1 - \frac{1}{2} (k_0d) \Delta \right]. \] (5)

where \( \Delta \ll 1 \). Using Eqs. (2) to (5), Eq. (1) simplifies to
\[ \Psi = \frac{S}{4\pi D} \frac{e^{-k_0d}}{d} \left[ \left[ 1 - \frac{1}{2} k_0d \left( \frac{R_s + 2R_b}{d^2} + \frac{R_s + 2R_b}{R_0} (\cos \alpha)^2 \right) \right] \right. \\
- \left[ 1 - \frac{1}{2} k_0d \left( \frac{(R_s + 2R_b)^2}{d^2} + \frac{R_s + 2R_b}{R_0} (\cos \alpha)^2 \right) \right] \\
\times \left. \left( 1 + \frac{R_s + R_b}{R_0 - R_s} \right) \right]. \] (6)

which can be further derived to the form of (the derivation is detailed in Appendix \( \Delta \))
\[ \frac{\partial \ln (\Psi \cdot d^2)}{\partial d} = - \left\{ k_0 + \frac{1}{2k_0R_b(R_0 - R_s)} \left[ \frac{2R_0 - R_s + 2R_b}{2R_bR_b(R_0 - R_s)} \right] \cos \alpha \cdot d \right\}. \] (7)

Equation (7) characterizes the decay rate of photon fluence along the direction defined by angle \( \alpha \), with respect to the line-of-sight source–detector distance \( d \). For the case-longi configuration, the detector locates at \((R_0, 0, z)\), so \( \alpha = \pi/2 \) and \( d_{\bot} = 0 \), and then Eq. (7) becomes
\[ \frac{\partial \ln (\Psi \cdot d^2)}{\partial d} = - \left\{ k_0 + \frac{1}{2k_0R_b(R_0 - R_s)} \left[ \frac{2R_0 - R_s + 2R_b}{2R_bR_b(R_0 - R_s)} \right] \right\}. \] (8)

For the case-azi configuration, the detector locates at \((R_0, \phi, 0)\), so \( \alpha = 0 \) and \( d_{\bot} = d \), and then Eq. (7) becomes
\[ \frac{\partial \ln (\Psi \cdot d^2)}{\partial d} = \left\{ k_0 + \frac{1}{2k_0R_b(R_0 - R_s)} \left[ \frac{2R_0 - R_s + 2R_b}{2R_bR_b(R_0 - R_s)} \right] \right\}. \] (9)

The first term \( k_0 \) in the right-hand side of Eqs. (8) and (9) characterizes the decay rate of photon fluence along a straight line on a semi-infinite interface. It is clear by Eq. (8) that the photon fluence along the longitudinal direction on a concave interface decays faster than the photon fluence along a straight line on the semi-infinite interface. However, the decay rate of photon fluence (comparing to \( k_0 \)) along the azimuthal direction on a concave interface as described by Eq. (9) is implicit owing to the two terms of opposite signs after \( k_0 \). It can be shown that the third term at the right-hand side of Eq. (9) is greater in magnitude than the second term for a general diffusion regime; therefore Eq. (9) actually accounts for the smaller decay rate of photon fluence along the azimuthal direction on a concave interface than that along a straight line on the semi-infinite interface.

From Eq. (7) it is straightforward to conclude that if the coordinates of the detector \((\alpha, d_{\bot})\) with respect to the source satisfy the condition of
\[ \cos \alpha = \frac{1}{k_0d_{\bot}} \frac{R_0}{2R_0 - R_s + 2R_b}. \] (10)

then the decay rate of photon fluence over the line-of-sight source–detector distance \( d \) on the concave interface is identical to that over the same \( d \) on the semi-infinite interface. Equation (10) implies that \( \alpha \) changes as the detector displaces azimuthally away from the source.

B. Analytic Representation of the Spiral Paths Associated with Convex Geometry of Large Radii
Consider the convex geometry shown in Fig. 2(B). A source illuminating into the tissue at \((R_0, 0, 0)\) can be represented by an isotropic source at \((R_0 + R_s, 0, 0)\). An extrapolated boundary in the imaginary "semi-infinite geometry" will be placed at \( R_s = 2AD \) inward from the source \((R_0, 0, 0)\). For the equivalent isotropic source at \((R_0 + R_s, 0, 0)\), its image source with respect to the extrapolated boundary of the imaginary "semi-infinite geometry" locates at \((R_0 - R_s - 2R_b, 0, 0)\).

Denote \( l_s \) as the distance from the detector \((R_0, \phi, z)\) to the equivalent “real” isotropic source at \((R_0 + R_s, 0, 0)\), and \( l_i \) as the distance from the detector \((R_0, \phi, z)\) to the “image” source \((R_0 - R_s - 2R_b, 0, 0)\) associated with the imaginary semi-infinite geometry. For \( R_0 \gg d \gg R_s, R_b \), the photon fluence rate at the detector position can be expressed by [15]
\[ \Psi = \frac{S}{4\pi D} \frac{e^{-k_0l_s}}{l_s} - \frac{S}{4\pi D} \frac{e^{-k_0l_i}}{l_i} \frac{2R_0 - R_s - 2R_b}{R_0 + R_s}. \] (11)

and we have
\[ l_r = d \sqrt{1 + \left( \frac{(R_s + 2R_b)^2}{d^2} + \frac{R_s + 2R_b}{R_0} (\cos \alpha)^2 \right)}. \] (12)

\[ l_i = d \sqrt{1 + \left( \frac{(R_s + 2R_b)^2}{d^2} - \frac{R_s + 2R_b}{R_0} (\cos \alpha)^2 \right)}. \] (13)

Since
\[ \sqrt{\frac{R_0 - R_s - 2R_b}{R_0 + R_s}} = \left( 1 - \frac{2R_s + 2R_b}{R_0 + R_s} \right)^{1/2} = 1 - \frac{R_s + R_b}{R_0 + R_s}. \] (14)

using Eqs. (12) to (14) and (5), Eq. (11) simplifies to
\[
\Psi = \frac{S}{4\pi D} e^{-kd} \left\{ \left[ 1 - \frac{1}{2} k_0 d \left( \frac{R_0^2}{d^2} + \frac{R_a}{R_0} (\cos \alpha)^2 \right) \right] \right. \\
\left. - \left[ 1 - \frac{1}{2} k_0 d \left( \frac{(R_a + R_b)^2}{d^2} - \frac{R_a + 2R_b}{R_0} (\cos \alpha)^2 \right) \right] (1 - \frac{R_a + R_b}{R_0 + R_a}) \right\},
\]

(15)

which can be further derived to the form of (the derivation is detailed in Appendix B)

\[
\frac{\partial \ln(\Psi \cdot d^2)}{\partial d} = -\left\{ k_0 - \frac{1}{2k_0 R_a} \left( \frac{R_a + R_b}{R_0 + R_a} \right) \right. \\
+ \left. \left[ \frac{2R_0 + R_a - 2R_b}{2R_0 R_a (R_0 + R_a)} \right] \cos \alpha \cdot d_{\perp} \right\}.
\]

(16)

Equation (16) characterizes the decay rate of photon fluence along the direction defined by angle \( \alpha \), with respect to the line-of-sight source–detector distance \( d \). For the case-longi configuration, the detector locates at \( (R_0, 0, z) \), so \( \alpha = \pi/2 \) and \( d_{\perp} = 0 \), and then Eq. (16) becomes

\[
\frac{\partial \ln(\Psi \cdot d^2)}{\partial d} = -\left\{ k_0 - \frac{1}{2k_0 R_a} \left( \frac{R_a + R_b}{R_0 + R_a} \right) \right\}
\]

(17)

For the case-azi configuration, the detector locates at \( (R_0, \phi, 0) \), so \( \alpha = 0 \) and \( d_{\perp} = d \), and then Eq. (16) becomes

\[
\frac{\partial \ln(\Psi \cdot d^2)}{\partial d} = -\left\{ k_0 - \frac{1}{2k_0 R_a} \left( \frac{R_a + R_b}{R_0 + R_a} \right) + \left[ \frac{2R_0 + R_a - 2R_b}{2R_0 R_a (R_0 + R_a)} \right] d_{\perp} \right\}.
\]

(18)

The first term \( k_0 \) in the right-hand side of Eqs. (17) and (18) characterizes the decay rate of photon fluence along a straight line on a semi-infinite interface. It is clear by Eq. (17) that the photon fluence along the longitudinal direction on a convex interface decays slower than the photon fluence along a straight line on the semi-infinite interface. However, the decay rate of photon fluence (comparing to \( k_0 \)) along the azimuthal direction on a convex interface described by Eq. (18) is inexplicit owing to the two terms of opposite signs after \( k_0 \). It can be shown that the third term at the right-hand side of Eq. (18) is greater in magnitude than the second term for the general diffusion regime; therefore Eq. (18) actually accounts for the greater decay rate of photon fluence along the azimuthal direction on a convex interface than that along a straight line on the semi-infinite interface.

From Eq. (16) it is straightforward to conclude that if the coordinates of the detector \( (\alpha, d_{\perp}) \) with respect to the source satisfy the condition of

\[
\cos \alpha = \frac{1}{k_0 d_{\perp}} \frac{R_0}{2R_0 + R_a - 2R_b},
\]

(19)

then the decay rate of photon fluence over line-of-sight source–detector distance \( d \) on the convex interface is identical to that over the same \( d \) on the semi-infinite interface. Equation (19) also implies that \( \alpha \) changes as the detector is displaced azimuthally away from the source.

3. SPIRAL PATHS ASSOCIATED WITH CONCAVE AND CONVEX GEOMETRIES OF SMALL RADII

For concave or convex geometries of small radii, analytic derivation of the spiral paths could become much more complicated. Should an analytic approximation of the spiral paths be reached, the resulting profiles would likely be much more inaccurate owing to the approximation imposed by a smaller radial dimension. In [17], the spiral paths of concave or convex geometry of a smaller radial dimension were found numerically based on the general analytic results given in [15]. The method and the found spiral paths are summarized in Fig. 3. First, a uniform grid is established on the cylindrical interface, and the source is fixed at one node. A detector has three options of moving away from the source: along the azimuthal direction, along the longitudinal direction, and along the diagonal of the previous two directions. For each possible future location of the detector, the photon fluence rate at that position is compared with the case in the semi-infinite geometry for the same line-of-sight distance of the detector from the source. The position with the least difference of the evaluated photon fluence rate from the semi-infinite geometry is chosen as the next starting position of the detector. The trace of moving the detector on the interface forms the spiral paths. In both concave and convex geometries, the spiral paths have two lobes symmetric to the source location, and each lobe is symmetric with respect to a middle sagittal plane containing the source. The spiral paths are shown to contain four identical quadrants. The MC and FEM solution of photon diffusion confirmed that the decay rate of photon fluence along the spiral paths was indeed equal to that along a straight line on a semi-infinite interface [17].

Fig. 3. (Color online) spiral paths for concave and convex geometries of centimeter-order radii are calculated based on analytic results derived in [15]. For a fixed source, a detector has three directions to move away from the source: along the azimuthal direction, along the longitudinal direction, and along the diagonal of the above two directions. For each possible future location of the detector, the photon fluence rate at that position is compared with the case in the semi-infinite geometry for the same line-of-sight distance of the detector from the source, and the position with the least difference in the evaluated photon fluence rate is the next starting position of the detector. The shown complete sets of the spiral profile for concave geometry (upper) and convex geometry (lower) are computed for a cylinder radius of \( R_0 = 1.5 \) cm and optical properties of \( \mu_a = 0.02 \) cm\(^{-1} \), \( \mu_s = 5 \) cm\(^{-1} \), and \( \alpha = 1.86 \).
4. PERTURBATION TO PHOTON FLUENCE RATE IN CONCAVE OR CONVEX GEOMETRIES—ANALYTIC TREATMENT

The spiral paths are demonstrated in concave and convex geometries for homogeneous-medium cases. However, it is questionable that the spiral paths associated with homogeneous-medium cases will hold for the medium containing heterogeneity. Practically, however, it may only be possible to examine the spiral paths in limited cases of medium heterogeneity. To facilitate the examination by analytic means, this section employs perturbation-based analysis to derive the general form of the photon fluence rate in concave or convex geometry that contains a single heterogeneity in an otherwise homogeneous medium.

We start with the equation of steady-state photon diffusion in an infinite medium as

$$\mu_a(\vec{r})\Psi(\vec{r}) - \nabla \cdot [D(\vec{r})\nabla \Psi(\vec{r})] = S(\vec{r}).$$  \hspace{1cm} (20)

where $\Psi(\vec{r})$ is the photon fluence rate at position $\vec{r}$, and $S(\vec{r})$ is the source term. The optical heterogeneity to a homogeneous medium of absorption coefficient $\mu_a$ and diffusion coefficient $D_0$ may be represented by

$$\mu_a(\vec{r}) = \mu_a + \delta \mu_a(\vec{r}).$$  \hspace{1cm} (21)

$$D(\vec{r}) = D_0 + \delta D(\vec{r})$$  \hspace{1cm} (22)

and the resulted photon fluence rate is expressed by

$$\Psi(\vec{r}) = \Psi_0(\vec{r}) + \Psi_{SC}(\vec{r}),$$  \hspace{1cm} (23)

where $\Psi_0(\vec{r})$ is the photon fluence rate for homogeneous medium that satisfies the equation of

$$\mu_a \Psi_0(\vec{r}) - D_0 \nabla^2 \Psi_0(\vec{r}) = S(\vec{r})$$  \hspace{1cm} (24)

and $\Psi_{SC}(\vec{r})$ represents a perturbation. By using Eqs. (21)–(23) we convert Eq. (20) to

$$[\mu_a + \delta \mu_a(\vec{r})][\Psi_0(\vec{r}) + \Psi_{SC}(\vec{r})] - D_0 \nabla^2[\Psi_0(\vec{r}) + \Psi_{SC}(\vec{r})] - \nabla \cdot [\delta D(\vec{r}) \nabla [\Psi_0(\vec{r}) + \Psi_{SC}(\vec{r})]] = S(\vec{r}).$$  \hspace{1cm} (25)

Subtracting Eq. (24) from Eq. (25) leads to

$$D_0 \nabla^2 \Psi_{SC}(\vec{r}) - \mu_a \Psi_{SC}(\vec{r}) = \delta \mu_a(\vec{r})[\Psi_0(\vec{r}) + \Psi_{SC}(\vec{r})] - \nabla \cdot [\delta D(\vec{r}) \nabla [\Psi_0(\vec{r}) + \Psi_{SC}(\vec{r})]].$$  \hspace{1cm} (26)

For a weak heterogeneity [18,19], i.e.,

$$\Psi_{SC}(\vec{r}) \ll \Psi_0(\vec{r}),$$  \hspace{1cm} (27)

Eq. (26) becomes

$$\nabla^2 \Psi_{SC}(\vec{r}) - \frac{\mu_a}{D_0} \Psi_{SC}(\vec{r}) = \frac{\delta \mu_a(\vec{r})}{D_0} \Psi_0(\vec{r}) - \frac{1}{D_0} \nabla \cdot [\delta D(\vec{r}) \nabla \Psi_0(\vec{r})].$$  \hspace{1cm} (28)

The Green function of Eq. (28) satisfies the equation of

$$\nabla^2 G(\vec{r}, \vec{r'}) - \frac{\mu_a}{D_0} G(\vec{r}, \vec{r'}) = -\delta(\vec{r} - \vec{r'}).$$  \hspace{1cm} (29)

We denote the source location as $\vec{r}_s$, the heterogeneity location as $\vec{r}'$, and the detector location as $\vec{r}_d$. The photon fluence rate measured at $\vec{r}'$ associated with a source at $\vec{r}_s$ is denoted as $\Psi_0(\vec{r}', \vec{r}_s)$, and $G(\vec{r}', \vec{r}_s)$, in Eq. (29) represents the response at $\vec{r}_s$ owing to an impulse at $\vec{r}'$.

We now consider a concave geometry of radius $R_0$ and the extrapolated boundary condition based on Part I of this study. For a directional source at $\vec{r}_s(R_0, \theta_s, z_s)$ there is an equivalent isotropic source at $\vec{r}_s(R_0 - R_a, \theta_s, z_s)$, and a heterogeneity at $\vec{r}'(\rho', \phi', z')$ assuming that the heterogeneity locates deeper than $R_a$ from the interface boundary, i.e., $\rho' < R_0 - R_a$, we have

$$\Psi_0(\vec{r}', \vec{r}_s) = \frac{S}{D_0} \frac{1}{2\pi^2} \int_0^\infty \mathrm{d}k \left\{ \cos[k(z' - z_s)] \right\} \times \sum_{m=0}^\infty \epsilon_m I_m(k_{\text{eff}}) K_m(k_{\text{eff}}(R_0 - R_a))$$

$$\times \left\{ 1 - \frac{I_m(k_{\text{eff}}(R_0 - R_a)) K_m(k_{\text{eff}} + R_a))]}{K_m(k_{\text{eff}}(R_0 + R_a))] I_m(k_{\text{eff}}(R_0 + R_a))] \right\} \cos[m(\phi' - \phi_s)].$$  \hspace{1cm} (30)

where $I_m$ and $K_m$ are the modified Bessel functions of the first and second kinds, respectively, $k_{\text{eff}} = \sqrt{k^2 + k_0^2}$, and

$$\epsilon_m = \begin{cases} 2 & m > 0 \cr 1 & m = 0 \end{cases}.$$  \hspace{1cm} (31)

For the heterogeneity at $\vec{r}'(\rho', \phi', z')$ and a detector at $\vec{r}_d(R_0, \phi_d, z_d)$, note $\rho' < R_0$, we have

$$G(\vec{r}_d, \vec{r}') = \frac{1}{2\pi^2} \int_0^\infty \mathrm{d}k \left\{ \cos[k(z_d - z')] \right\} \sum_{m=0}^\infty \epsilon_m I_m(k_{\text{eff}}) K_m(k_{\text{eff}})$$

$$\times \left\{ 1 - \frac{I_m(k_{\text{eff}}) K_m(k_{\text{eff}} + R_a))}{K_m(k_{\text{eff}}) I_m(k_{\text{eff}}(R_0 + R_a))] \right\} \cos[m(\phi_d - \phi')].$$  \hspace{1cm} (32)

Similarly we consider a convex geometry of radius $R_0$ and the extrapolated boundary condition. For a directional source at $\vec{r}_s(R_0, \theta_s, z_s)$ there is an equivalent isotropic source at $\vec{r}_s(R_0 + R_a, \theta_s, z_s)$, and a heterogeneity at $\vec{r}'(\rho', \phi', z')$ assuming that the heterogeneity locates deeper than $R_a$ from the interface boundary, i.e., $\rho' > R_0 + R_a$, we have
\[
\Psi_0(\vec{r}, \vec{r}_s) = \frac{S}{D} \frac{1}{2\pi^2} \int_0^\infty dk \left\{ \cos[k(z' - z_s)] \right. \\
\times \sum_{m=0}^\infty \epsilon_m I_m(k_{\text{eff}}(R_0 + R_s)) K_m(k_{\text{eff}}k) \\
\left. \cdot \left( 1 - \frac{I_m(k_{\text{eff}}(R_0 - R_s)) K_m(k_{\text{eff}}R_0)}{K_m(k_{\text{eff}}(R_0 - R_s)) I_m(k_{\text{eff}}R_0)} \right) \right\} \cos[m(\phi' - \phi_s)]. \tag{33}
\]

For the heterogeneity at \( \vec{r}'(\phi', \phi', z') \) and a detector at \( \vec{r}_s(R_0, \phi_d, z_d) \), note \( \rho' > R_0 \), we have

\[
G(\vec{r}_d, \vec{r}) = \frac{1}{2\pi^2} \int_0^\infty dk \left\{ \cos[k(z_d - z')] \right. \\
\times \sum_{m=0}^\infty \epsilon_m I_m(k_{\text{eff}}R_0) K_m(k_{\text{eff}}k) \\
\left. \cdot \left( 1 - \frac{I_m(k_{\text{eff}}(R_0 - R_s)) K_m(k_{\text{eff}}R_0)}{K_m(k_{\text{eff}}(R_0 - R_s)) I_m(k_{\text{eff}}R_0)} \right) \right\} \cos[m(\phi_d - \phi')]. \tag{34}
\]

The solution to Eq. (28), representing the change to the photon fluence rate measured at \( \vec{r}_s \) associated with a source at \( \vec{r}_d \) by the heterogeneity at \( \vec{r}' \), is then

\[
\Psi_{\text{SC}}(\vec{r}_d, \vec{r}_s) = -\frac{1}{D_0} \iiint_V G(\vec{r}_d, \vec{r}) \delta \mu_a(\vec{r}) \Psi_0(\vec{r}', \vec{r}_s) d^3r' + \frac{1}{D_0} \iiint_V G(\vec{r}_d, \vec{r}) \nabla \cdot (\delta D(\vec{r}) \nabla \Psi_0(\vec{r}', \vec{r}_s)) d^3r'. \tag{35}
\]

In Eq. (35), the first term of integration is associated with the absorption heterogeneity and the second term of integration is associated with the diffusion heterogeneity. Appendix C shows that the second term can be transformed, and by that transformation Eq. (35) changes to

\[
\Psi_{\text{SC}}(\vec{r}_d, \vec{r}_s) = -\frac{1}{D_0} \iiint_V G(\vec{r}_d, \vec{r}) \delta \mu_a(\vec{r}) \Psi_0(\vec{r}', \vec{r}_s) d^3r' \\
- \frac{1}{D_0} \iiint_V \delta D(\vec{r}) \nabla G(\vec{r}_d, \vec{r}') \cdot \nabla \Psi_0(\vec{r}', \vec{r}_s) d^3r'. \tag{36}
\]

It is worthwhile to notice that there is a mistake seen in analytic descriptions of some previous works similar in form to Eq. (36), such as Eq. (2) in [19] and Eq. (11.63) in [20], regarding the sign associated with the second term of integration. The detailed accounting in Appendix C shall clarify the “-” sign, rather than a “+” sign, associated with the second term of integration related to the diffusion heterogeneity.

For an inclusion of volume \( V \) and a uniform contrast over the background medium, we define the absorption strength of the inclusion with respect to the background medium as

\[
\delta \mu_a = \frac{\| \delta \mu_a \bullet V \|}{\mu_a} \tag{37}
\]

and the scattering strength of the inclusion with respect to the background medium as

\[
\delta P_s = \frac{\| \delta P_s \bullet V \|}{P_s}. \tag{38}
\]

Equation (37) implies that the same level of absorption perturbation to the photon fluence rate could be caused by either a smaller anomaly with stronger absorption contrast or a larger anomaly with weaker absorption contrast. Equation (38) implies that the same level of scattering perturbation to the photon fluence rate could be caused by either a smaller anomaly with stronger scattering contrast or a larger anomaly with weaker scattering contrast. Then Eq. (36) becomes

\[
\Psi_{\text{SC}}(\vec{r}_d, \vec{r}_s) = -\delta \mu_a \frac{\mu_a}{D_0} G(\vec{r}_d, \vec{r}) \Psi_0(\vec{r}', \vec{r}_s) \\
- \frac{\delta P_s}{D_0} \nabla G(\vec{r}_d, \vec{r}') \cdot \nabla \Psi_0(\vec{r}', \vec{r}_s). \tag{39}
\]

The gradient operator in Eq. (39) can be expanded in cylindrical coordinates as

\[
\nabla G(\vec{r}_d, \vec{r}') \cdot \nabla \Psi_0(\vec{r}', \vec{r}_s) = \left[ \frac{\partial G(\vec{r}_d, \vec{r}')}{\partial \rho'} \frac{\partial \Psi_0(\vec{r}', \vec{r}_s)}{\partial \rho'} \\
+ \frac{\partial G(\vec{r}_d, \vec{r}')}{\partial \phi'} \frac{\partial \Psi_0(\vec{r}', \vec{r}_s)}{\partial \phi'} \\
+ \frac{\partial G(\vec{r}_d, \vec{r}')}{\partial z'} \frac{\partial \Psi_0(\vec{r}', \vec{r}_s)}{\partial z'} \right]. \tag{40}
\]

5. PERTURBATION TO PHOTON FLUENCE RATE BY A WEAK TARGET ALIGNED AZIMUTHALLY WITH THE SPIRAL PATHS—NUMERICAL EVALUATION BASED ON ANALYTIC TREATMENT

This section aims to evaluate the photon fluence rate along the spiral paths identified for homogeneous-medium cases, when the medium contains a weak heterogeneous inclusion whose center is aligned azimuthally with one location on the spiral paths. The perturbation analysis discussed in the previous section will be numerically implemented for the weak inclusion. For concave and convex geometries, the partial derivatives in Eq. (40) can be numerically approximated using a central difference scheme, after \( \Psi_0(\vec{r}', \vec{r}_s) \) and \( G(\vec{r}_d, \vec{r}') \) are quantified based on the numerical methods demonstrated in [15,16].

As the evaluation of spiral paths with inclusion in concave...
or convex geometry has to involve evaluating the photon fluence rate along a straight line in a semi-infinite geometry with identical inclusion, the gradient operator in Eq. (39) will be expanded in Cartesian coordinates for the semi-infinite geometry, and the resulting partial derivatives will be found similarly by a central difference scheme.

We consider a spherical anomaly of 0.15 cm in radius and 0.25 cm in depth that is aligned with one quadrant of the spiral paths, as shown in Fig. 4. The position of the anomaly is chosen so that in the concave geometry [Fig. 4(A)] the azimuthal angle between the anomaly center and the source is π/2. In the semi-infinite geometry [Fig. 4(B)] and the convex geometry [Fig. 4(C)], the position of the anomaly is chosen such that the line-of-sight distance between the source and the projection of the anomaly center onto the straight line or spiral-path (hence the physical boundary) is kept the same as that in the concave geometry. Table 1 lists the four sets of optical parameters assigned to the single anomaly, which include positive μₐ, positive μ₀ₛ, negative μₐ, and negative μₐ contrast with respect to those of the background medium that is not necessarily identical in the four cases. The radii of both concave and convex applicators are set as 1.5 cm, and A = 1.86 is chosen.

The results of numerical evaluation based on the four cases of contrasts specified in Table 1 are given in Fig. 5. In each of the figure parts from 5(A) to 5(D), the photon fluence rates are compared among four configurations: (1) along a straight line on the semi-infinite interface for homogeneous medium, which is used as the reference; (2) along a straight line on the semi-infinite interface with the anomaly; (3) along the spiral profile on the concave interface with the anomaly; (4) along the spiral profile on the convex interface with the anomaly. The photon fluence curves for the four configurations are shown indistinguishable at the macroscopic scale near the 5 cm range for d. To examine the microscopic differences of the photon fluence curves, the curves corresponding to a 0.1 cm range of d and centering at the azimuthal coordinate of the anomaly are magnified as the inset in each figure part. Under the magnification, it is found that (1) the photon fluence curves associated with the anomaly are clearly distinguished from the reference; (2) the photon fluence curves associated with the anomaly of absorption contrast are still indistinguishable among the three geometries; and (3) the

Table 1. Four Sets of Optical Parameters for Evaluating the Change to Photon Fluence Rate by an Anomaly of Weak Contrast to the Background Medium

<table>
<thead>
<tr>
<th>Set</th>
<th>Positive μₐ contrast</th>
<th>Positive μ₀ₛ contrast</th>
<th>Negative μₐ contrast</th>
<th>Negative μ₀ₛ contrast</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.025</td>
<td>0.025</td>
<td>0.05</td>
<td>0.05</td>
</tr>
<tr>
<td>2</td>
<td>0.025</td>
<td>0.025</td>
<td>0.025</td>
<td>0.025</td>
</tr>
<tr>
<td>3</td>
<td>0.05</td>
<td>0.05</td>
<td>0.025</td>
<td>0.025</td>
</tr>
<tr>
<td>4</td>
<td>0.025</td>
<td>0.025</td>
<td>0.025</td>
<td>0.025</td>
</tr>
</tbody>
</table>

Fig. 5. (Color online) Photon fluence rate when one weak anomaly resides in the otherwise homogeneous background medium. The anomaly possesses (A) positive μₐ contrast, (B) positive μ₀ₛ contrast, (C) negative μₐ contrast, and (D) negative μ₀ₛ contrast over the background. The shown curves of photon fluence are plotted for (1) along a straight line on semi-infinite interface of homogeneous medium, (2) along a straight line on semi-infinite interface having the anomaly aligned with the straight line, (3) along the spiral profile on concave interface having the anomaly aligned with the spiral profile, and (4) along the spiral profile on convex interface having the anomaly aligned with the spiral profile.
photon fluence curves associated with the anomaly of scattering contrast are distinguishable among the three geometries, with the curves of concave and convex geometries locating very close to and at the opposite sides of the curve of semi-infinite geometry.

6. CHANGE TO PHOTON FLUENCE RATE BY A STRONG TARGET ALIGNED AZIMUTHALLY WITH THE SPIRAL PATHS—NUMERICAL EVALUATION BASED ON FINITE-ELEMENT METHOD

As the perturbation analysis becomes increasingly inaccurate for increasing contrast strength of the anomaly, FEM computation based on a software package of near infrared fluorescence and spectral tomography (NIRFAST) [21] is implemented to evaluate the photon fluence rate along the spiral paths when a strong anomaly resides in the medium.

The FEM meshing domain is illustrated in Figs. 6(A), 6(B), and 6(C) for concave, semi-infinite, and convex geometries, respectively. In the concave geometry, the meshing volume is a cylinder of 14 cm in height and 1.5 cm in radius, which is discretized into 76620 nodes and 349697 tetrahedral elements. The surface containing the spiral profile is set with higher node density. In the semi-infinite geometry, the meshing volume is a rectangle of 15 × 11 × 5.5 cm³, which is discretized into 88941 nodes and 496211 elements. The straight line for evaluating the photon fluence rate is set with higher node density. In the convex geometry, the meshing domain is the volume between two concentric cylinders of 15 cm in height, with 1.5 cm inner radius and 6 cm outer radius. The meshing volume is discretized into 83312 nodes and 437039 tetrahedral elements. The surface containing the spiral profile is set with denser nodes.

Table 2. Four Sets of Optical Parameters Used for Evaluating the Change to Photon Fluence Rate by an Anomaly of Strong Contrast to the Background Medium

<table>
<thead>
<tr>
<th>Set</th>
<th>Positive μₐ (cm⁻¹)</th>
<th>Background μₐ (cm⁻¹)</th>
<th>Anomaly μₐ (cm⁻¹)</th>
<th>Anomaly μₛ (cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.025</td>
<td>10.0</td>
<td>0.1</td>
<td>10.0</td>
</tr>
<tr>
<td>2</td>
<td>Positive μₛ</td>
<td>0.025</td>
<td>10.0</td>
<td>0.025</td>
</tr>
<tr>
<td>3</td>
<td>Negative μₐ</td>
<td>0.1</td>
<td>10.0</td>
<td>0.025</td>
</tr>
<tr>
<td>4</td>
<td>Negative μₛ</td>
<td>0.025</td>
<td>20.0</td>
<td>0.025</td>
</tr>
</tbody>
</table>

We consider a spherical anomaly of 0.4 cm in radius and 0.5 cm in depth that is aligned azimuthally with one quadrant of the spiral paths. The positions of the anomaly in concave, semi-infinite, and convex geometries are chosen following the same rules as in Section 5. Table 2 lists the four sets of optical parameters assigned to the single anomaly, which include positive μₐ, positive μₛ, negative μₐ, and negative μₛ contrasts with respect to those of the background medium that is not necessarily identical in the four cases. The four sets of anomaly defined in Table 2 have approximately 57 times of positive absorption strength, 57 times of positive scattering strength, 28 times of negative absorption strength, and 95 times of negative scattering strength, respectively, of the ones defined in Table 1, when counting the difference in volume.

The results of FEM simulation based on the four cases of contrasts as specified in Table 2 are given in Fig. 7. In each of the figure parts from 7(A) to 7(D), the photon fluence rates are compared among four configurations as with Fig. 5. At the macroscopic scale near the 5 cm range for d, the photon fluence curves for the three geometries with the anomaly are distinguishable from the reference except for negative μₐ contrast; however, the photon fluence curves for the three geometries with the anomaly are nearly indistinguishable. At the microscopic level similar to that in Fig. 5, the photon fluence curves of the concave and convex geometries are very close to and at the opposite sides of the curve of semi-infinite geometry, for anomaly of either absorption or scattering contrast.

7. DISCUSSION

Our previous studies have suggested and demonstrated the existence of spiral paths in the concave and convex geometries for homogeneous-medium conditions. As stated earlier, the spiral paths refer to the equivalence of a unique set of directions on the concave and convex interfaces to a straight line on a semi-infinite interface, in terms of the decay rate of photon fluence with respect to the line-of-sight distance between a source and a detector positioned for probing a homogeneous medium. Such equivalence of the spiral directions in concave or convex geometries to a straight line in a semi-infinite geometry may very well be limited to only the specific set of parameters. For concave and convex geometries of large radii, Eqs. (10) and (19) represent the spiral paths by means of the angle α. It is unmistakable that α is a function of Rₒ, and α should also be affected by Rₛ and Rₛ, which collectively are determined by the optical properties of medium and tissue-applicator interface. It is therefore...
imperative to examine the actual profile of spiral paths associated with different geometric and optical parameters.

Figure 8 investigates the spiral paths associated with different sets of geometric and optical parameters. Since the four limbs of the spiral paths in both concave and convex geometries are symmetric with regard to the midsagittal plane containing the source, only one quadrant of the spiral paths is to be investigated. The spiral paths found for concave geometry are grouped in the left column and for convex geometry in the right column. The set of baseline parameters are $R_0 = 1.5$ cm, $A = 1.86$, $\mu_a = 0.025$ cm$^{-1}$, and $\mu_s = 10$ cm$^{-1}$, and each of the plots from (A) to (H) has one parameter differing from the baseline parameters. Specifically, (A) and (B) correspond to changing radius from 1, 1.5, to 2 cm; (C) and (D) correspond to changing the value of the $\mu_a$ parameter from 0.025, 0.1 cm$^{-1}$; and (E) and (F) correspond to changing $\mu_s$ from 5, 10, to 20 cm$^{-1}$. The most salient feature observed from Fig. 8 is that the spiral profile develops much deeper into the $z$ direction in the convex geometry than in the concave geometry, for the otherwise identical set of parameters. The value of the $\mu_a$ parameter seems to have little effect on the profile of spiral paths in both geometries. The spiral profile is shown to relate to other parameters; however, it is affected considerably less in convex geometry than in concave geometry.

As this study has also investigated whether the spiral paths found for the homogeneous medium specific to a given set of optical parameters would be valid for the same geometry if the medium contains heterogeneity, two observations are noted. At the macroscopic scale, the photon fluence curves for the three geometries associated with the anomaly are nearly indistinguishable from each other even for the strong anomaly considered, indicating that the spiral paths is a good approximation macroscopically. At a sufficiently detailed microscopic scale, the photon fluence curves for the three geometries associated with the anomaly do become separated; however, the photon fluence curves of the concave and convex geometries seem to locate at the opposite sides of the curve of semi-infinite geometry. As the numerical evaluation based on the analytic treatment involves summing modified Bessel functions of finite orders, and the FEM is implemented at finite resolution of the elements, limited precision is expected for the numerical results shown, as expressed by the slight oscillatory behavior of the curves associated with concave or convex geometries visible at microscopic scales. The deviation of the photon fluence curve of concave or convex geometry from that of semi-infinite geometry may be related to the slight variance of the spiral paths with respect to the actual optical properties, indicating that the spiral paths could be considered a good approximation to a straight line, but it is not identical to a straight line in semi-infinite geometry. Apparently the deviation of the photon fluence curve of concave or convex geometry from that of semi-infinite geometry is to become smaller as the radial dimension of the concave or convex applicator is to be increased. This study examined the change to photon fluence rate along the spiral paths of concave and convex geometries.
identified for homogeneous medium cases when only one anomaly is introduced into the medium. The perturbation analysis, being linear in its nature, can in principle be applied to multiple anomalies. However, the results based on numerical implementation of the perturbation-based analytic approach will become increasingly inaccurate if anomalies with large volume or strong contrast are included owing to the nonlinearity between the photon fluence and $\mu_a$ or $\mu_s'$. Certainly FEM would facilitate more accurate evaluation for multiple anomalies of various contrasts. This study is also specific to the case of having the only anomaly aligned azimuthally with the spiral paths. If the same anomaly is placed off from the position aligning with the spiral paths, the change to the photon fluence rate measured along the spiral paths by the anomaly is expected to be less than that shown in Figs. 5 and 7. In that case the photon fluence curves associated with the three geometries with the anomaly as studied in Figs. 4 and 6 will become less distinguishable. Therefore the approximation by spiral paths could become more accurate for an inclusion not aligned with the spiral paths than one aligned with the spiral paths.

8. CONCLUSIONS

This study continued the work of examining steady-state photon diffusion in a concave or convex geometry. The analysis in either of these two geometries has implications to diffuse optical sensing of externally applicable or internally applicable tissue medium. The study specifically complemented our previous prediction that, on the tissue-applicator interface of either concave or convex geometry there exists a unique set of spiral paths, along which the steady-state photon fluence rate decays at a rate equal to that along a straight line on a planar semi-infinite interface, for the same line-of-sight source–detector distance. This phenomenon, referred to as spiral paths, is demonstrated analytically for concave or convex geometry of large radial dimension, and numerically for concave or convex geometry of small radial dimension. This study also examined the spiral paths when the medium contained heterogeneity. Although the heterogeneity being investigated is limited to an anomaly with either positive or negative contrast of absorption or scattering coefficient over the background medium, by aligning the anomaly azimuthally with the spiral paths the anomaly has the maximum sensitivity.
to the change to photon fluence rate. For an anomaly of weak contrast strength the effect of it to the photon fluence rate along the spiral paths is calculated by a well-established perturbation analysis. Our revisiting of the perturbation analysis for numerical implementation in cylindrical coordinates helped identify a mistake appearing in similar analyses in some previous works. As the perturbation analysis is limited to weak-target cases, the change by an anomaly of strong contrast to the photon fluence rate along the spiral paths is instead computed by using PEM. For all investigated heterogeneous-medium cases the photon fluence rate along the homogeneous-medium associated spiral paths is macroscopically indistinguishable from that along a straight line on a semi-infinite interface, though microscopically the discrepancy is observed.

APPENDIX A: DERIVATION OF EQ. (7) FROM EQ. (6)

Equation (5) is rewritten here as

\[
\Psi = \frac{S}{4\pi D} e^{-k_d d} \left[ -\frac{1}{2} k_0 d \left( \frac{R_k^2}{2\alpha} \right)^2 + \frac{R_k}{R_0} (\cos \alpha)^2 \right] \left[ 1 - \frac{1}{2} k_0 d \left( \frac{R_k + 2R_b}{d^2} + \frac{R_k + 2R_b}{R_0} (\cos \alpha)^2 \right) \right] \left( \frac{1}{R_0 - R_a} \right). \tag{A1} \]

Equation (A1) can be further simplified as

\[
\Psi = \frac{S}{4\pi D} e^{-k_d d} \left[ 1 - \frac{k_0 R_k^2 + k_0 R_d (\cos \alpha)^2 - 1}{2d} \frac{R_0}{R_k (R_0 - R_a)} \frac{R_k}{R_0} (\cos \alpha)^2 - \frac{R_k + 2R_b}{R_0 - R_a} \frac{d^2}{2d} \frac{R_0}{R_k (R_0 - R_a)} \frac{R_k}{R_0} (\cos \alpha)^2 \right] = \frac{S}{2\pi D} e^{-k_d d} \left[ \frac{k_0 R_k R_b (R_a + R_b)}{d} \left( \frac{R_k}{R_0} \frac{R_k}{R_0} (\cos \alpha)^2 - \frac{R_k + 2R_b}{R_0 - R_a} \frac{d^2}{2R_0 R_k (R_0 - R_a)} (\cos \alpha)^2 \right) \right] = \frac{S}{2\pi D} e^{-k_d d} \left[ \frac{k_0 R_k R_b (R_a + R_b)}{d} \frac{d^2}{2R_0 R_k (R_0 - R_a)} (\cos \alpha)^2 \right] = \frac{S}{2\pi D} e^{-k_d d} \left[ \frac{k_0 R_k R_b (R_a + R_b)}{d} \frac{d^2}{2R_0 R_k (R_0 - R_a)} (\cos \alpha)^2 \right]. \tag{A2} \]

Under the assumption that \( R_0 \gg R_a, R_b, d \), based on Taylor expansion, Eq. (A2) can be approximated as

\[
\Psi = \frac{S}{2\pi D} e^{-k_d d} k_0 R_b (R_a + R_b) \exp \left\{ -\frac{d}{2k_0 R_a (R_0 - R_a)} + \frac{d^2}{2R_0 R_b R_a (R_0 - R_a)} \right\} (\cos \alpha)^2 + \left( \frac{R_a + 2R_b}{4R_0 R_b (R_0 - R_a)} \right). \tag{A3} \]

By multiplying both sides of Eq. (A3) with \( d^2 \), we have

\[
\Psi d^2 = \frac{S}{2\pi D} k_0 R_b (R_a + R_b) e^{(2\pi D/k_0 R_a)\cdot d^2} \exp \left\{ -\frac{d}{2k_0 R_a (R_0 - R_a)} + \frac{d^2}{2R_0 R_b R_a (R_0 - R_a)} \right\} (\cos \alpha)^2 d^2. \tag{A4} \]

Taking the natural logarithm, Eq. (A4) leads to

\[
\ln(\Psi d^2) = -k_0 d - \frac{d}{2k_0 R_a (R_0 - R_a)} + \frac{d^2}{2R_0 R_b R_a (R_0 - R_a)} \left( \frac{R_a + 2R_b}{4R_0 R_b (R_0 - R_a)} \right) (\cos \alpha)^2 d^2 + \ln \left[ \frac{S}{2\pi D} k_0 R_b (R_a + R_b) \right] + \left( \frac{R_a + 2R_b}{4R_0 (R_0 - R_a)} \right). \tag{A5} \]

Taking the derivative with respect to \( d \) and substituting \( d_{\perp} = d \cdot \cos \alpha \), Eq. (A5) leads to

\[
\frac{\partial}{\partial d} \ln(\Psi \cdot d^2) = -\left\{ k_0 + \frac{1}{2k_0 R_a (R_0 - R_a)} \right\} \left[ \frac{2R_0 - R_a + 2R_b}{2R_0 R_b (R_0 - R_a)} \right] \cos \alpha \cdot d_{\perp}. \tag{A6} \]

APPENDIX B: DERIVATION OF EQ. (16) FROM EQ. (15)

Equation (15) is rewritten here as

\[
\Psi = \frac{S}{4\pi D} e^{-k_d d} \left[ 1 - \frac{1}{2} k_0 d \left( \frac{R_k^2}{d^2} + \frac{R_k}{R_0} (\cos \alpha)^2 \right) \right] \left[ 1 - \frac{1}{2} k_0 d \left( \frac{R_k + 2R_b}{d^2} + \frac{R_k + 2R_b}{R_0} (\cos \alpha)^2 \right) \right] \left( \frac{1}{R_0 - R_a} \right). \tag{B1} \]

Equation (B1) can be further simplified as
ψ = \frac{S}{4\pi D} e^{-k_0 d} \left[ \frac{k_0 R_a^2 - k_0 R_b d}{2 R_0} (\cos \alpha)^2 - 1 + k_0 (R_a + 2 R_b) d \frac{R_0}{2 R_0} \right] \left( \cos \alpha \right)^2 + \frac{R_a + R_b}{R_0 + R_a} - \frac{k_0 (R_a + 2 R_b) R_a + R_b}{2 d} \frac{R_0}{R_0 + R_a} \\
+ \frac{k_0 R_b d}{2 R_0} \frac{R_a + R_b}{R_0 + R_a} (\cos \alpha)^2 \\
= \frac{S}{4\pi D} e^{-k_0 d} \left[ 2k_0 R_b (R_a + R_b) \frac{d}{d} (\cos \alpha)^2 + \frac{k_0 (R_a + 2 R_b) d}{R_0} (\cos \alpha)^2 - \frac{k_0 (R_a + 2 R_b) R_a + R_b}{2 d} \frac{R_0}{R_0 + R_a} \right] \\
= \frac{S}{4\pi D} e^{-k_0 d} \left[ 2k_0 R_b (R_a + R_b) \frac{d}{d} (\cos \alpha)^2 - \frac{d}{2k_0 R_b (R_a + R_b)} \frac{d}{d} (\cos \alpha)^2 - \frac{(R_a + 2 R_b) d^2}{4 R_b R_0 (R_a + R_b)} (\cos \alpha)^2 - \frac{(R_a + 2 R_b)^2}{4 R_b (R_a + R_b)} \right] \\
\text{(B2)}

Under the assumption that \( R_0 \gg R_a, R_b, d \), based on Taylor expansion, Eq. (B2) can be approximated as

\[ \psi = \frac{S}{4\pi D} 2k_0 R_b (R_a + R_b) e^{\frac{d}{2k_0 R_b (R_a + R_b)}} \left[ -k_0 d + \frac{d}{2k_0 R_b (R_a + R_b)} \right] \left[ - \frac{d^2}{2 R_0 R_0} + \frac{(R_a + 2 R_b) d^2}{4 R_b R_0 (R_a + R_b)} \right] (\cos \alpha)^2 = \frac{(R_a + 2 R_b)^2}{4 R_b (R_a + R_b)} \]

\text{(B3)}

By multiplying both sides of Eq. (B3) with \( d^2 \), we have

\[ \psi d^2 = \frac{S}{2\pi D} k_0 R_b (R_a + R_b) e^{\frac{d}{2k_0 R_b (R_a + R_b)}} \exp \left[ -k_0 d + \frac{d}{2k_0 R_b (R_a + R_b)} \right] \left[ - \frac{d^2}{2 R_0 R_0} + \frac{(R_a + 2 R_b) d^2}{4 R_b R_0 (R_a + R_b)} \right] (\cos \alpha)^2 \]

\text{(B4)}

Taking the natural logarithm, Eq. (B4) leads to

\[ \ln(\psi d^2) = -k_0 d + \frac{d}{2k_0 R_b (R_a + R_b)} + \left[ - \frac{1}{2 R_0 R_0} + \frac{R_a + 2 R_b}{4 R_b R_0 (R_a + R_b)} \right] (\cos \alpha)^2 d^2 + \ln \left[ \frac{S}{2\pi D} k_0 R_b (R_a + R_b) \right] - \frac{(R_a + 2 R_b)^2}{4 R_b (R_a + R_b)} \]

\text{(B5)}

Taking the derivative with respect to \( d \) and substituting \( d = d \cdot \cos \alpha \), Eq. (B5) leads to

\[ \frac{\partial}{\partial(d)} \ln(\psi d^2) = -\left\{ k_0 - \frac{1}{2k_0 R_b (R_a + R_b)} + \frac{2 R_b + R_a - 2 R_b}{2 R_b R_0 (R_a + R_b)} \cos \alpha \cdot d \right\} \]

\text{(B6)}

**APPENDIX C: DERIVATION OF EQ. (36) BY FOLLOWING THE APPROACH IN [18]**

Equation (35) is rewritten here as

\[ \Psi_{SC}(\tilde{r}_a, \tilde{r}_s) = -\frac{1}{D_0} \iiint_V G(\tilde{r}_a, \tilde{r}_s) \delta \mu_a(\tilde{r}) \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r} + \frac{1}{D_0} \iiint_V G(\tilde{r}_a, \tilde{r}) \nabla \cdot \{ \delta D(\tilde{r}) \nabla \Psi_0(\tilde{r}, \tilde{r}_s) \} d^3 \tilde{r}. \]

\text{(C1)}

The second integration part can be expanded as

\[ \iiint_V G(\tilde{r}_a, \tilde{r}_s) \nabla \cdot \{ \delta D(\tilde{r}) \nabla \Psi_0(\tilde{r}, \tilde{r}_s) \} d^3 \tilde{r} = \iiint_V G(\tilde{r}_a, \tilde{r}_s) \nabla \delta D(\tilde{r}) \cdot \nabla \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r} + \iiint_V G(\tilde{r}_a, \tilde{r}_s) \delta D(\tilde{r}) \nabla^2 \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r}. \]

\text{(C2)}

Applying Green's first identity \[ \iiint_V (\phi \nabla^2 \psi + \nabla \phi \cdot \nabla \psi) d^3 x = \oint_S (\phi \nabla \psi) d^2 a, \] it can be seen that

\[ \iiint_V G(\tilde{r}_a, \tilde{r}_s) \delta D(\tilde{r}) \nabla^2 \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r} = \oint_S G(\tilde{r}_a, \tilde{r}_s) \delta D(\tilde{r}) \nabla \Psi_0(\tilde{r}, \tilde{r}_s) d^2 a - \iiint_V \nabla \{ G(\tilde{r}_a, \tilde{r}_s) \delta D(\tilde{r}) \} \cdot \nabla \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r}. \]

\text{(C3)}

The surface integral in the above derivation is eliminated because we have the freedom to choose the surface at infinity, where \( G(\tilde{r}_a, \tilde{r}_s) \) decays to zero. Hence,

\[ \iiint_V G(\tilde{r}_a, \tilde{r}_s) \delta D(\tilde{r}) \nabla^2 \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r} = -\iiint_V \nabla \{ G(\tilde{r}_a, \tilde{r}_s) \delta D(\tilde{r}) \} \cdot \nabla \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r}
\]
\[ = -\iiint_V G(\tilde{r}_a, \tilde{r}_s) \nabla \delta D(\tilde{r}) \cdot \nabla \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r} - \iiint_V \delta D(\tilde{r}) \cdot \nabla G(\tilde{r}_a, \tilde{r}_s) \cdot \nabla \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r}. \]

\text{(C4)}

Substituting Eq. (C4) into Eq. (C2) leads to

\[ \frac{1}{D_0} \iiint_V G(\tilde{r}_a, \tilde{r}_s) \nabla \cdot \{ \delta D(\tilde{r}) \nabla \Psi_0(\tilde{r}, \tilde{r}_s) \} d^3 \tilde{r} = -\frac{1}{D_0} \iiint_V \delta D(\tilde{r}) \cdot \nabla G(\tilde{r}_a, \tilde{r}_s) \cdot \nabla \Psi_0(\tilde{r}, \tilde{r}_s) d^3 \tilde{r}. \]

\text{(C5)}

Substituting Eq. (C5) into Eq. (C1) leads to
\[
\Psi_{\text{NC}}(\vec{r}_d, \vec{r}_s) = -\frac{1}{D_0} \iiint_{V} G(\vec{r}_d, \vec{r}) \delta \rho_d(\vec{r}) \Psi_d(\vec{r}, \vec{r}_s) d^3r' - \frac{1}{D_0} \iiint_{V} \delta D(\vec{r}) \nabla G(\vec{r}_d, \vec{r}) \cdot \nabla \Psi_d(\vec{r}, \vec{r}_s) d^3r'.
\]

(C6)

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