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A Specific Feature of the Procedure for Determination of Optical Properties of Turbid Biological Tissues and Media in Calculation for Noninvasive Medical Spectrophotometry

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Introduction

In contemporary medical engineering industry, one of the key problems of development of methods, apparatuses, and devices for optical spectroscopy of biological tissues is the compilation of effective computation algorithms providing maximal accuracy and reliability of determination of initial optical properties of the object of interest from experimental data [14, 18]. Optical properties of biological tissues can be determined from radiation fluxes measured experimentally by solving inverse problems of scattering [11], which employ different methods of description of radiation propagation medium. In turbid light-scattering biological media (most biological media are turbid [22]), numerical models of transition theory and light-scattering in turbid media should be used [8, 20]. The models have a limited number of solutions. Therefore, approximate solutions are often used for practical purposes in photometry of turbid media. For example, flux Kubelka–Munk (KM) approaches are widely used in the practice of noninvasive spectrophotometry, because they are simple and illustrative. Moreover, the KM models allow the final calculation equations to be derived in explicit analytical form [8, 12, 17, 18, 21-24]. In terms of transition theory and KM models, internal optical properties of turbid media are completely characterized by linear optical extinction and scattering coefficients. The linear optical extinction and scattering coefficients are determined coefficients of differential equations describing the model.

In optics, the KM models are purely photometric and phenomenological models based on heuristic principles providing separation of radiation field into discrete rectangular fluxes. The principles also support the validity of linear equation of energy balance for each flux in medium element [2, 4-8, 24]. In the simplest case, two one-dimensional flux KM models are considered. Such model represents one-dimensional radiation propagation medium with two oppositely directed fluxes $F_+(x)$ and $F_-(x)$ [8, 13, 24]. Because this model is photometric (energy) and one-dimensional, it disregards wave properties of radiation. In this case, the classical KM model is described by two coupled linear differential equations of the first order [8]:

$$\begin{cases} \mathrm{d}F_+(x)/\mathrm{d}x = -(K+S)F_+(x) + SF_-(x) \\ \mathrm{d}F_-(x)/\mathrm{d}x = (K+S)F_-(x) - SF_+(x), \end{cases} \quad (1)$$

in general case, for $K \neq 0$ the solution is:

$$F_+(x) = C_1\mathrm{e}^{-\alpha x} + C_2\mathrm{e}^{\alpha x};\ F_-(x) = C_1A_-\mathrm{e}^{-\alpha x} + C_2A_+\mathrm{e}^{\alpha x}, \quad (2)$$

where C_1 and C_2 are integration constants determined from boundary conditions; K and S are linear (transport) extinction coefficients and radiation scattering by medium element dx, respectively; $\alpha = (K(K + 2S))^{1/2}$; $A_+ = (K + 2S + \alpha)/(K + 2S - \alpha)$; $A_- = 1/A_+$. Calculation of transport coefficients is the task of the inverse problem of biomedical optics, particularly in the practice of noninvasive medical spectrophotometry [14].

The disadvantages of the KM model are uncertain area of application and low accuracy [8]. Low accuracy is particularly significant for the problem of development of computation algorithms for spectrophotometric medical diagnostic devices. For example, a branch of modern noninvasive spectrophotometry, optical oxihemometry (tissue oximetry) is a method of measurement of concentration of hemoglobin fractions in blood using their spectra [9]. The measurements are noninvasive and transdermal, using properties of backscattered and transmitted radiation in biological tissues with further calculation of blood extinction coefficients in different spectral ranges.

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Calculated values are compared with tabular values of spectral extinction coefficients for model solutions of whole hemolyzed blood verified using accurate methods of laboratory spectrophotometry [28]. These methods are based on spectrophotometry of dilute solutions of blood and Bouguer's law:

$$F(x) = F_0 \cdot e^{-\mu_a x}, \quad (3)$$

where F_0 is incident light flux; $F(x)$ is measured light flux passed through the cuvette; μ_a is blood solution extinction coefficient (solutions of hemoglobin fractions); x is light path length in the cuvette (usually 1 cm).

In laboratory spectrophotometry light scattering in the cuvette is neglected because of low blood concentration in solutions. This allows use of Eq. (3) in direct determination of μ_a of a solution. In noninvasive spectrophotometry of biological tissues, light scattering in the tissue cannot be neglected. This makes the calculation of μ_a and respective computation algorithms more sophisticated (e.g., algorithms based on Eqs. (1)). This raises the problem of correspondence between the transport extinction coefficient K determined from the KM model using inverse algorithms and parameter μ_a of the Bouguer law.

This problem has been discussed in [4, 8, 12, 13, 16]. Equation (4) derived in [25] is widely cited in the literature and used in practice:

$$K \approx 2\mu_a. \quad (4)$$

The accuracy of the standard two-flux KM approach was estimated to be 80-85% [12].

Analysis of the literature [5, 7, 13, 16] shows that this problem remains unsolved. It was shown at Vladimirskii Moscow Regional Scientific-Research Clinical Institute (Moscow, Russia) that the accuracy of the KM approach for some particular cases (ideal scattering, single scattering) can be increased by accurate measuring of transport coefficients of Eq. (1) using actual optical and physical properties of medium element Δx [7, 13, 23, 26]. For single scattering the following equation was derived:

$$K = \mu_a. \quad (5)$$

This equation is obviously valid for vanishingly small scattering. This suggests that the accuracy of other flux single scattering KM approaches is higher provided that actual optical and physical properties of medium elements are taken into account in Eq. (1) [5]. The goal of this work was to consider the problems of accuracy and reliability of the procedure for determination of optical per-unit-length properties of light-scattering biological tissues and media in noninvasive medical spectrophotometry. The problem of correspondence between the transport extinction coefficient K determined from KM model and parameter μ_a of the Bouguer law is also considered.

Basic Model Problem and Its Solution

The model of one-dimensional scattering medium is a layer of thickness H_0 with non-reflecting (crumbly) borders. This layer is exposed from the left to a light flux F_0 (Fig. 1).

Let the linear extinction coefficient be μ_a. Scattering of the medium is simulated by infinitely thin plane reflecting borders (heterogeneities $r_1, r_2, \ldots, r_n$). These borders reflect incident radiation with reflection coefficient R and transmit radiation with coefficient $(1 - R)$. Let the heterogeneities be spread uniformly at distance h; the first and the last heterogeneities are at distance $h/2$ from the external borders of the layer. This model is a good approximation of biological tissue, provided that the number of heterogeneities is sufficiently large.

Such models have long been known in physics and optics as pile models [27]. In contrast to the Stokes problem, which considers a pile of thick plates, infinitely thin reflecting heterogeneities included in one thick plate are considered in this work. In contrast to the Stokes problem, reflection from external medium is neglected, because the borders are considered crumbly[1].

A modified pile model was selected because the radiation field distribution in an n-layer pile can be derived rigorously using simple photometric equations. Let us consider exponential attenuation of fluxes $F_+(x)$ and $F_-(x)$ along their path between heterogeneities and radiation reflection and transmission at the borders of the heterogeneities. The resulting distribution of radiation field inside and outside the pile can be used in the KM model.

Let local frame of references be introduced for each interval i at $x > h/2$ between heterogeneities: $z_i(z_i \in [0, h])$, where $i = 1, 2, 3, \ldots, n$ is the number of heterogeneities to the left of the interval (Fig. 2). For each i-th interval between heterogeneities, the fluxes $F_+^i(z_i)$ and $F_-^i(z_i)$ can be calculated from Eq. (3) as:

[1] Crumbly external borders correspond to coarse surface of biological tissue [15] or surface of powdered materials [5]. Reflection from such surfaces is negligible as compared to back-scattered radiation. For one-dimensional models the term "crumbly external border" is arbitrary; it is used in this work for the sake of illustration.

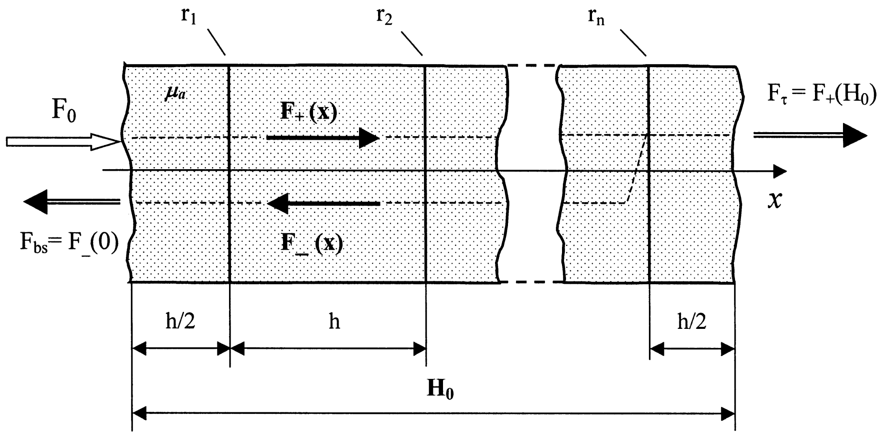

Fig. 1. Model representation of one-dimensional scattering medium.

$$F_+^i(z_i) = F_+^i(0)\cdot e^{-\mu_a z_i};\ F_-^i(z_i) = F_-^i(0)\cdot e^{\mu_a z_i}, \qquad (6)$$

where $F_+^i(0)$ and $F_-^i(0)$ are unknown values of fluxes at the left end of the interval. The values are determined for flux coupling at the ends of the intervals. At the total number of heterogeneities and intervals $n = N$, an additional $2N$ values of border fluxes $F_+^i(0)$ and $F_-^i(0)$ should be found.

Coupling conditions are derived from laws of radiation transmission and reflection at the interface between the media and addition of unidirectional fluxes (Fig. 2):

$$F_+^i(0) = F_+^{i-1}(h)\cdot(1 - R) + F_-^i(0)\cdot R$$

$$F_-^{i-1}(0) = F_+^{i-1}(h)\cdot R + F_-^i(0)\cdot(1 - R), \qquad (7)$$

where $F_-^{i-1}(h) = F_-^{i-1}(0)\cdot e^{-\mu_a z_i}$ at $1 < i \le N$;

$$F_+^{i-1}(h) = \begin{cases} F_+^{i-1}(0)\cdot e^{-\mu_a h} \text{ at } i > 1 \\ F_0\cdot e^{-\mu_a h/2} \text{ at } i = 1 \text{ (first heterogeneity).} \end{cases}$$

Because flux from the right is absent, the closing condition for $F_-^{i=N}(0)$ is:

$$F_-^{i=N}(0) = F_+^{i=N}(h)\cdot R\cdot e^{-\mu_a h}. \qquad (8)$$

Solution of Eqs. (7) and (8) with respect to $2N$ unknown fluxes $F_+^i(0)$ and $F_-^i(0)$ is reduced to solution of a set of $2N$ linear algebraic equations [19], which is rather simple.

The fluxes at external (crumbly) borders of pile (total back-scattered flux F_{bs} and transmitted flux F_τ) after calculation of $F_+^i(z_i)$ and $F_-^i(z_i)$ from Eq. (6) can be determined from:

$$F_{bs} = F_-(0) = F_0\cdot R\cdot e^{-\mu_a h} + F_-^{i=1}(0)\cdot(1 - R)\cdot e^{-\mu_a h/2},$$

$$F_\tau = F_+(H_0) = F_+^{i=N}(h)\cdot(1 - R)\cdot e^{-\mu_a h/2}, \qquad (9)$$

where F_0 is external radiation flux incident to the pile model from the left.

The solution of the problem using the KM method requires explicit solutions of Eq. (1) using actual optical and physical properties of the model: μ_a, R, N, and H_0. These solutions cannot be found phenomenologically because even if Eqs. (4) and (5) are valid, *a priori* expression for S is problematic [13]. A more rigorous approach is based on derivation of all expressions.

Let the set of simultaneous equations (1) be recast as:

$$\begin{cases} dF_+(x)/dx = -\beta_1 F_+(x) + \beta_2 F_-(x) \\ dF_-(x)/dx = -\beta_1 F_-(x) - \beta_2 F_+(x). \end{cases} \qquad (10)$$

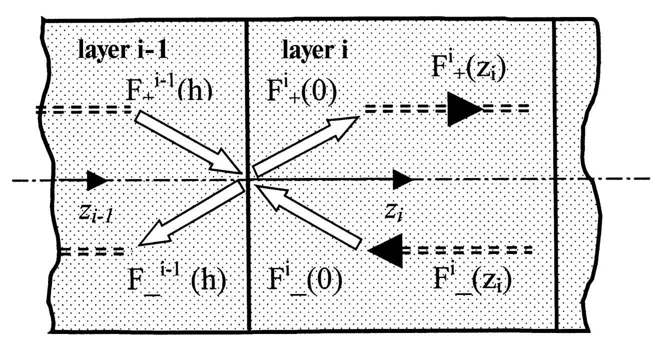

Fig. 2. Local frame of references and determination of fluxes in the *i*-th pile layer.

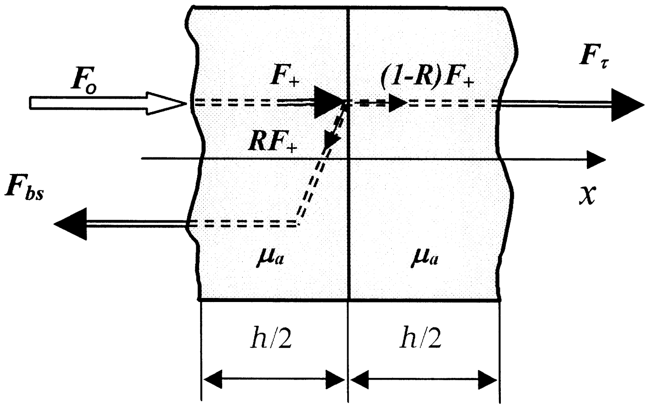

Fig. 3. A layer of medium with one heterogeneity in the middle.

Consider the explicit expression for radiation transformation coefficients β_1 and β_2 with respect to parameters μ_a, R, N, and H_0 of the pile model and solution of Eqs. (10), (6), (9) for fluxes F_{bs} and F_τ. For the sake of simplicity consider Gurevich equations [6] for F_{bs} and F_τ in two-flux approximation[2]:

$$F_{bs} = F_0 \cdot P \cdot (1 - e^{-2LH_0})/(1 - P^2 e^{-2LH_0});$$

$$F_\tau = F_0 \cdot e^{-LH_0} \cdot (1 - P^2)/(1 - P^2 e^{-2LH_0}), \quad (11)$$

where $L = (\beta_1^2 - \beta_2^2)^{1/2}$; $P = (\beta_1 - L)/\beta_2$. Regardless of layer thickness (H_0) and external flux (F_0), parameter:

$$[1 + (F_{bs}/F_0)^2 - (F_\tau/F_0)^2]/[2(F_{bs}/F_0)] = J = \text{const}, \quad (12)$$

is invariable, i.e., it is a photometric invariant typical of medium element Δx. Because Eqs. (11) and (12) are valid for any layer of any scattering medium, it is safe to suggest that they are valid for our model $H_0 = h$ with only one heterogeneity. A layer of medium with one heterogeneity in the middle is shown in Fig. 3. Expressions for F_{bs} and F_τ can be derived using parameters μ_a, R, N, and H_0. Introduction of mean density of heterogeneities gives:

$$\mu_\rho = N/H_0, \quad (13)$$

at $h = 1/\mu_\rho$ for photometric propagation of radiation fluxes in one layer with one heterogeneity:

$$F_{bs} = F_0 \cdot R \cdot e^{-\mu_a/\mu_\rho}; \; F_\tau = F_0(1 - R) \cdot e^{-\mu_a/\mu_\rho}. \quad (14)$$

Let Eq. (11) be identical to Eq. (14) for similar radiation fluxes. Replacing in Eq. (11) H_0 by $h = 11/\mu_\rho$ and eliminating F_0 in the left and right parts of the equations, we obtain a set of two simultaneous algebraic equations with two variables β_1 and β_2. Expressions for β_1 and β_2 can be easily derived:

$$\beta_1 = \omega \cdot \frac{\mu_a - \mu_\rho \ln(1-R) + \mu_\rho \ln\left(1 - \omega + \sqrt{\omega^2 - R^2 e^{-2\mu_a/\mu_\rho}}\right)}{\sqrt{\omega^2 - R^2 e^{-2\mu_a/\mu_\rho}}},$$

$$\beta_2 = R \cdot e^{-\mu_a/\mu_\rho} \cdot$$

$$\cdot \frac{\mu_a - \mu_\rho \ln(1-R) + \mu_\rho \ln\left(1 - \omega + \sqrt{\omega^2 - R^2 e^{-2\mu_a/\mu_\rho}}\right)}{\sqrt{\omega^2 - R^2 e^{-2\mu_a/\mu_\rho}}}, \quad (15)$$

where $\omega = [1 - (1 - 2R) \cdot e^{-2\mu_a/\mu_\rho}]/2$.

Dependence of transport coefficients in Eq. (10) on actual optical and physical properties of medium is not obvious *a priori*. For β_1 this dependence is not analogous to $\beta_1 = (K + S)$ in Eq. (1):

$$\beta_1 = k\mu_a + \beta_2,$$

where k is any numerical coefficient, because it follows from Eq. (15) that:

$$\beta_1 = [\omega \cdot e^{2\mu_a/\mu_\rho} \cdot \beta_2]/R.$$

Equation (15) can be compared to expressions derived in [7, 13, 23, 26]. For medium with $\mu_a = 0$ an exact expression was derived [26]:

$$\beta_1 = \beta_2 = \beta_m = \mu_\rho R/(1 - R). \quad (16)$$

For Eq. (15):

$$\lim_{\mu_a \to 0} \beta_1 = \lim_{\mu_a \to 0} \beta_2 = \beta_m,$$

in the absence of absorption, Eq. (15) tends to Eq. (16). Single scattering equations derived in [7] can be recast as:

$$\beta_1 = \mu_a - \mu_\rho \cdot \ln(1 - R),$$

$$\beta_2 = R \cdot e^{-\mu_a/\mu_\rho} \cdot [2\mu_a - \mu_\rho \ln(1 - R)]/[1 - R \cdot e^{-2\mu_a/\mu_\rho}]. \quad (17)$$

[2] Strictly speaking, Gurevich equations differ from initial differential Eqs. (1) and (10). However, the solution of Eq. (11) for fluxes F_{bs} and F_τ is identical to the solution of Eq. (10) for a general system of flux equations.

This is consistent with Eq. (15) in the absence of absorption.

The set of simultaneous equations (10) and Eq. (15) can be solved similarly to Eq. (2) and set of simultaneous equations (1) with parameters:

$$\alpha = L = (\beta_1^2 - \beta_2^2)^{1/2};$$

$$A_+ = [\beta_1 + \beta_2 + \alpha]/[\beta_1 + \beta_2 - \alpha] \text{ and } A_- = 1/A_+. \quad (18)$$

Integration constants C_1 and C_2 in Eq. (2) are found from boundary conditions:

$$F_+(0) = F_0 \text{ and } F_-(H_0) = 0. \quad (19)$$

The radiation field distribution inside and at the borders of the model medium can be calculated by solving the set of simultaneous equations (10), Eqs. (2), (15), (18), and (19).

Numerical Examples and Discussion

Let us consider numerical examples. The field of unit radiation $F_0 = 1$ for model medium with various parameters is shown in Fig. 4. The parameters are: $N = 3$, $H_0 = 1.5$ cm; $R = 0.4$; $\mu_a = 0.5$ cm^{-1}. In calculations the following equations were used: Eqs. (6)-(9) and KM method equations (10), (15), (18), and (19). Results of the single scattering (SS) approximation based on Eqs. (10) and (17) and KM classical model were considered for comparison using *a priori* relationships:

$$\beta_1 = \mu_a + \beta_2; \ \beta_2 = \beta_m = \mu_\rho R/(1 - R). \quad (20)$$

Vertical lines indicate three heterogeneities in the medium. Radiation flux distribution in this model is piecewise continuous (stepwise) with indefinite derivatives in breaking points of the first order. Therefore, the KM approach has no accurate solution regardless of medium parameters, because this method operates with fluxes with definite first and second derivatives. According to [3], if N is large ($N \to \infty$), any piecewise continuous function would tend to a smooth function. Therefore, the KM functions are reduced to a smooth function. Solution of Eq. (15) gives accurate values of backscattered and transmitted fluxes, i.e., for fluxes F_{bs} and F_τ measured experimentally. The difference is maximal for F_{bs}. Therefore, if approximation and/or model are selected incorrectly, optical properties of the medium are reconstructed from F_{bs} with maximum error.

Let us consider calculation error of F_{bs} as function of optical properties of the model medium. The ratio of fluxes F_{bs} to accurate value F_{bs} for different approxima-

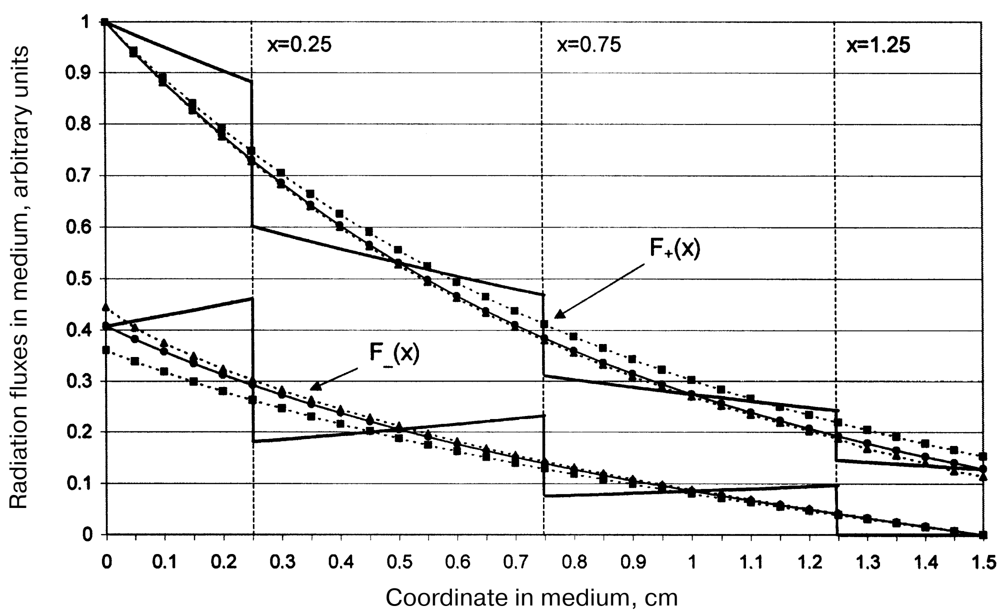

Fig. 4. Field of unit radiation $F_0 = 1$ for model medium with parameters: $N = 3$, $H_0 = 1.5$ cm; $R = 0.4$, $\mu_a = 0.5$ cm^{-1}; exact solution (solid line); model solution using Eqs. (10) and (15) (circles); SS approximation using Eqs. (10) and (17) (rectangles); classical KM method using Eqs. (10) and (20) (triangles).

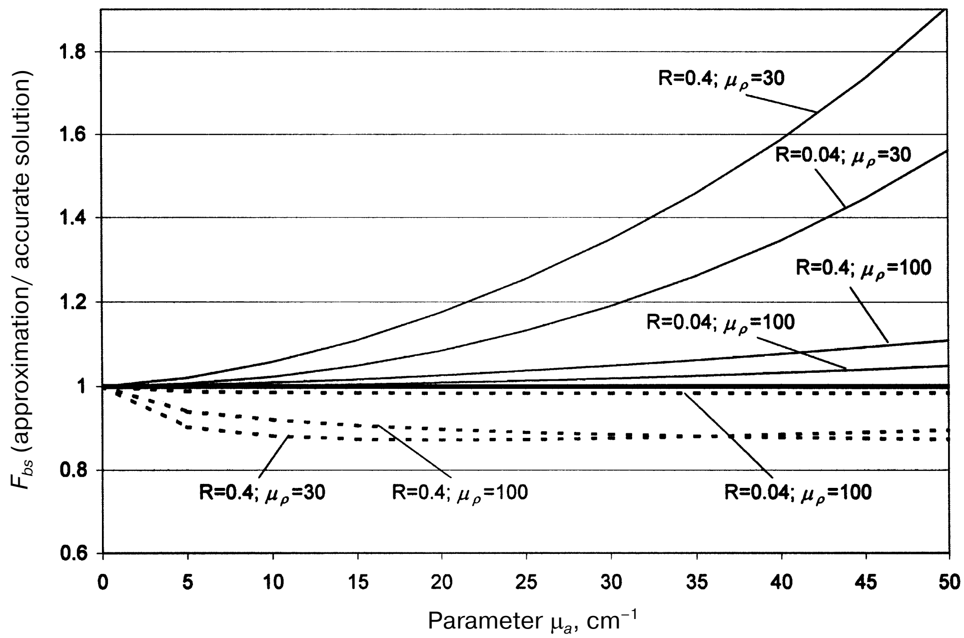

Fig. 5. Ratio between approximate and accurate values of F_{bs} for different approximations and optical properties of medium. Calculation for semi-indefinite layer: SS approximation using Eqs. (10) and (17) (dashed line); classical KM method using Eqs. (10) and (20) (solid line).

tions and optical properties of medium is shown in Fig. 5. Calculation was made for the semi-indefinite layer ($H_0 \rightarrow \infty$). The SS approximation of F_{bs} using Eqs. (10), (15), and (17) and classical KM method using Eqs. (10) and (20) together with Eqs. (6)-(9) were used. As expected, the ratio of flux calculated using Eqs. (10) and (15) and the result of accurate photometric calculation was 1 (error is absent). Other approximations give error increasing with R, μ_a and decreasing with μ_ρ. Generally, the error could be up to 20-30%.

The solution of the set of simultaneous equations (10) and Eq. (15) gives the exact value of flux F_{bs} over all range of parameters μ_a, R, N, and H_0. Therefore, *a priori* separation of β_1 into two independent coefficients K and S is not correct for initial KM models (1). This is true for the general transition equation. The classical transition equation *a priori* can be separated into two parameters μ_a and μ_s, where μ_s is a linear scattering coefficient similar to S [1, 2, 8]. True optical properties of medium elementary element were discussed in [2]. It follows from Eq. (15) and the pile model that scattering and absorption of radiation in the medium elementary element cannot be divided into two independent processes. Eq. (15) at $R < \mu_a/\mu_\rho < 1$ for β_1 can be divided into two independent parameters:

$$\beta_1 = \mu_a + R\mu_\rho \cong \mu_a - \mu_\rho \ln(1 - R), \qquad (21)$$

which is similar to Eq. (17). Equation (4) is doubtful. Solution of the general transition equation was not compared in [25] with the solution of a set of simultaneous equations (1). Solution of the set of simultaneous equations (1) was compared with solution of 22-flux model, and Eq. (4) was solved approximately. The KM model (1) at $R \rightarrow 0$ or $\mu_\rho \rightarrow 0$ is reduced to the Bouguer law (3). Equations (15) at $R \rightarrow 0$ give:

$$\beta_1 = \mu_a; \ \beta_2 = 0. \qquad (22)$$

If Eq. (4) is valid regardless of medium scattering, the KM model (1) in the absence of scattering gives twice larger exponent of the Bouguer law (3) than the transition equation, which is doubtful.

Thus, the set of simultaneous equations (10) in combination with Eq. (15) give a more substantiated result. Coefficients β_1 and β_2 in Eq. (10) are effective optical parameters (single scattering approximation (17), scatteringless approximation (22), approximation (16), etc.). Reconstruction of actual optical properties of the medium from measuring data F_{bs} in computation algorithms of diagnostic devices requires standard determination of β_1 and β_2 and solution of the set of simultaneous equations (15). The set of simultaneous equations (15) for different models is written differently.

The set of simultaneous equations (15) is widely discussed in the literature on biomedical optics. Similar expressions were derived in [12, 18, 21, 22]. In contrast to set of simultaneous equations (15), these expressions were derived in the invariant form rather than explicitly like Eq. (12). Using correlation between coefficients

$$\beta_1 = \beta_2 \cdot J, \quad (23)$$

which can be easily derived from Eq. (15) due to the following equation[3]

$$J = (\omega \cdot e^{2\mu_a/\mu_\rho})/R, \quad (24)$$

Eq. (1) was substituted into Eq. (23) together with

$$\beta_1 = K + S; \beta_2 = S,$$

in [18, 21, 22].

This substitution gave the erroneous expression

$$K = S(J - 1).$$

However, this expression would be valid for the model considered in this work if Eqs. (21) and (5) were valid.

Let us consider Eq. (23). A similar expression was derived in [10]. For optical tomography this expression simplifies the problem of the inverse task to one independent variable. It follows from Eq. (23) that this expression may have a broader meaning.

Conclusion

In the transition theory and KM flux models based on heuristic initial differential equations, it is somewhat incorrect to postulate for the general case of any model medium that the first coefficient in the right part of the equations represents separated parameters μ_a and μ_s (K and S). This causes errors in calculation of direct problems and calculation of backscattered light flux and reconstruction of optical properties of medium from measured data. Reconstruction of actual optical properties of medium from measuring data in computation algorithms of diagnostic devices requires standard determination of various parameters and solution of the set of simultaneous equations (15). Calculation of transport coefficients is the task of the inverse problem of biomedical optics, particularly in the practice of noninvasive medical spectrophotometry.

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[3] Because invariant J does not depend on medium thickness, Eq. (24) can be derived from Eq. (12) by simple substitution of fluxes from Eq. (14) for layer h with one heterogeneity.

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