Improved Kubelka-Munk approach for determination of tissues' optical properties in biomedical noninvasive reflectance spectroscopy

Lapaeva L.G., Rogatkin D.A.

Moscow Regional Research & Clinical Institute "MONIKI"
Shepkina str., 61/2, Moscow, 129110, RF
tel. 7-495-631-73-17, email: laserrog@mtu-net.ru

ABSTRACT

The Kubelka-Munk (KM) two-flux light transport one-dimensional (1D) model is, evidently, the most widely used transport theory in biomedical optics because of its simplicity and existence of its clear analytical solution. Moreover, the KM approach is a good approximation of the general radiative transport equation in the case of 1D theoretical tasks. But it is well known that the KM model doesn't allow anyone to obtain an exact solution, especially in cases of highly-absorbing and weakly-scattering media. In the most of publication it is assumed that the light must be diffuse on a surface as well as within the medium for a correct application of the KM equations. However, in our opinion, there is no any reason to separate light radiation on diffuse and collimated components in a simple 1D theoretical model. So, the root of the problem of the model accuracy may be located in a far another field. As we reported in our previous publications more correct results with the use of KM basic approach in some special cases of turbid media can be yielded by means of some modification of original KM equations. In this work we propose a general improvement of 1D two-flux KM model for any cases of scattering and absorbing media to reach an exact analytical solution of any theoretical 1D light propagation and scattering problem in application to biomedical noninvasive reflectance spectroscopy.

Keywords: backscattering, absorption, biomedical spectroscopy, transport theory, Kubelka–Munk approach.

1. INTRODUCTION

The original KM model is a well-known two-flux model[1] with two fluxes $F_+(x)$ and $F_-(x)$ of light traveling into the medium in forward and reverse directions. The optical properties of medium are described by transport absorption (K) and scattering (S) coefficients. The KM differential equations describing the radiant energy balance on dx of medium are:

$$\begin{cases} dF_+(x)/dx = -(K+S)F_+(x) + SF_-(x) \\ dF_-(x)/dx = (K+S)F_-(x) - SF_+(x) \end{cases} . \quad (1)$$

System (1) has an exact analytical solution:

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

where:

$$\alpha = \sqrt{K(K+2S)}\,;\ A_+ = (K+2S+\alpha)/(K+2S-\alpha)\,;\ \ A_- = 1/A_+ .$$

For biomedical noninvasive spectroscopy it is interesting to find a backscattered F_{bS}= *F_(0)* or a transmitted by a tissue flux F_τ= *F+(H0)* with the next calculation of *S* and/or *K*. Transport coefficients *S* and *K* determine optical properties of tissue, so the correct calculation of them is the key step of the next correct medical diagnosis. One of the applications of noninvasive medical spectroscopy is the tissues reflectance oximetry. The main point of this technique is a comparison of calculated *K* from a real patient examination with those one which obtained in laboratory experiments for oxy- and/or deoxy- hemoglobin fractional solutions. A conventional setup of the laboratory "in vitro" spectrophotometry experiment is:

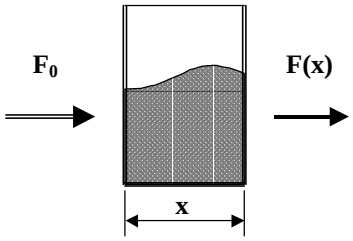

Fig.1. Conventional setup of the laboratory spectrophotometry experiment (in vitro).

With the use of well-known Bouguer Law (BL):

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

a transport absorption coefficient (μ_a) for different hemoglobin fractions can easy be calculated form (3) because in this case the light scattering into the weak-concentrated solution can be neglected. For noninvasive medical spectroscopy there is a high scattering into the tissues, so another than (3) calculation algorithms, for example system (1), must be applied to find out *S* and *K*. So, the main our question is: Can we consider *K* of the KM model equivalent μ_a of the BL? And the next question is: can KM model provide an exact F_{bS} and F_τ values to calculate *K* accurately? From the literature[2] we know:

$$K \approx 2\mu_a . \tag{4}$$

But, if so, in a case of *S=0* the KM equations (1) will yield as a solution a BL with a twice absorption, that is quite doubt. From the other hand, the KM model is assumed to be valid in the case of the diffuse irradiation only. But what is the difference between diffuse and collimated light in the 1D problem?

This and some other questions push researchers to investigate and modify KM approach during a long time[3–6]. In this paper we proposed a general, simple and exact analytical method to improve a 1D two-flux KM model for any cases of scattering and absorbing media. It allowed us to reach in a closed form an exact analytical solution of any theoretical 1D light scattering problem in application to biomedical noninvasive spectroscopy, i.e. in application to calculate accurately backscattered and transmitted by a tissue radiation fluxes. Our approach allowed to determine real relations between μ_a and KM model's transport coefficients (*K* and *S*) as well.

2. SIMPLE THEORETICAL PROBLEM

Let's take into consideration a simple model of scattering media as shown in figure 2. We assume a homogenous medium with transport absorption coefficient μ_a and a number of reflecting heterogeneities r_i (i = 1, 2, 3….n) into it. In a case of n>>1 such model is a good approximation of any 1D media with a multiple scattering caused by multiple light reflections between heterogeneities. Moreover, this task has an exact photometric solution for any $F_i(x)$ with the use of the BL and reflecting boundary conditions on all heterogeneities. It allows anyone to test any 1D theoretical model.

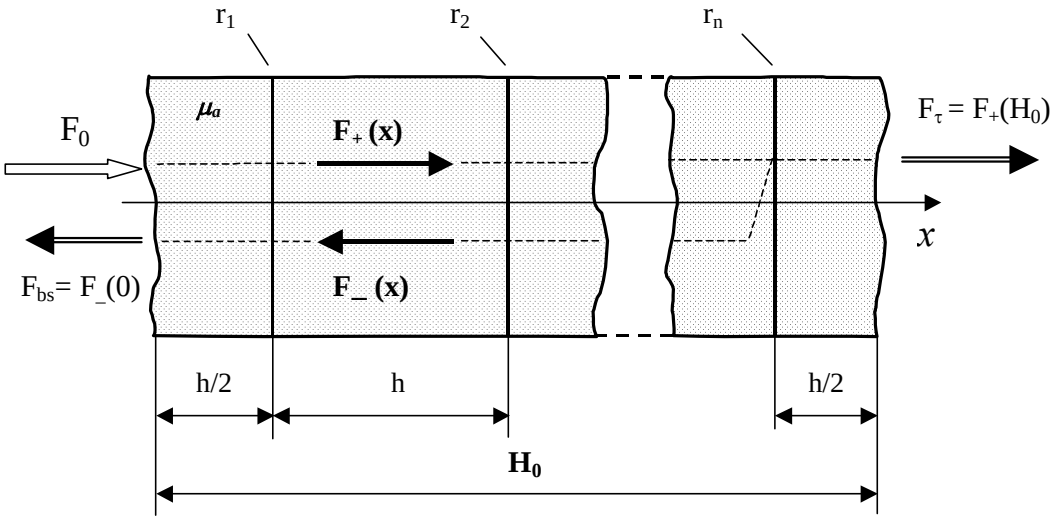

Fig.2. Geometry of the problem.

Let's introduce a local coordinate system z_i ($z_i \in [0,h]$) for each layer between r_i. Let all $r_1=r_2=\ldots r_n=R$ and n=N. Then:

$$F_+^i(z_i) = F_+^i(0)\cdot e^{-\mu_a z_i} \quad \text{and} \quad F_-^i(z_i) = F_-^i(0)\cdot e^{\mu_a z_i}\ , \tag{5}$$

Boundary magnitudes of fluxes for each i-th layer can be calculated with the use of geometry in a fig.3 as follows:

$$\begin{aligned} F_+^i(0) &= F_+^{i-1}(h)\cdot(1-R) + F_-^i(0)\cdot R \\ F_-^{i-1}(h) &= F_+^{i-1}(h)\cdot R + F_-^i(0)\cdot(1-R)\,, \end{aligned} \tag{6}$$

where: $F_-^{i-1}(h) = F_-^{i-1}(0)\cdot e^{\mu_a z_i}$ $(1< i \le N)$; $F_+^{i-1}(h) = \begin{cases} F_+^{i-1}(0)\cdot e^{-\mu_a h} & (i>1) \\ F_0\cdot e^{-\mu_a h/2} & (i=1) \end{cases}$; $F_-^{i=N}(0) = F_+^{i=N}(h)\cdot R\cdot e^{-\mu_a h}$.

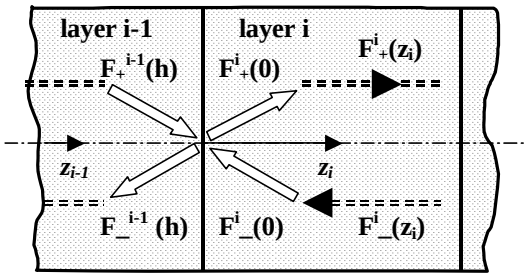

Fig.3. Geometry of internal boundary processes.

From all of that it is easy to yield:

$$F_{bs} = F_-(0) = F_0 \cdot R \cdot e^{-\mu_a h} + F_-^{i=1}(0) \cdot (1-R) \cdot e^{-\mu_a h/2} \ ;$$
$$F_\tau = F_+(H_0) = F_+^{i=N}(h) \cdot (1-R) \cdot e^{-\mu_a h/2} \quad . \tag{7}$$

Now we will try to use the KM approach for the same model. We'll consider the general representation of the system (1) as follows:

$$\begin{cases} dF_+(x)/dx = -\beta_1 F_+(x) + \beta_2 F_-(x) \\ dF_-(x)/dx = \beta_1 F_-(x) - \beta_2 F_+(x) \end{cases} \tag{8}$$

and will try to find out an accurate dependences of coefficients β_1 and β_2 on real optical properties of our model – N, H_0, R and μ_a. The system (8) has a well-known solution in terms of backscattered and transmitted radiation[7]:

$$F_{bs} = F_0 \cdot P \cdot \frac{1-e^{-2LH_0}}{1-P^2 e^{-2LH_0}} \ ; \quad F_\tau = F_0 \cdot e^{-LH_0} \cdot \frac{1-P^2}{1-P^2 e^{-2LH_0}} \ , \tag{9}$$

where: $L = \sqrt{\beta_1^2 - \beta_2^2}$ and $P = (\beta_1 - L)/\beta_2$. (10)

Equations (9) are valid for any thickness H_0 of medium, so they are valid for our model and thickness of picked out one layer "h" as it is shown in a fig.4:

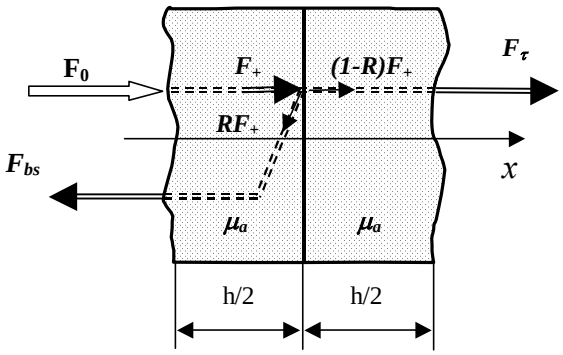

Fig.4. One scattering layer of 1D phantom of turbid media.

Introducing a transport density of heterogeneities

$$\mu_\rho = N/H_0 \tag{11}$$

as well as taking into consideration the external boundary conditions in the simplest form

$$F_+(0) = F_0 \ ; \quad F_-(H_0) = 0 \tag{12}$$

we obtain our general dependencies:

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

$$\beta_2 = R \cdot e^{-\mu_a/\mu_\rho} \cdot \frac{\mu_a - \mu_\rho \ln(1-R) + \mu_\rho \ln(1-\omega+\sqrt{\omega^2 - R^2 e^{-2\mu_a/\mu_\rho}})}{\sqrt{\omega^2 - R^2 e^{-2\mu_a/\mu_\rho}}}, \qquad (13)$$

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

Thus, in a light of our questions, in a common case we can't write $\beta_1 = k\mu_a + \beta_2$ where *k* is any constant, because as it follows from (13):

$$\beta_1 = \frac{\omega \cdot e^{\mu_a/\mu_\rho}}{R} \cdot \beta_2 \quad . \qquad (14)$$

3. CALCULATIONS

In order to test our results let's consider a visual simple numeric example: F_0=1; N=3; H_0=1.5cm; R=0.4; μ_a=0.5cm^{-1}. For this example fig. 5 represents radiant fluxes magnitudes versus a depth of our media phantom. An exact photometric solution (5)-(7) is denoted by stepped bold solid line. Our approach with the use of (8)-(13) is denoted by solid line with dark circles. For comparison, a single scattering approximation (SSA) of KM method[6] as well as the standard multiple scattering (SMS) KM approach with coefficients [5]:

$$K = \mu_a \qquad \text{and} \qquad S = \frac{R\mu_\rho}{1-R}. \qquad (15)$$

also were calculated and denoted in fig. 5 by dotted lines with square and triangle markers accordingly. As it follows from numeric results (fig.5), with respect to exact solution, only our approach can give the same result (without error) on external boundaries of our 1D scattering medium phantom. Any other KM approach (SSA or SMS) shows an error in calculated fluxes on boundary surfaces. And this mistake, especially for F_{bS} , increases with the increase of μ_a . Figure 6 shows this tendency for F_{bS} in a case of half-infinite medium. In fig.6 we presented relations of different KM approximations results and exact photometric one versus μ_a. Our approach has relation "1" along all values of μ_a (solid bold line). Classic SMS KM approach has the biggest error (solid lines) when μ_a >20 cm^{-1} and when there are not a lot of heterogeneities into the medium. A middle miscalculation appears for SSA of KM method (dotted lines) with a tendency to decreasing errors when a reflection on boundary surfaces of heterogeneities falls down.

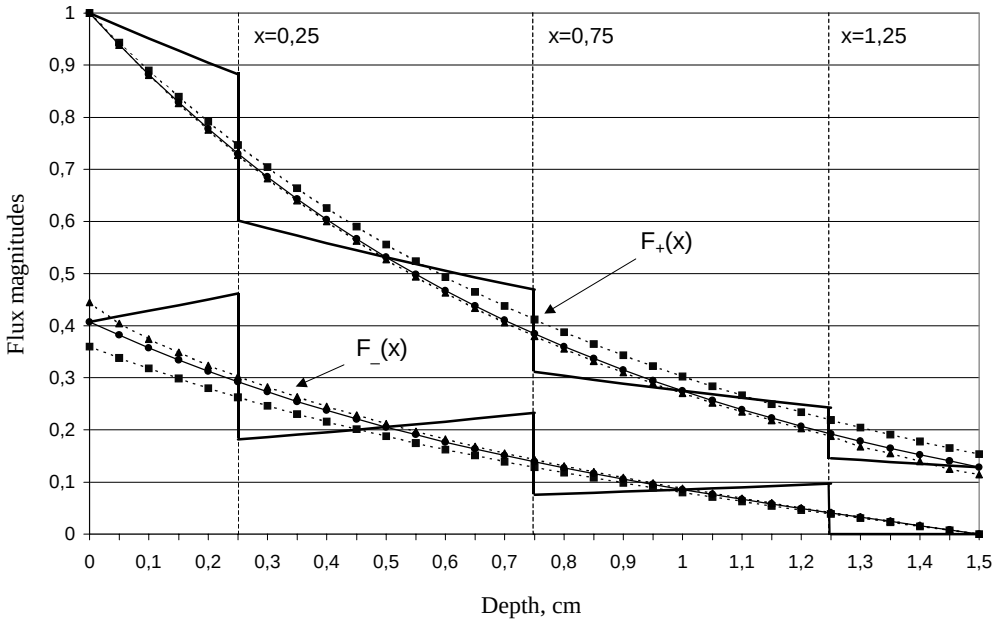

Fig. 5. Results of numeric calculation example.

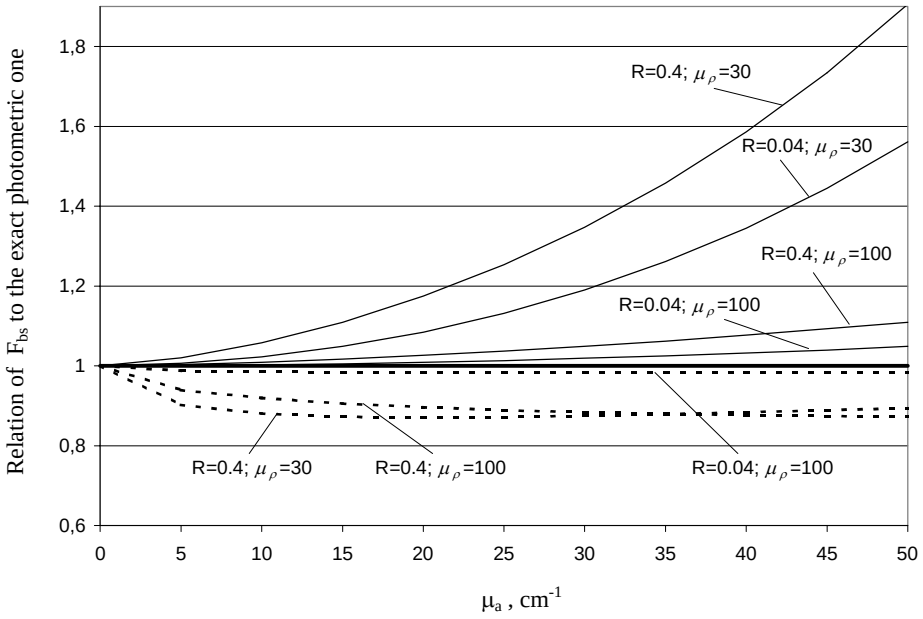

Fig. 6. Errors in F_{bs} with the increase of absorption.
Solid lines – SMS KM method; dotted lines – SSA of KM.

4. DISCUSSION

In our opinion, we have yielded quite interesting result, especially equations (13). They show, that in the general light transport theory there are a number of tasks where we can't separate easily absorption and scattering transport coefficients in equations (*K* and *S* in the KM approach). Such separation and independence of *K* on *S* in the classical transport theory is a consequence of the accepted radiant energy balance formalism into the elementary volume of medium. But in a number of cases, for our 1D model in instance, both an absorption and scattering processes are not independent. Moreover, it comes into operation the so-called (and today quite forgotten) in photometry ***Invariant*** [7]:

$$\frac{1+(F_{bs}/F_0)^2-(F_\tau/F_0)^2}{2(F_{bs}/F_0)} = J = const$$

because it could be shown from (13) that:

$$\beta_1 = \beta_2 \cdot J \qquad (16)$$

$$\text{or} \qquad \beta_1 = \frac{\omega \cdot e^{\mu_a/\mu_\rho}}{R} \cdot \beta_2 \quad .$$

Namely the use of (16) by a number of authors leads to a small error in some publications. Substituting into (16) as we now see in a general case the wrong values

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

they obtain (for example [8], eq. 1.24) the wrong formula

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

which is used then, in that number, in the applied biomedical oximetry and spectroscopy. The numerical error, as we see in fig. 5-6, is not very much for low absorption and strong scattering – the main situation in the biomedical optics. But for another situation and media this mistake can increase dramatically. And quite wrong will be the procedure to use a twice absorption $2\mu_a$ for substitution it into "*K*" of KM classical approach.

5. CONCLUSION

First of all, we can conclude that there is a complex dependence of KM differential equations' coefficients β_1 and β_2 on real optical properties of medium. In a general case we can't represent the first coefficient of KM equations (β_1) as a sum of two independent transport parameters *K* and *S*. To calculate, for example, a correct theoretical value of backscattered flux on a boundary surface of our 1D medium (that is important for a medical noninvasive spectroscopy) we had to use the complex formulas (13) for preliminary calculation of system's coefficients β_1 and β_2. Only with the use of that our modified KM approach, as it was shown, can provide an exact result for any boundary fluxes.

From the other hand, we can see now that <u>the answer on our main question is:</u> $K=\mu_a$. Only such equivalence gives a minimum miscalculation in F_{bS} if, of course, not to take into consideration our more correct and accurate equations (13).

ACKNOWLEGMENTS

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