Mathematical modelling of optical radiation transport in biological tissues under the conditions of moveable integrating spheres registration

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Abstract. To describe the propagation of radiation in biological tissue, it is crucial to know the tissue’s optical characteristics. Integrating spheres method is widely used for experimental determination of optical properties of biological tissues. In this method, radiation scattered by the test sample in forward and backward directions is detected by the integrating spheres, along with the radiation that passed through the sample without scattering. In order to increase information content of the measurements, a moveable integrating spheres method was proposed, allowing one to register scattered radiation at different distances from sample surface to sphere ports. In this work, using the multilayer Monte Carlo method a numerical simulation of radiation propagation in a turbid medium was carried out under the conditions of detecting scattered radiation by moveable and stationary integrating spheres. Random errors were added to the direct problem solution in order to simulate experimental inaccuracies. The corresponding inverse problems were solved and the errors arising in the determination of optical properties (albedo, scattering anisotropy, optical depth) were compared in the cases of moveable and fixed spheres. It is shown that the same error in the inverse problem input data leads to smaller root-mean-square deviation from the true values when reconstructing albedo and anisotropy with the moveable spheres method, compared to the classical stationary spheres approach.

1. Introduction
Laser radiation is widely used in various fields of medicine, such as ophthalmology (laser vision correction), urology (laser lithotripsy) or dermatology (removal of port-wine stains and cosmetic skin defects) [1,2]. In order to optimise spectral, temporal and energetic parameters of medical laser radiation, physical and mathematical modelling of interaction between light and biological tissues is used.

There are several approaches to describing interaction between optical radiation and turbid media. Propagation of monochromatic radiation in an isotropic macroscopically homogeneous medium without inelastic scattering can be described using the stationary light transfer equation:

\[\hat{s} \nabla L(r, \hat{s}) = - (\mu_a + \mu_s) L(r, \hat{s}) + \mu_s \int \frac{p(\hat{s}, \hat{s}' ) L(r, \hat{s}') d\omega'}{4\pi} + S(r, \hat{s}). \] (1)
In this equation, $L(r, \hat{s})$ is the brightness of radiation, propagating in the direction $\hat{s}$ at the point with the radius-vector $r$, $S(r, \hat{s})$ is the radiation source term; the integration is performed over the solid angle $d\omega'$. Medium is characterised by its optical properties (generally, depending on the radiation wavelength): scattering and absorption coefficients $\mu_s$ and $\mu_a$ and the scattering phase function $p(\hat{s}, \hat{s}')$. To describe boundary conditions, the refractive index $n$ (a real number) is introduced. In some cases, dimensionless parameters may be used: scattering anisotropy $g$ (mean cosine of the scattering angle), optical albedo $a = \mu_s/(\mu_s + \mu_a)$ and sample’s optical depth $\tau = l(\mu_s + \mu_a)$ (where $l$ is the sample thickness). In order to perform correct modelling of radiation propagation, the problem of determining optical properties of biological tissues turns out to be crucial.

Integrating spheres method is one of the classical techniques for determining optical properties of biological tissues. In this method, a flat sample of studied tissue is irradiated by a collimated laser beam, and using the integrating spheres with their ports close to the sample surface, forward- and back-scattered radiation is detected. Radiation that passed through the sample without scattering is also registered. Optical properties of the sample (absorption and scattering coefficients, scattering anisotropy) are then reconstructed with the help of mathematical modelling of laser-tissue interaction using the Monte Carlo method [3], inverse adding-doubling method [4] or multi-stream models [5]. Recently, an original moveable integrating spheres method was proposed [6], where measurements are conducted at different distances between sample surface and ports of spheres that detect forward- and back-scattered radiation. In this case information content of measurement results can be increased significantly, and the idea was put forward that this method may substantially reduce the errors in optical properties determining.

In this paper, numerical simulations of radiation propagation in a turbid medium under the conditions of detecting scattered radiation by moveable and stationary integrating spheres were carried out. In order to simulate experimental inaccuracies, the random errors were added to the simulation results; the inverse problems were solved to reconstruct the values of the sample’s optical properties. The errors, arising in the cases of scattered radiation detection by moveable and fixed spheres, were compared.

2. Formulation of the problem

Numerical simulations were carried out for the problem, where collimated radiation is normally incident on a flat sample surface that consists of a scattering medium 1 mm thick (with optical characteristics $a = 0.9$, $\tau = 1.0$, $g = 0.9$, $n = 1.5$, which are typical for biological tissues) sandwiched between two transparent glass slides 1 mm thick (with $n = 1.6$). After the interaction with the sample, the radiation was registered using three integrating spheres with diameters $D = 10$ cm and port diameters $d = 13$ mm (see Fig. 1): two moveable spheres for detection of forward- and back-scattered radiation, or diffuse transmission and reflection ($T$ and $R$ respectively) and one sphere for measuring the collimated radiation ($T_c$).

![Figure 1](image.png)

Figure 1. Scheme of the experiment for determining sample optical properties using moveable integrating spheres.

The mathematical modelling of radiation transport in the sample was performed using the multilayer Monte Carlo method [7]. Propagation of a bunch of photons in the sample was
modelled, dependencies of diffuse transmission and reflection fractions $T(z_T)$ and $R(z_R)$ on the distances between the sample surface and the sphere ports $z_T$ and $z_R$ were obtained (see Fig. 2), along with the collimated radiation fraction $T_c$, detected by the stationary sphere at a great distance from the sample. In the case of the fixed integrating spheres, three numbers $T(0)$, $R(0)$, $T_c$ were obtained as the simulation results.

Figure 2. Dependencies of radiation fractions detected by moveable integrating spheres on the distance between the sphere port and the sample surface.

To compare the efficiencies of the moveable and fixed integrating spheres methods, the error obtained in determining the set of optical properties $(a, \tau, g)$ in both cases was investigated. To do this, random absolute error with normally distributed magnitude (dispersion $\sigma = 10^{-3}$) was added to the data acquired by solving the direct problem (to every value of dependencies $R(z)$ and $T(z)$, and $T_c$). For moveable spheres, the distance $z$ was varied from 0 mm to 20 mm with a step of 2 mm.

Next, the distribution of the values of optical properties determined by solving the inverse problem was studied. The solution was obtained according to the following algorithm:

(i) Calculating the value of optical depth $\tau$ from $T_c$ according to Beer-Lambert formula;
(ii) Acquiring the initial approximation $a_0$ and $g_0$ from $R(0)$ and $T(0)$ values using inverse adding-doubling algorithm [8];
(iii) Determining of the values $a$ and $g$ that best describe the dependencies $R(z)$ and $T(z)$ (or match the values $R(0)$ and $T(0)$ in the case of fixed spheres), obtained by solving the direct problem with Monte Carlo method, using Nelder-Mead minimisation algorithm [9] (with starting points $a_0$ and $g_0$).

3. Simulation results
Figure 3 shows the box plot of the results of determining albedo $a$ and scattering anisotropy $g$ for the cases of moveable and fixed integrating spheres. It can be seen that the dispersion of $a$ and $g$ values, obtained by using the moveable integrating spheres method, is less than the dispersion in the classical approach. An overestimation of the results compared to the initial values of $a$ and $g$ is also observed in the case of fixed spheres.
Figure 3. Results of determining of albedo $a$ and scattering anisotropy $g$ obtained using the method of moveable integrating spheres (red) and classical fixed spheres (green).

The values of standard deviations $\sigma$ of the obtained parameters from their initial values ($a = 0.9$, $\tau = 1.0$, $g = 0.9$) are presented in Table 1. The errors in determining the optical depth $\tau$ are of the same order of magnitude in both cases: this is due to the fact that the value $\tau$ is derived from the value of the collimated radiation fraction $T_c$, which was calculated in the same way for both methods.

Table 1. Standard deviations of albedo $a$, scattering anisotropy $g$ and optical depth $\tau$ from their initial values in the conditions of solving the inverse problem by the methods of moveable and fixed integrating spheres.

|                      | Fixed spheres | Moveable spheres |
|----------------------|---------------|------------------|
| $\sigma_a \times 10^{-6}$ | 205           | 5.2              |
| $\sigma_g \times 10^{-6}$ | 183           | 4.1              |
| $\sigma_{\tau} \times 10^{-6}$ | 9.6           | 7.4              |

4. Conclusions
In this work, numerical simulations of the problem of light propagation in turbid medium and its registration by the moveable and stationary integrated spheres were carried out using the multilayer Monte Carlo method. To take into account errors that might arise in the course of a real experiment, the random errors with normal distribution were added to the calculated values. In order to determine optical properties of the sample from the obtained data, an inverse Monte Carlo algorithm with an initial approximation using the inverse adding-doubling method was implemented.

Based on the modelling, the errors in determining optical properties with the moveable integrating spheres were estimated. For the sample of scattering tissue ($l = 1$ mm, $a = 0.9$, $g =$
0.9, $\tau = 1.0$, $n = 1.5$) sandwiched between the transparent glass slides ($l = 1$ mm, $n = 1.6$) a set of parameters $a$, $\tau$, $g$ can be determined with the root-mean-square error of the order $10^{-6}$. It was also shown that with the same error in the input data, the root-mean-square deviation from the true values when determining albedo and scattering anisotropy with the method of moveable spheres is less compared to the classical approach. Thus, the method of moveable integrating spheres can be used to minimise the influence of the measurement error on the results of determining the optical properties of biological tissues.

5. References

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