Radiative transfer through multi-layered medium: high-frequency experiments and theory

Andrei Dergatchev, Rene A. Bolt and Frits F.M. de Mul
University of Twente, Department of Applied Physics,
P.O. Box 217, Enschede, 7500 AE, the Netherlands

ABSTRACT

Development of efficient analytical and numerical techniques for the determination of optical parameters of biotissues on the base of measured data is a crucial part of successful implementation of non-invasive diagnosis techniques in clinical conditions. Widely used approximations, like diffusion approximation (DA), were shown to fail in most real-life circumstances due to simplifications of modeling or neglect of various involved phenomena, like boundary effects, tissue inhomogeneity, skin roughness and deviations of optical properties of skin in time due to physiological effects.

In this work we compare experimental results with results of numerical simulations. For our measurements, we used both spatial-resolved and frequency-domain techniques. To describe propagation of photons we numerically solved the radiative transfer equation (RTE). We found that the Monte-Carlo method (MC) is too time-consuming for large source-detector separations. We achieved flexibility in preparation of experimental medium with tissue-simulating sample containing several homogeneous layers.

Our objective is the investigation of accuracy in determining unknown structures and optical coefficients from measured data, based on the realistic model of the tissue described in the RTE.

Keywords: Transport theory, discrete ordinates method

1. INTRODUCTION

In this contribution we present results of both high-frequency measurements and numerical simulations of radiative transfer through a multi-layered tissue-simulating sample. Investigation of radiative transfer through multi-layered sample is important for successful development of methods of non-invasive diagnosis. The ability to carry out the diagnosis procedure removes the necessity to physically interact with, or penetrate into, tissue, thus providing important advantages for many industrial technological applications. Another attractive field of possible applications of non-invasive technologies lies in the diagnosis of biotissues for various medical applications. The absence of physical interaction with biotissue means the preservation of the patient from pain and possible infections.

Detecting multiple-scattered photons it is not possible to directly measure optical parameters of hidden layers. Instead, a beam of radiation is incident into tissue and reflected radiation is observed. Observable quantities include various parameters such as intensity, angular distribution, time of flight distribution of detected photons etc. The solution of the problem of accurate measurement of such parameters is a first step in the diagnosis procedure.

From the viewpoint of medical applications, it is important to study a phenomenon of radiative transfer through multiple layers of homogeneous material, since it corresponds to real structure of human biotissue. While development of optical coherence tomography during last years provided a great tool for monitoring of surface and under-surface layers, layers located at depth more then 1 mm can not be accurately monitored and thus other techniques are required for such cases as monitoring of brain, cancer or blood vessels to name a few. We use results of experiments with multi-layered tissue-simulating phantom for testing of how successfully theoretical model based on radiative transfer theory (RTT) describes observed data.

2. THEORY

The ability to estimate optical parameters of inner tissue layers on the base of measured characteristics of radiation reflected from tissue is based upon the capability of accurate theoretical description of the phenomenon of propagation of radiation through scattering medium. Generally speaking, propagation of photons in media is a very complicated process. During

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propagation in the medium, photons are scattered and absorbed by particles of medium. The speed of propagation of photons is determined by the refractive index of the medium. The characteristics of a single scattering event - i.e. which direction the photon will take after scattering on a particle - is determined by the characteristics of the particles in medium. It is usually estimated basing on Mie theory. Direction of propagation of photons is also changed on boundaries between layers in the medium. In a case when the size of medium is not sufficiently large, reflectance of photons from boundaries must be taken into account. Also, the resulting detected radiation depends on the numerical aperture of the source fiber, determining with which angle the beam of incident photons will expand in medium.

So, besides scattering and absorption, the characteristics of a single scattering event (conveniently described as a phase function), the structure of the medium, boundary conditions between different layers in the medium and on its boundaries, various characteristics of the incident beam of radiation and the refractive index of the medium, all influence the distribution of photons. It is not possible to find analytical solutions describing such distribution for all but a very limited set of simple cases. Existing analytical approaches fail to include all these parameters in approximate solution. For example, we have shown[1] that boundary conditions influence the observed signal at a level which is measurable with high-accuracy techniques. So, for the description of real-life situations it is necessary to use a general analytical or numerical approach which will be capable of taking into account all important parameters for the particular case in consideration.

As we have said already, RTT does not provide an analytical solution for the intensity reflected from the medium in the general case of boundary conditions and spatial distribution of optical parameters. However, there were several numerical methods developed for the solution of the radiative transfer equation (RTE) which give approximated solution for reflected radiation. RTE is widely encountered in nuclear physics (neutron transport, reactor shielding) and atmospherical optics.

The final stage of the diagnosis procedure consists of finding a correspondence between measured parameters of the radiation reflected from medium with those theoretically predicted (for one or other structure and values of optical parameters of tissue) and determination of such spatial structure and quantitative values of optical parameters which are in a better agreement with experiment.

Besides precise experiments, accurate theoretical description of the phenomenon of radiative transfer is a key issue for successful diagnosis.

Despite major theoretical effort, to the moment there is no general approach which allows direct solution of the reverse problem of diagnosis, i.e. direct derivation of optical parameters of tissue basing on experimentally observed parameters. For the estimation of optical parameters and structure of inner layers of tissue practically everywhere an iterative procedure is used, during which at each step the convergence of computed to experimentally observed radiation reflected from tissue is achieved using slight deviation of structure and optical parameters of a model of tissue and recalculation till the difference between numerical solution and experiment becomes smaller than some predefined parameter. For this method, development of time-efficient approaches may require additional development of theoretical model of the phenomenon.

Another developed approach for tackling the solution of the reverse problem is used when structure and optical parameters of tissue under investigation are known from independent experiments. Then, it is possible to precalculate theoretically expected spatial distributions of optical parameters, which is dramatically accelerating the procedure of diagnostics, because of a considerable reduction of the region of initial uncertainty in unknown optical parameters and structure of tissue under investigation. And in some cases it is possible to use analytical formulas developed on the base of the diffusion approximation (DA) of RTE. In this case it is possible to estimate optical parameters basing directly on measured data. However, an accuracy of such approach is dependent critically on applicability of the DA to experimental conditions.

In present article we use the first approach, as we model a situation when diagnosis is to be performed on tissue about which no pre-measured optical parameters and estimation of structure is available.

3. PROBLEM FORMULATION

Consider a point source of collimated radiation and several detectors with known diameter and aperture function. We use a source to irradiate a scattering and absorbing medium and we use detectors to measure light reflected back from the surface of the medium from the same side where the source is placed. We want to determinate characteristics (such as amplitude, degree of polarization, angular dependence, pathlength distribution of detected photons etc) of detected radiation depending on optical parameters and structure of medium.

Various approaches exist for solution of this problem[4,5,8], analytical, approximated and numerical. We are looking for the general case of optical parameters (scattering, absorption coefficients and phase function), in which case analytical and approximated methods can not provide accurate predictions in general case.

In a reverse problem, one wants to determine (optical) parameters and structure of an unknown medium from measured parameters of reflected radiation (transmission mode can be also used but is more difficult to implement in biological applications).

The original time-dependent radiative transfer equation for the number $\varphi(\mathbf{r},\mathbf{\Omega},\mathbf{t})$ of photons per unit time per steradian in position $\mathbf{r}$ in direction $\mathbf{\Omega}$ is:

$$\left[\frac{1}{c}\frac{\partial}{\partial t}+\Omega\bullet\nabla+\mu_t\right]\varphi(r,\Omega,t)=\varepsilon(r,\Omega,t)+\frac{\mu_s'}{4\pi}\int\varphi(r,\Omega,t)p(r,\Omega\bullet\Omega')d\Omega' \quad (1)$$

where $\mu_t=\mu_t(\mathbf{r})$ is total attenuation coefficient, $\mu_s=\mu_s(\mathbf{r})$ is scattering coefficient, $p(\mathbf{r},\mathbf{\Omega}\bullet\mathbf{\Omega}')=p(\mathbf{r},\mathbf{\Omega}\bullet\mathbf{\Omega}',\mathbf{r})$ is scattering phase function, c is speed of light in the medium, $\varepsilon(\mathbf{r},\mathbf{\Omega},\mathbf{t})$ describes internal sources. The integral is taken over whole solid angle.

4. DERIVATION OF EQUATIONS FOR PARAMETERS OF AMPLITUDE-MODULATED SIGNAL

Numerical solution of the original RTE (1) is a formidable task because of memory requirements - one need to store 3D spatial data, times 2D angular data times 1D time data, which sums up to unacceptable requirements (100X100X100 for spatial distribution times 80 angular times 8 bytes already sums up to 640 MB and we haven't even took into account time) if one is looking for accurate high-resolution estimations. For frequency-domain applications, however, it is possible to simplify numerical calculations. We note that for sinusoidally amplitude-modulated radiation source of the form:

$$\varepsilon(r,\Omega,t)=\varepsilon_0+\varepsilon_1\sin\omega t \quad (*)$$

we are looking for a solution of the RTE in the form

$$\varphi(r,\Omega,t)=\varphi_0+\varphi_1(r,\Omega)\sin(\omega t+\delta(r,\Omega)) \quad (**)$$

because typical intensities are too small to cause any non-linear effects in biotissue. $\varphi_1(r,\Omega)$ is a modulation and $\delta(r,\Omega)$ is a phase shift. So, instead of determination of time-dependent variable $\varphi(r,\Omega,t)$ we are solving equations for two time-independent variables $\varphi_1(r,\Omega)$ and $\delta(r,\Omega)$.

Substituting (**) into original equation (1) we get :

$$\frac{\omega}{c}\varphi_1\cos(\omega t+\delta)+\Omega\nabla\varphi_0+\Omega\nabla\varphi_1\sin(\omega t+\delta)+\varphi_1\Omega\nabla\delta\cos(\omega t+\delta)+\mu_t\varphi_0+\mu_t\varphi_1\sin(\omega t+\delta)=$$
$$\varepsilon_0+\varepsilon_1\sin\omega t+\mu_s\int d\Omega' p(\Omega,\Omega')\varphi_0+\mu_s\int d\Omega' p(\Omega,\Omega')\varphi_1(r,\Omega')\sin(\omega t+\delta(r,\Omega'))$$

And splitting for $\sin\omega t$ and $\cos\omega t$ parts which must be equal to each other for both sides of the equation, we get 2 equations:

$$-\frac{\omega}{c}\varphi_1\sin\delta+\Omega\nabla\varphi_1\cos\delta-\varphi_1\Omega\nabla\delta\sin\delta+\mu_t\varphi_1\cos\delta=\varepsilon_1+\mu_s\int d\Omega' p(\Omega,\Omega')\varphi_1(r,\Omega')\cos\delta(r,\Omega')$$

and

$$\frac{\omega}{c}\varphi_1\cos\delta+\Omega\nabla\varphi_1\sin\delta+\varphi_1\Omega\nabla\delta\cos\delta+\mu_t\varphi_1\sin\delta=0+\mu_s\int d\Omega' p(\Omega,\Omega')\varphi_1(r,\Omega')\sin\delta(r,\Omega')$$

which by multiplication with $\sin\delta$ and $\cos\delta$ and addition and subtraction of resulting expressions can be further transformed to:

$$\Omega\nabla\varphi_1 + \mu_t\varphi_1 = \varepsilon_1\cos\delta + \mu_s\int d\Omega' p(\Omega,\Omega')\varphi_1(r,\Omega')\cos(\delta(r,\Omega') - \delta(r,\Omega))$$

and (2)

$$\frac{\omega}{c}\varphi_1 + \varphi_1\Omega\nabla\delta = \mu_s\int d\Omega' p(\Omega,\Omega')\varphi_1(r,\Omega')\sin(\delta(r,\Omega') - \delta(r,\Omega)) - \varepsilon_1\sin\delta$$

5. DESCRIPTION OF SIDOM (SOURCE-ITERATION DISCRETE ORDINATE METHOD)

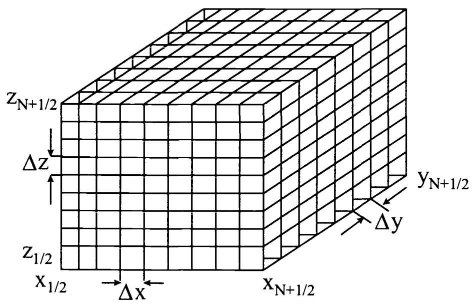

Illustration of spatial discretization

The SIDOM[2] was originally developed for applications in nuclear physics for calculations of neutron transport. It is a method for numerical solution of the radiative transfer equation (RTE) which can be derived from transport theory.

The SIDOM can be used for arbitrary spatial distribution of μ'_s, μ_t, $p(\mathbf{r},\Omega\bullet\Omega')$ and c (which depends on refractive index of medium), for arbitrary kind of single-scattering phase function $p(\mathbf{r},\Omega\bullet\Omega')$ and source function $\varepsilon(\mathbf{r},\Omega,\mathbf{t})$. This makes it one of rare universe approaches for solution of RTE. To find a numerical solution of the RTE, first we introduce angular discretization - instead of a continuous 4π solid angle we are looking for solution of the RTE in a limited number N of angular directions in each point of the space variable **r**. As a second step, we similarly introduce spatial discretization in **R**, so we aim to determine a distribution of particles in a discrete number of points in 3D $\varphi(x_i,y_j,z_k)$ - $\varphi_{i,j,k}$ for brevity for each of N angular directions - $\varphi_{i,j,k,n}$. The possible number of space coordinates and angular directions is limited by practical considerations, such as memory available to store all unknowns.

After the discretization step, we rewrite the original RTE equation in discrete form. To do so, we need to estimate the derivatives numerically. This can be done using well known diamond difference relation, however it was shown[5,6] that this approach leads to numerical instabilities in the overall computation scheme. Therefore[2], less accurate but always stable one-side difference scheme is used:

$$\left.\frac{\partial\varphi}{\partial z}\right|_{i,j,k,n} \approx \frac{\varphi_{i,j,k,n} - \varphi_{i,j,k-1,n}}{\Delta z};\ \left.\frac{\partial\varphi}{\partial y}\right|_{i,j,k,n} \approx \frac{\varphi_{i,j,k,n} - \varphi_{i,j-1,k,n}}{\Delta y};\ \left.\frac{\partial\varphi}{\partial x}\right|_{i,j,k,n} \approx \frac{\varphi_{i,j,k,n} - \varphi_{i-1,j,k,n}}{\Delta x} \quad (3)$$

Thus finally the time-independent RTE in its discrete form becomes:

$$\mu_n\frac{\varphi_{i,j,k,n} - \varphi_{i-1,j,k,n}}{\Delta x} + \eta_n\frac{\varphi_{i,j,k,n} - \varphi_{i,j-1,k,n}}{\Delta y} + \xi_n\frac{\varphi_{i,j,k,n} - \varphi_{i,j,k-1,n}}{\Delta z} + \sigma^t_{i,j,k}\varphi_{i,j,k,n} = q_{i,j,k,n} \quad (4)$$

where μ_n η_n and ξ_n are directional cosines corresponding to *n*th angular direction, σ_t and σ_s are total attenuation and scattering coefficients in volume element $\Delta x\Delta y\Delta z$, and $q_{i,j,k,n}$ is so called "source-term", responsible for the title of the method itself. The formula for $q_{i,j,k,n}$ is:

$$q_{i,j,k,n} = \sigma^s_{i,j,k}\sum_{n'=1}^{N} phase\_f[n,n']\varphi_{i,j,k,n'} + \varepsilon_{i,j,k,n} \quad (5)$$

where $\varepsilon_{i,j,k,n}$ is local sources in $\Delta x\Delta y\Delta z$.
For a given distribution of $q_{i,j,k,n}$ one can derive a relation between $\varphi_{i,j,k,n}$ and its neighbors $\varphi_{I-1,j,k,n}$ $\varphi_{i,j-1,k,n}$ $\varphi_{i,j,k-1,n}$:

$$\varphi_{i,j,k,n} = \frac{q_{i,j,k,n} + \frac{\mu_n}{\Delta x}\varphi_{i-1,j,k,n} + \frac{\eta_n}{\Delta y}\varphi_{i,j-1,k,n} + \frac{\xi_n}{\Delta z}\varphi_{i,j,k-1,n}}{\sigma^t_{i,j,k} + \frac{\mu_n}{\Delta x} + \frac{\eta_n}{\Delta y} + \frac{\xi_n}{\Delta z}} \qquad (6)$$

The SIDOM approaches the unknown distribution of $\varphi_{i,j,k,n}$ by iteration on $q_{i,j,k,n}$ and recalculation of $\varphi_{i,j,k,n}$ on each new iteration step until the solution is converged so that relative changes in $\varphi_{i,j,k,n}$ become smaller than some predefined value.

The most important issue for phase shift calculation is a determination of boundary conditions for the phase. The problem is, that, while one can sufficiently accurately put intensity (and hence modulation) of the incoming signal at large distances from the source to zero, this can not be true for its phase, so some other approaches must be considered. In the present contribution we have put the phase shift of the incoming beam at the n'th iteration equal to the phase shift of the outcoming beam at the (n-1)'th iteration, following the approximation that at large distances from the source the photons are scattered nearly isotropically and thus their phase is nearly independent of the angular direction. In this work we present numerical and experimental results for boundaries at 3.2 cm and at 10 cm from source, where such an approximation was shown to be valid.

In our *in vivo* experiments with human tissue, we measured phase shift approximately 5° at 20MHz at 15 mm source/detector separation. It means that for the whole volume of propagation of photons from source till the distances where the intensity of multiple scattered beam becomes negligible, one can use a linearized approximation $\sin\delta \approx \delta$ (due to small magnitude of the δ) which substantially simplified solution of the set of equations (2). In the present contribution we present experimental and numerical results for modulation frequency 20 MHz where we experimentally showed such an approximation to be true for biotissue.

6. EXPERIMENTS

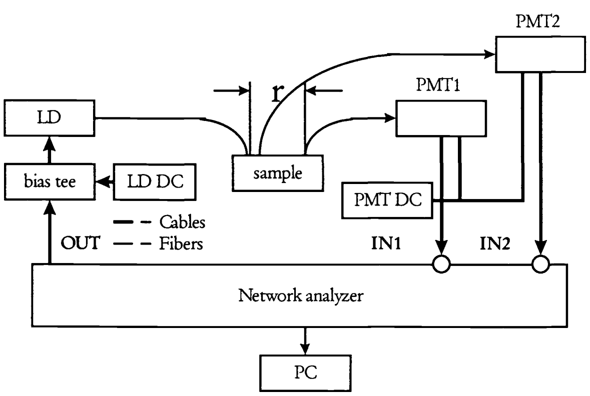

Fig. 1. Experimental setup.

Our experimental setup (Fig. 1) consists of a radiation source - Toshiba TOLD 9441MC laser diode; 2 detectors - Hamamatsu H6779-01 PMT; HP 4396B network analyzer; voltmeter and multi-layered tissue-simulating sample. Using the analyzers's internal AC source to modulate the amplitude of the laser diode radiation and fast PMT to measure radiation reflected from the sample we measure the relative phase shift and modulation depth between analyzers' inputs IN1 and IN2. Our setup is similar to that of Tromberg[3].

The light from the laser diode is focused into the fibre, and another end of fibre is fixed on the surface of the top layer of the multi-layered sample. Detection fibers are also placed on the surface of sample, with their opposite sides being coupled into the PMTs.

Our sample holder contains a set of plastic layers of various thicknesses. Internally each layer has a cylindrically symmetric hole with diameter of a 20 cm. To separate layers with liquid sample from each other we use 0.25 mm plastic sheet. With such construction we are capable to build multi-layered samples of arbitrary structure, using plastic layers of different thickness.

As tissue-simulating sample we use a suspension of Intralipid in water.

For our experiments we used various combinations of layers thicknesses and optical parameters (scattering and absorption coefficients). We used a reference fiber to take into account slight instability of the laser diode and of its power supply. We measured the intensity and the phase of reflected radiation at various distances from the source fiber. We changed the thickness of the layers, changed optical parameters (scattering coefficient) of layers, swept over a range of distances from the source fiber and measured the intensity and the phase of reflected signal.

7. RESULTS

In our previous work[9] we presented experimental and numerical results for the intensity of the reflected signal for the two-layered sample. In this work we present results for the phase. We used a multi-layered cylindrical sample (diameter 20 cm) containing layers with different scattering (for experiments presented here μ'_s was in the range 0.2 mm^{-1}– 1.0 mm^{-1}).

We made a set of measurements with the two-layered geometry with the top layer having different thickness and scattering coefficient. We measured a dependence of phase upon source-detector separation (@20MHz) or modulation frequency.

In fig.2 experimental results are presented for 2-layered system with different reduced scattering coefficient of the top layer.

In fig. 3 experimental results are shown for 2-layered system with varying thickness of the top layer.

In fig.4 results are plotted for 2 cases of scattering coefficients for two cases of thickness of the top layer. We observed that a) at large source-detector separations (20 mm) and b) for the case when reduced scattering coefficient of the top layer is higher then that of the bottom layer, gradient of detected phase isn't significantly different when thickness of the top layer is varying between 1.5 and 4.5 mm. In contrast, for the case when μ'_s of the top layer was smaller then μ'_s of the bottom layer, we observe a considerable change in the gradient of the phase increasing thickness of less scattering layer from 1.5 mm to 4.5 mm. Our interpretation of observed results is that at source-detector separation as large as 20 mm, main part of pathlength of detected photons comes from propagation in the bottom layer and layer of 1.5 mm thickness introduces rather slight dependence on the reduced scattering coefficient of the top layer (fig.3). When thickness of the top layer is 4.5 mm, a dependence on its scattering gets larger (fig. 2). However, higher scattering together with the increase of pathlength simultaneously causes higher losses, thus decreasing relative contribution of photons with higher pathlength (due to higher scattering of the top layer) in detected signal. For the case of μ'_s of the top layer being smaller then μ'_s of the bottom layer, part of detected signal which represents photons with smaller pathlength due to smaller scattering of the top layer doesn't get similarly dumped.

In figs. 5 and 6 numerical results are shown for configuration corresponding to that of our measurements, except that in numerical simulations we found it to be more convenient to change optical parameters of the bottom layer instead of the top layer, so what in measurements is higher scattering of the top layer in simulations is smaller scattering of the bottom layer.

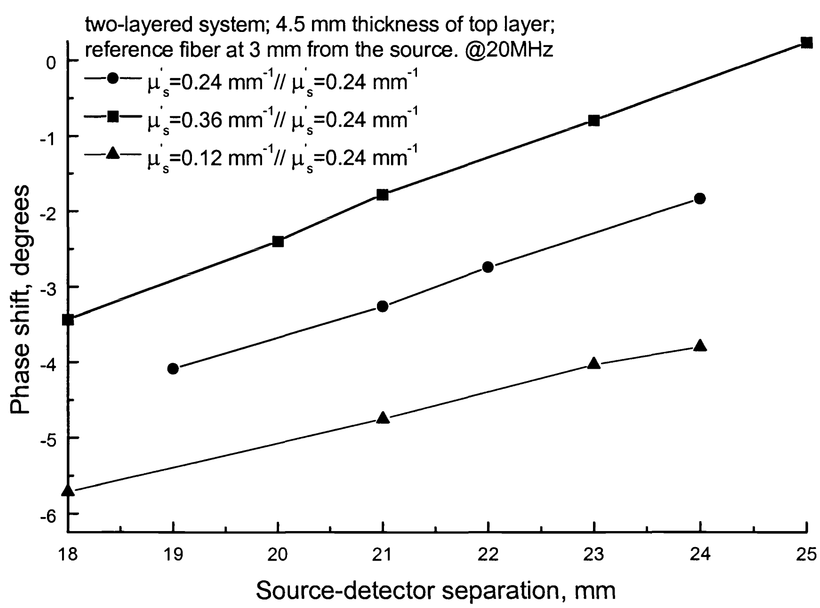

Fig. 2. 20 cm diameter sample holder. Experimental results with different scattering of the top layer. Dependence on source-detector separation. Phase shift uncertainty is 0.05 degree.

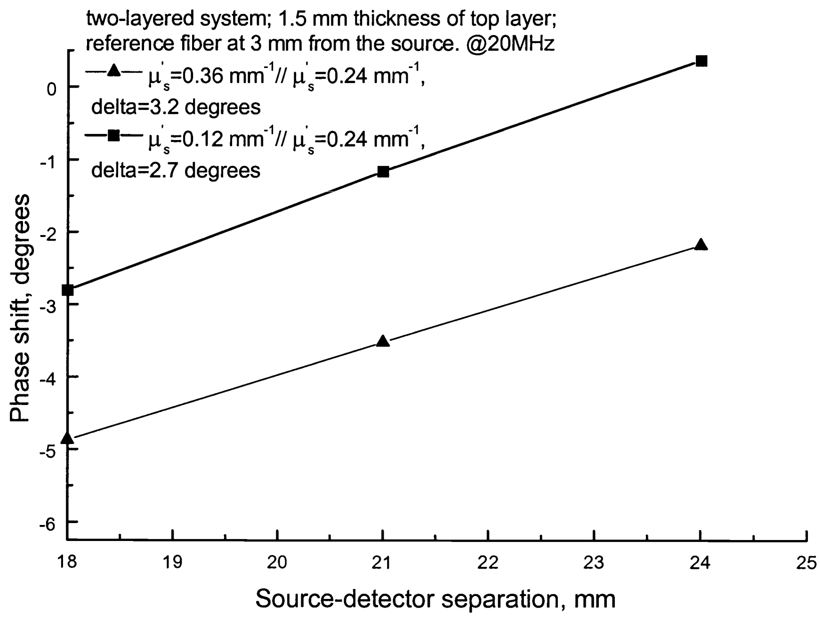

Fig. 3. 20 cm diameter sample holder. Experimental results with various thickness of the top layer. Dependence on source-detector separation. Phase shift uncertainty is 0.05 degree.

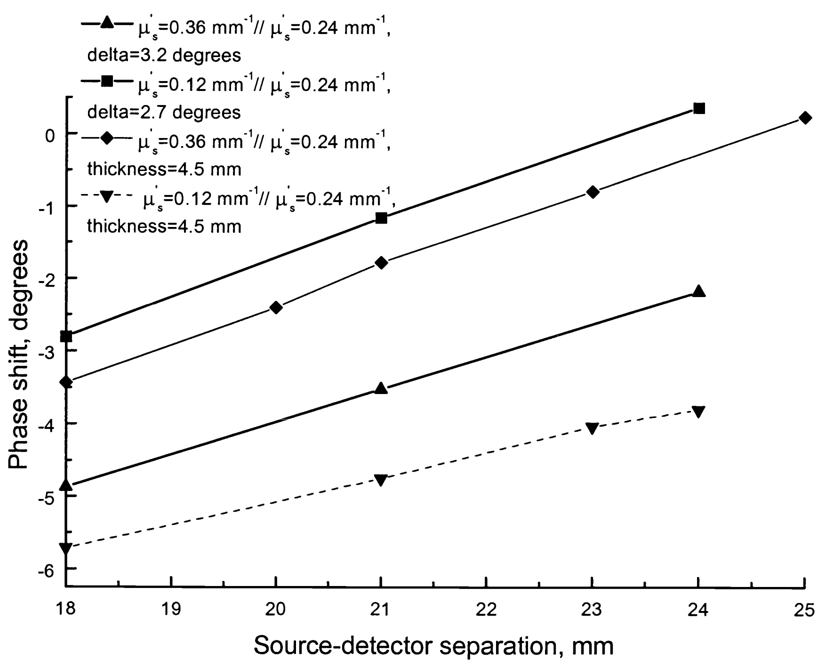

Fig. 4. 20 cm diameter sample holder. Experimental results with various thickness of the top layer and scattering. Dependence on source-detector separation. Phase shift uncertainty is 0.05 degree.

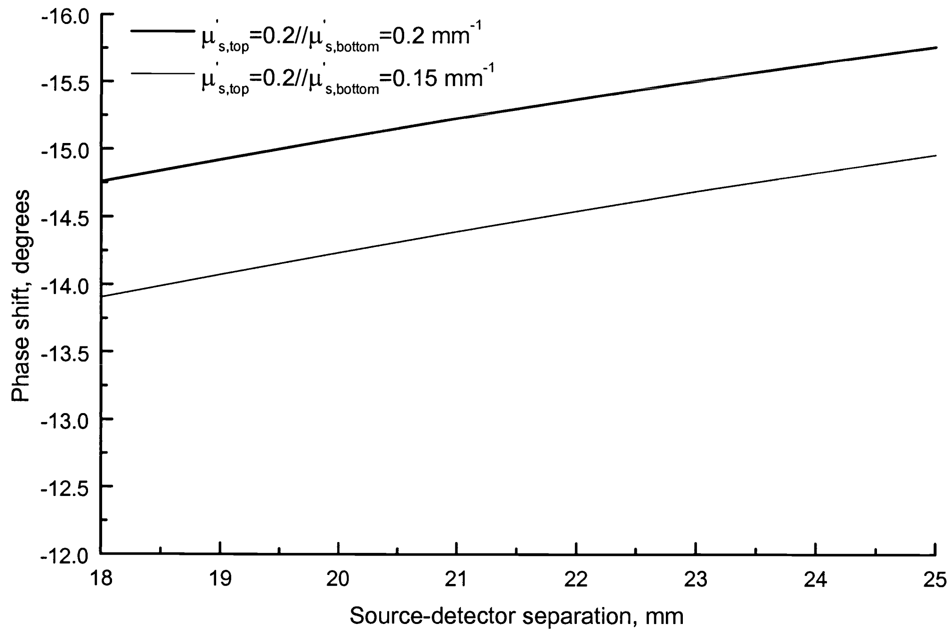

Fig. 5. 6.4 cm diameter sample holder. Numerical results for phase shift at 20 Mhz.
Dependence of phase vs source-detectors separation for case of different optical parameters of the bottom layer.

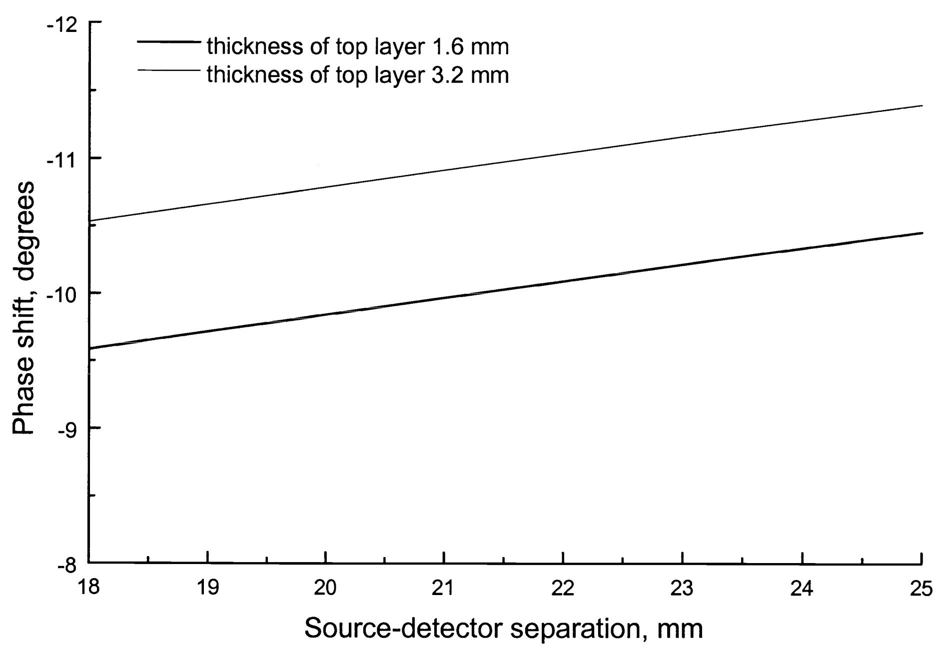

Fig. 6. 6.4 cm diameter sample holder. Numerical results for phase shift at 20 Mhz.
Dependence of phase vs source-detectors separation for case of different thicknesses of the top layer.

Also, 0.25 mm plastic layer was not described - we used just one layer over another. Nevertheless, good qualitative agreement was found (cf fig.6 and fig.4). We see that calculated gradient of phase shift is close to that to actually measured. Calculated difference in phase shift for different values of scattering of the top layer is approx. 1 degree - a bit smaller then that measured. We believe that this is partly because of conservative boundary conditions we used, which are underestimating phase of in-coming intensity, which has significant influence at the top boundary where one is conducting measurements. We plan to investigate another approximations for boundary conditions of phase.

Also, we observe that calculated difference in phase shift for different thicknesses of the top layer (fig.6) is close to that experimentally observed (fig.4), even though our approximation for boundary conditions isn't the best possible.

When approximation $\sin\delta \approx \delta$ holds, and with boundary conditions for phase which we used, phase shift computed according to procedure described here will produce linear dependence of phase vs modulation frequency. From experimental results we know that indeed phase shift is close to linear dependence upon modulation frequency in the frequency range of order of tens of megahertz.

Numerical results were obtained using Sun HPC450 workstation.

8. CONCLUSIONS

Our experimental investigation of frequency-domain technique applied to multi-layered sample manifests that layered system exhibits strongly different behavior when optical parameters of top/bottom differ and this behavior can be used to significantly accelerate the diagnosis using different source-detector separations and different modulation frequencies.

Our results show that SIDOM can be used for numerical solution of derived set of frequency-domain radiative-transfer equations in realistic multi-layered case. Additional considerations are required for increase of accuracy of numerical solution[5] and decrease of computational time[7].

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