Determination of optimal source-detector separation in measuring chromophores in layered tissue with diffuse reflectance

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Based on analysis of the relation between mean penetration depth and source-detector separation in a three-layer model with the method of Monte-Carlo simulation, an optimal source-detector separation is derived from the mean penetration depth referring to monitoring the change of chromophores concentration of the sandwiched layer. In order to verify the separation, we perform Monte-Carlo simulations with varied absorption coefficient of the sandwiched layer. All these diffuse reflectances are used to construct a calibration model with the method of partial least square (PLS). High correlation coefficients and low root mean square error of prediction (RMSEP) at the optimal separation have confirmed correctness of the selection. This technique is expected to show light on noninvasive diagnosis of near-infrared spectroscopy.

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In the applications of near infrared spectroscopy used for diagnostic goals, it is essential to study penetration depth of diffused photons re-emitting from irradiated tissue[1−6]. Penetration depth, which represents the maximum depth travelled by photons before they are absorbed or escape from the sample surface, plays an important role in giving detailed information of tissue, especially referring to the noninvasive measurement of variations of chromophore in tissue. Feng *et al.* studied the penetration depth with numerical simulations for homogeneous media[7]. Hiraoka *et al.* studied this problem in non-homogeneous media[8]. Measurements of penetration depth have been also carried out by Cui *et al.*[9], Sassaroli *et al.*[10], and Tsai *et al.*[11]. Del Bianco *et al.* have investigated the penetration depth by studying the time-resolved probability function derived from the diffusion equation analytical expression[12].

In this paper, penetration depth of diffused photons re-emitting from the sample surface is investigated with Monte-Carlo simulation method in a three-layer medium. We suppose a thin layer sandwiched by a slab and a semi-infinite layer. The distribution and average value of penetration depth at different separations from the source to the detector are investigated, and the ratio of photons whose penetration depth is in the "sandwiched" layer is also investigated. As a result, we find an optimal source-detector separation to observe the change of chromophore concentration of this layer. In the end, we verify the correctness of the selection of the optimal separation with the method of partial least square (PLS) regression.

A cylindrical coordinate originated at the point of the incident light is adopted to orient the photons. We divide the r and z directions into Nr and Nz grids respectively, with increment of Δr and Δz. As we focus on the penetration depth as a function of source-detector separation r in this presentation, a two-dimensional (2D) array, $R[r][d]$ is set to score photons that re-emit at the place of r away from light source and have penetrated into a depth of d.

When photons migrate in turbid medium, their weight W_i will be lost according to equation $\Delta W_i = (\mu_\mathrm{a}/\mu_\mathrm{t})W_i$ with μ_a and μ_t being the absorption coefficient and total attenuation coefficient, respectively, once the photons reach the interaction sites. After photons re-emit from the surface of medium, we score their weight W_i into the corresponding array $R[r][d]$ according to its source-detector distance r and penetration depth d

$$R[r][d] = \sum_{i=1}^{N_d} W_i, \quad (1)$$

where N_d means the number of total photons re-emitting at separation r.

And the mean depth of photons re-emitting from r, $\bar{d}(r)$, can be calculated by

$$\bar{d}(r) = \frac{\sum\limits_{d} d \cdot R[r][d]}{\sum\limits_{d} R[r][d]}. \quad (2)$$

We perform the Monte-Carlo simulation on a three-layer model, and the parameters of each layer, including absorption coefficient, scattering coefficient, anisotropy factor, thickness, and refractive index are listed in Table 1.

The simulation result shows the linear relationship between the penetration depth and the source-detector separation, as shown in Fig. 1. We can see that photons with the mean penetration depth in the range of layer 2, mainly concentrate in the ring with inner radius of 2.8 mm and outer radius of 3.2 mm. For a further investigation, we have calculated the ratio of photon number with mean penetration depth in layer 2 to total number of photons reflected in different position. As shown in

Table 1. Parameters of Each Layer of the Medium

Layer	Absorption Coefficient (mm^{-1})	Scattering Coefficient (mm^{-1})	Anisotropy Factor	Refractive Index	Thickness (mm)
1	0.45	14.0	0.873	1.37	1.0
2	1.00	14.0	0.873	1.37	0.1
3	0.18	9.2	0.873	1.37	infinite

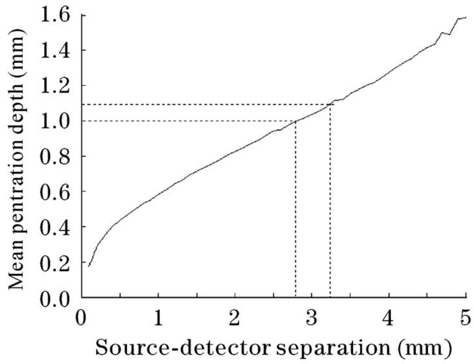

Fig. 1. Mean penetration depth of photons re-emitting from the surface of medium versus source-detector separation.

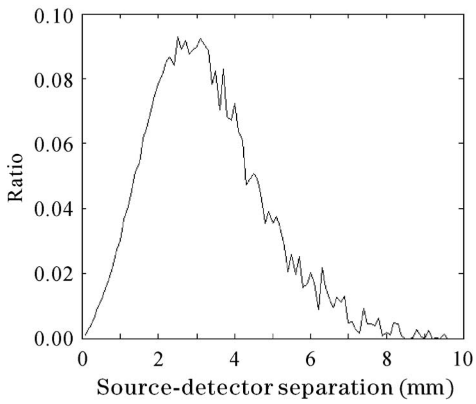

Fig. 2. Ratio of photon number with depth within layer 2 to total number of photons reflected.

Fig. 2, at the source-detector separation around 3.2 mm, the maximum ratio is close to 0.09, which means photons re-emitting from this position can reflect the information of layer 2 in the maximum extent.

From the above analysis, we can conclude that the point around 3.0 mm between source and detector is the optimal separation to monitor the change of absorption coefficient of layer 2.

In order to verify the results, Monte-Carlo simulations have been performed for 80 times with absorption coefficient of layer 2 varied from 0.8 to 1.2 mm^{-1} with interval of 0.05 mm^{-1}. The other settings of Monte-Carlo program are kept constant. For each run, data of diffused reflectance at different source-detector separations ($R_d(r)$) can be obtained. In the following, we take the different absorption coefficients as the variable vector, and $R_d(r)$ at different r as dependent variable vectors. Thus, 100 groups of data including the same variable vector and a dependent variable for different r

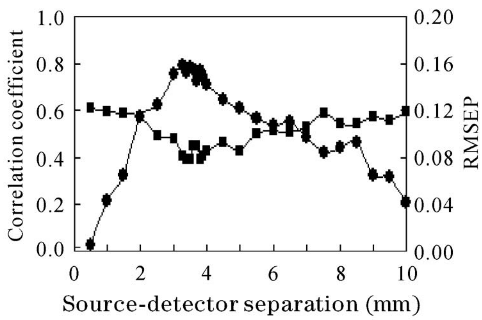

Fig. 3. Correlation (dots) and RMSEP (squares) of the calibration model using all diffuse reflectance at different source-detector separations.

can be used to build calibration models. The models are constructed with the method of PLS.

The correlation coefficient and root mean square error of prediction (RMSEP), which are the two key factors to estimate capability of the calibration models, are shown in Fig. 3 as a function of r. We can find from the figure that correlation coefficient rises up from near source, and reaches the maximum at r equaling to 3.2 mm, and then begins to decrease, which means diffuse reflectance of r equaling to 3.2 mm has a better correlation than those of other positions. RMSEP presents contrary tendency, it reaches the minimal value for r equal to 3.2 mm. Results of both correlation coefficient and RMSEP indicate that around 3.2 mm is optimal position to monitor information of layer 2.

Up to now, we have deduced a range between 2.8 and 3.2 mm as an optimal separation to monitor the change of chromopore of layer 2, and then obtained a result of 3.2 mm as the most correlative separation with the method of PLS. We can find that 3.2 mm resulted from the method of PLS equals to the separation corresponding to the depth of the bottom of layer 2. It can be explained that photons with a mean penetration depth into the bottom of layer 2 have more opportunities to interact with this layer, compared with those only reach the top of this layer. Therefore, the separation between the source and the detector corresponding to the bottom of the layer interested with the mean penetration depth is the optimal spacing to monitor the variations of chromophores of this layer.

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References

1. T. R. Cheatle, L. A. Potter, M. Cope, D. T. Delpy, P. D. C. Smith, and J. H. Scurr, British J. Surg. **78,** 405 (1991).
2. S. Fantini, M. A. Franceschini, J. B. Fishkin, B. Barbieri, and E. Gratton, Appl. Opt. **33,** 5204 (1994).
3. I. Tachtsidis, C. E. Elwell, T. S. Leung, C.-W. Lee, M. Smith, and D. T. Delpy, Physiol. Meas. **25,** 437 (2004).
4. R. Marbach, Th. Koschinsky, F. A. Gries, and H. M. Heise, Appl. Spectrosc. **47,** 875 (1993).
5. S. U. A. Muller, B. Mertes, C. F. Fischbacher, K. U. Vagemann, and K. Danzer, Int. J. Artif. Organs **20,** 285 (1997).
6. F. F. Jobsis, Science **198,** 1264 (1977)).
7. S. Feng, F. Zeng, and B. Chance, Proc. SPIE **1888,** 78 (1993).
8. M. Hiraoka, M. Firbank, M. Essenpreis, M. Cope, S. R. Arridge, P. van der Zee, and D. T. Delpy, Phys. Med. Biol. **38,** 1859 (1993).
9. W. Cui, C. Kumar, and B. Chance, Proc. SPIE **1431,** 180 (1991).
10. A. Sassaroli, C. Blumetti, F. Martelli, L. Alianelli, D. Contini, A. Ismaelli, and G. Zaccanti, Appl. Opt. **37,** 7392 (1998).
11. C. L. Tsai, Y. F. Yang, C. C. Han, J. H. Hsieh, and M. Chang, Appl. Opt. **40,** 5770 (2001).
12. S. Del Bianco, F. Martelli, and G. Zaccanti, Phys. Med. Biol. **47,** 4131 (2002).
13. L. H. Wang, S. L. Jacques, and L. Q. Zheng, Computer Methods and Programs in Biomedicine **47,** 131 (1995).