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An inverse biotechnology problem in estimating the optical diffusion and absorption coefficients of tissue

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Abstract

An inverse algorithm for biotechnology problem utilizing the conjugate gradient method is applied in the present study in determining the unknown spatial-dependent optical diffusion and absorption coefficients of the biological tissue based on irradiance and temperature measurements. The accuracy of this inverse problem is examined by using the simulated exact and inexact irradiance and temperature measurements in the numerical experiments. Results show that the estimation on the spatial-dependent diffusion and absorption coefficients can be obtained with any arbitrary initial guesses on a Pentium IV 1.4 GHz personal computer for the test cases considered in the present study.

1. Introduction

Lasers application in medicine, such as surgery, therapy and ophthalmology, emerged rapidly during the recent 20 years. For instance, small, unresectable tumors can be destroyed thermally using interstitial laser heating. This minimally invasive technique involves coupling laser energy to optical fibers implanted percutaneously in a tumor volume. Dowlatshahi et al. [1] and Amin et al. [2] used this kind of technique clinically. However the phenomena of radiation–tissue interaction is studied insufficiently.

As with most cancer therapy techniques, the purpose is to destroy a targeted tumor using interstitial laser heating while sparing surrounding normal biological tissue. This implies that thermal control is very important during the process. The temperature distribution of the tissue during laser heating depends on a heat generation term, which was induced by the product of irradiance and optical absorption coefficient of tissue. Meanwhile, based on the optical propagation equation [3], the irradiance of tissue depends on both optical diffusion and absorption coefficients. For this reason the determination of those two optical properties of tissue becomes important.

The direct biotechnology problems for optical propagation and heat transfer equations are concerned with the determination of irradiance and temperature of tissue when the initial and boundary conditions as well as thermophysical and optical properties of tissue are all specified. In contrast, the inverse biotechnology problem considered here involves the determination of the unknown spatial-dependent optical diffusion and absorption coefficients in a biological tissue from the knowledge of the irradiance and temperature measurements taken within the tissue.

The technique of conjugate gradient method (CGM) [4] has been shown its potential for solving many kinds of inverse problems and has been applied to many different applications. For instance, Huang and Chen [5] used boundary element method and conjugate gradient method to estimate the boundary heat fluxes for an irregular domain. Huang and Wang [6] used CGM in estimating surface heat fluxes for a three-dimensional inverse heat conduction problem. Huang and Chen [7] used same technique in estimating surface heat fluxes for a three-dimensional inverse heat convection problem. Huang and Chin [8] used CGM in a two-dimensional inverse problem of imaging the thermal conductivity of

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Nomenclature

$C(r)$	effective volumetric heat capacity
$D(r)$	optical diffusion coefficient
J_1, J_2	functional defined by Eqs. (3a) and (3b)
J'_1, J'_2	gradient of functional defined by Eqs. (18) and (20)
$k(r)$	effective thermal conductivity
P_1, P_2	direction of descent defined by Eqs. (5a) and (5b)
$Q(r)$	heat generation rate by laser irradiation
r	dimensionless coordinate
S	point optical source
t	dimensionless time
$T(r,t)$	estimated dimensionless temperature
$Y(r,t)$	measured dimensionless temperature

Greek symbols

β_1, β_2	search step sizes
γ_1, γ_2	conjugate coefficients
$\delta(\cdot)$	Dirac delta function
$\lambda_1(r,t)$, $\lambda_2(r)$	Lagrange multipliers defined by Eqs. (15) and (19)
$\mu_a(r)$	optical absorption coefficient
$\phi(r)$	estimated dimensionless irradiance
$\Phi(r)$	measured dimensionless moisture
ΔT, $\Delta\phi$	direct problem in variations defined by Eqs. (7) and (11)
η_1, η_2	convergence criteria

Superscript

n	iteration index

a non-homogeneous medium. Huang [9] applied the CGM in a non-linear inverse vibration problem in estimating the unknown external forces for a system with displacement-dependent parameters. However, the inverse biotechnology problem in determining the optical properties for biological tissue is very limited in the literature.

The conjugate gradient method derives its basis from the variational principles [4] and transforms the original direct problem to the solution of two subproblems, namely, the direct problem in variations and the adjoint problem, which will be discussed in detail in this study.

2. Direct problem

To illustrate the methodology for developing expressions for use in determining two unknown spatial-dependent optical diffusion and absorption coefficients for a biological tissue, we consider the following physical problem. A tissue of radius $\bar{r}_0$ in cylindrical coordinate is subjected to a constant irradiance $\bar{\phi}(\bar{r}_0)$ at outer boundary. Initially the temperature of the tissue is equal to $\overline{T}(\bar{r},0)$. For time $t>0$, the boundary surface at $\bar{r}_0$ is subjected to a constant temperature $\overline{T}(\bar{r}_0,\bar{t})$.

In order to obtain the dimensionless optical propagation and heat transfer equations, the following dimensionless quantities should be defined

$$r=\frac{\bar{r}}{\bar{r}_0};\quad \phi(r)=\frac{\bar{\phi}(\bar{r})}{\bar{\phi}_r};\quad D(r)=\frac{\overline{D}(\bar{r})}{\overline{D}_r};\quad \mu_a(r)=\frac{\bar{r}_0^2\bar{\mu}_a(\bar{r})}{\overline{D}_r};$$

$$k(r)=\frac{\bar{k}(\bar{r})}{\bar{k}_r};\quad T(r,t)=\frac{\overline{T}(\bar{r},\bar{t})}{\overline{T}_r};\quad C(r)=\frac{\overline{C}(\bar{r})}{\overline{C}_r};\quad S=\frac{\bar{r}_0^2\overline{S}}{\overline{D}_r\bar{\phi}_r};$$

$$Q(r)=\mu_a(r)\phi(r)=\frac{\bar{r}_0^2\overline{Q}(\bar{r})}{\bar{k}_r\overline{T}_r};\quad t=\frac{\bar{k}_r\bar{t}}{\overline{C}_r\bar{r}_0^2}$$

here ϕ is the irradiance, D and μ_a represent the optical diffusion and absorption coefficients, respectively, k and C denote the effective thermal conductivity and volumetric heat capacity, respectively, T is the temperature, S and Q represent the point optical source and heat generation rate by laser irradiation, respectively, and t denotes the dimensionless time. The subscript r represents the reference quantity.

The dimensionless formulations for optical propagation equation and heat transfer equation can be expressed as:

$$-\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left[r^2D(r)\frac{\mathrm{d}\phi(r)}{\mathrm{d}r}\right]+\mu_a(r)\phi(r)=S\delta(r),\quad \text{in } 0\leqslant r\leqslant 1 \tag{1a}$$

$$\frac{\mathrm{d}\phi(r)}{\mathrm{d}r}=0;\quad \text{at } r=0 \tag{1b}$$

$$\phi=\phi(1);\quad \text{at } r=1 \tag{1c}$$

and

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2k(r)\frac{\partial T(r,t)}{\partial r}\right]+\mu_a(r)\phi(r)=C(r)\frac{\partial T(r,t)}{\partial t},\quad \text{in } 0\leqslant r\leqslant 1,\ t>0 \tag{2a}$$

$$\frac{\partial T(r,t)}{\partial r}=0;\quad \text{at } r=0 \tag{2b}$$

$$T=T(1,t);\quad \text{at } r=1 \tag{2c}$$

$$T=T(r,0);\quad \text{for } t=0 \tag{2d}$$

Here $\delta(\cdot)$ is the Dirac delta function. The direct problems considered here are concerned with calculating the tissue's irradiance and temperature when the optical diffusion and absorption coefficients, $D(r)$ and $\mu_a(r)$, thermal properties and initial and boundary condition are known. The Crank–Nicolson finite difference method can be used to solve these direct problems.

3. Inverse problem

For the inverse problem considered here, the optical diffusion and absorption coefficients, $D(r)$ and $\mu_a(r)$, are regarded as being unknown, but everything else in Eqs. (1) and (2) is known. In addition, the measured irradiance and temperature distributions within the space domain are considered available from the techniques of non-contact measurements.

It is obvious that the undetermined coefficients $D(r)$ and $\mu_a(r)$ both appear in Eq. (1), however, it is impossible to use only Eq. (1) to estimate simultaneously for $D(r)$ and $\mu_a(r)$. For this reason Eq. (2) is needed in this study. The sequence of the present inverse problem is as follows:

(a) Estimate $Q(r)$ from Eq. (2) using measured temperature distribution, here $Q(r) = \mu_a(r)\phi(r)$.
(b) Estimate $D(r)$ from Eq. (1) using the estimated $Q(r)$ and the measured irradiance distribution.
(c) Once $D(r)$ is obtained, $\phi(r)$ can also be determined. Therefore $\mu_a(r)$ is obtainable using $Q(r) = \mu_a(r)\phi(r)$.

Let the measured irradiance at position r be denoted by $\Phi(r)$, the measured temperature at position r and time t be denoted by $Y(r,t)$. Then this inverse problem can be stated as follows: by utilizing the above mentioned measured temperature and irradiance data $Y(r,t)$ and $\Phi(r)$, estimate the unknown diffusion coefficient, $D(r)$, and heat generation rate by laser irradiation, $Q(r)$, over the specified space domain. Finally the absorption coefficient $\mu_a(r)$ can be calculated using $Q(r) = \mu_a(r)\phi(r)$.

The solutions of the present inverse problem are to be obtained in such a way that the following two functionals are minimized:

$$J_1[Q(r)] = \int_{r=0}^{1}\int_{t=0}^{t_f} r^2[T(r,t) - Y(r,t)]^2\,\mathrm{d}t\,\mathrm{d}r \tag{3a}$$

$$J_2[D(r)] = \int_{r=0}^{1} r^2[\phi(r) - \Phi(r)]^2\,\mathrm{d}r \tag{3b}$$

Here $T(r,t)$ and $\phi(r)$ are the estimated (or computed) temperature and irradiance. These quantities are determined from the solution of the direct problems given previously by using the estimated diffusion coefficient $D(r)$ and heat generation rate by laser irradiation, $Q(r)$.

4. Conjugate gradient method for minimization

The following iterative process based on the conjugate gradient method [4] is now used for the estimation of diffusion coefficient $D(r)$ and heat generation rate by laser irradiation $Q(r)$ by minimizing the above two functionals $J_1[Q(r)]$ and $J_2[D(r)]$:

$$Q^{n+1}(r) = Q^n(r) - \beta_1^n P_1^n(r) \quad n = 0,1,2,\ldots \tag{4a}$$

$$D^{n+1}(r) = D^n(r) - \beta_2^n P_2^n(r) \quad n = 0,1,2,\ldots \tag{4b}$$

where β_1^n and β_2^n are the search step sizes in going from iteration n to iteration $n+1$, and $P_1^n(r)$ and $P_2^n(r)$ are the directions of descent (i.e. search directions) given by

$$P_1^n(r) = J_1'^n(r) + \gamma_1^n P_1^{n-1}(r) \tag{5a}$$

$$P_2^n(r) = J_2'^n(r) + \gamma_2^n P_2^{n-1}(r) \tag{5b}$$

which is a conjugation of the gradient directions $J_1'^n(r)$ and $J_2'^n(r)$ at iteration n and the directions of descent $P_1^{n-1}(r)$ and $P_2^{n-1}(r)$ at iteration $n-1$. The conjugate coefficient is determined from

$$\gamma_1^n = \frac{\int_{r=0}^{1}[J_1'^n(r)]^2\,\mathrm{d}r}{\int_{r=0}^{1}[J_1'^{n-1}(r)]^2\,\mathrm{d}r} \quad \text{with } \gamma_1^0 = 0 \tag{6a}$$

$$\gamma_2^n = \frac{\int_{r=0}^{1}[J_2'^n(r)]^2\,\mathrm{d}r}{\int_{r=0}^{1}[J_2'^{n-1}(r)]^2\,\mathrm{d}r} \quad \text{with } \gamma_2^0 = 0 \tag{6b}$$

To perform the iterations according to Eqs. (4), we need to compute the step sizes β_1^n and β_2^n and the gradients of the functionals $J_1'^n(r)$ and $J_2'^n(r)$. In order to develop expressions for the determination of these two quantities, two direct problems in variations and two adjoint problems are constructed as described below.

5. Direct problem in variations and search step sizes

Firstly, it is assumed that when $Q(r)$ undergoes a variation $\Delta Q(r)$, $T(r,t)$ is perturbed by $\Delta T(r,t)$. Then replacing in the direct problem $Q(r)$ by $Q(r) + \Delta Q(r)$, $T(r,t)$ by $T(r,t) + \Delta T(r,t)$, subtracting from the resulting expressions the direct problem and neglecting the second-order terms, the following direct problem in variations for the function $\Delta T(r,t)$ is obtained.

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 k(r)\frac{\partial \Delta T(r,t)}{\partial r}\right] + \Delta Q(r) = C(r)\frac{\partial \Delta T(r,t)}{\partial t},\quad \text{in } 0 \leqslant r \leqslant 1,\ t > 0 \tag{7a}$$

$$\frac{\partial \Delta T(r,t)}{\partial r} = 0; \quad \text{at } r = 0 \tag{7b}$$

$$\Delta T = 0; \quad \text{at } r = 1 \tag{7c}$$

$$\Delta T = 0; \quad \text{for } t = 0 \tag{7d}$$

We should note that the above direct problem in variations could also be solved by Crank–Nicolson finite difference method.

The functional $J_1[Q(r)]$ for iteration $n+1$ is obtained by rewriting Eq. (3a) as

$$J_1[Q^{n+1}(r)] = \int_{r=0}^{1}\int_{t=0}^{t_f} r^2[T(r,t;Q^n - \beta_1^n P_1^n) - Y(r,t)]^2\,\mathrm{d}t\,\mathrm{d}r \tag{8}$$

where we replaced $Q^{n+1}(r)$ by the expression given by Eq. (4a).

If the estimated temperatures $T(r,t;Q^n - \beta_1^n P_1^n)$ are linearized by a Taylor expansion, Eq. (8) takes the form:

$$J_1[Q^{n+1}(r)] = \int_{r=0}^{1}\int_{t=0}^{t_f} r^2[T(r,t;Q^n) - \beta_1^n \Delta T(P_1^n) - Y(r,t)]^2\,\mathrm{d}t\,\mathrm{d}r \tag{9}$$

where $T(r,t;Q^n)$ is the solution of the direct problem by using estimate $Q(r)$.

The function $\Delta T(P_1^n)$ is taken as the solutions of problem (7) by letting $\Delta Q(r) = P_1^n(r)$ in Eq. (7a).

Eq. (9) is differentiated with respect to β_1^n and equating it equal to zero to obtain the following search step size β_1^n:

$$\beta_1^n = \frac{\int_{r=0}^{1}\int_{t=0}^{t_f} r^2(T-Y)\Delta T\,\mathrm{d}r\,\mathrm{d}t}{\int_{r=0}^{1}\int_{t=0}^{t_f} r^2\Delta T^2\,\mathrm{d}r\,\mathrm{d}t} \tag{10}$$

Similarly, by perturbing $D(r)$ with $\Delta D(r)$, the second direct problem in variations can be obtained as

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left[r^2 D(r)\frac{\mathrm{d}\Delta\phi}{\mathrm{d}r}\right] + \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left[r^2 \Delta D(r)\frac{\mathrm{d}\phi}{\mathrm{d}r}\right] = 0, \quad \text{in } 0 \leqslant r \leqslant 1 \tag{11a}$$

$$\frac{\mathrm{d}\Delta\phi(r)}{\mathrm{d}r} = 0; \quad \text{at } r = 0 \tag{11b}$$

$$\Delta\phi = 0; \quad \text{at } r = 1 \tag{11c}$$

and the search step size β_2^n is obtained as

$$\beta_2^n = \frac{\int_{r=0}^{1} r^2(\phi - \Phi)\Delta\phi\,\mathrm{d}r}{\int_{r=0}^{1} r^2\Delta\phi^2\,\mathrm{d}r} \tag{12}$$

6. Adjoint problems and gradient equations

To obtain the adjoint problem for heat transfer equation, Eq. (2a) is multiplied by the Lagrange multiplier (or adjoint function) $\lambda_1(r,t)$ and the resulting expression is integrated over the time and correspondent space domains. Then the result is added to the right hand side of Eq. (3a) to yield the following expression for the functional $J_1[Q(r)]$:

$$J_1[Q(r)] = \int_{r=0}^{1}\int_{t=0}^{t_f} r^2[T(r,t) - Y(r,t)]^2\,\mathrm{d}t\,\mathrm{d}r + \int_{r=0}^{1}\int_{t=0}^{t_f} \lambda_1(r,t)\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 k(r)\frac{\partial T(r,t)}{\partial r}\right] + Q(r) - C(r)\frac{\partial T(r,t)}{\partial t}\right\}\mathrm{d}t\,\mathrm{d}r \tag{13}$$

Firstly, the variation ΔJ_1 is obtained by perturbing $Q(r)$ by $Q(r) + \Delta Q(r)$ and $T(r,t)$ by $T(r,t) + \Delta T(r,t)$ in Eq. (13), subtracting from the resulting expression the original Eq. (13) and neglecting the second-order terms. We thus find

$$\Delta J_1[Q(r)] = \int_{r=0}^{1}\int_{t=0}^{t_f} r^2 2[T(r,t) - Y(r,t)]\Delta T\,\mathrm{d}t\,\mathrm{d}r + \int_{r=0}^{1}\int_{t=0}^{t_f} \lambda_1(r,t)\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 k(r)\frac{\partial \Delta T(r,t)}{\partial r}\right] + \Delta Q(r) - C(r)\frac{\partial \Delta T(r,t)}{\partial t}\right\}\mathrm{d}t\,\mathrm{d}r \tag{14}$$

In Eq. (14), the second double integral term is integrated by parts; the initial and boundary conditions of the direct problem in variations are utilized. The vanishing of the integrands leads to the following adjoint problem for the determination of $\lambda_1(r,t)$:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 k(r)\frac{\partial \lambda_1(r,t)}{\partial r}\right] + 2(T - Y) + C(r)\frac{\partial \lambda_1(r,t)}{\partial t} = 0, \quad \text{in } 0 \leqslant r \leqslant 1, t > 0 \tag{15a}$$

$$\frac{\partial \lambda_1(r,t)}{\partial r} = 0; \quad \text{at } r = 0 \tag{15b}$$

$$\lambda_1(r,t) = 0; \quad \text{at } r = 1 \tag{15c}$$

$$\lambda_1(r,t) = 0; \quad \text{for } t = t_f \tag{15d}$$

Finally, the following integral term is left

$$\Delta J_1 = \int_{r=0}^{1} \Delta Q(r) \int_{t=0}^{t_f} \lambda_1(r,t)\,\mathrm{d}t\,\mathrm{d}r \tag{16}$$

From definition [4], the general structure of the residual functional variation in the Hilbert space L_2 can be presented as the functional increment and can be presented as

$$\Delta J_1 = \int_{r=0}^{1} \Delta Q(r) J_1'(r)\,\mathrm{d}r \tag{17}$$

A comparison of Eqs. (16) and (17) leads to the following expression for the gradient of functional J_1':

$$J_1'(r) = \int_{t=0}^{t_f} \lambda_1(r,t)\,\mathrm{d}t \tag{18}$$

The adjoint problem for $\lambda_1(r,t)$ is different from the standard initial value problems in that the final time condition at time $t = t_f$ is specified instead of the customary initial condition. However, this problem can be transformed to an initial value problem by the transformation of the time variable as $t^* = t_f - t$. Then the techniques of Crank–Nicolson finite difference method can be used to solve the above adjoint problem.

We note that $J_1'(r)$ is always equal to zero at $r = 1$ since $\lambda_1(1,t) = 0.0$, therefore if the value of $Q(1)$ cannot be predicted accurately before the inverse calculations, the estimated values of $Q(r)$ will deviate from exact values near $r = 1$. However, if we let $\lambda_1(1,t) = \lambda_1(1-\Delta r, t)$, where Δr denotes the space increment for use in finite difference calculation, the singularity at $r = 1$ can be avoided in the present study and a reliable inverse solutions can be obtained.

Similarly, to derive the adjoint problem for the optical propagation equation, Eq. (1a) is multiplied by the Lagrange multiplier (or adjoint function) $\lambda 2(r)$ and follow the same procedure as described previously. Eventually the adjoint equation can be derived as follows

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left[r^2 D(r)\frac{\mathrm{d}\lambda_2}{\partial r}\right] + 2(\phi - \Phi) = 0 \quad \text{in } 0 \leqslant r \leqslant 1 \tag{19a}$$

$$\frac{\mathrm{d}\lambda_2(r)}{\mathrm{d}r} = 0; \quad \text{at } r = 0 \tag{19b}$$

$$\lambda_2(r) = 0; \quad \text{at } r = 1 \tag{19c}$$

and the gradient equation is as follows

$$J_2'(r) = \frac{\mathrm{d}\lambda_2}{\mathrm{d}r}\frac{\mathrm{d}\phi}{\mathrm{d}r} \tag{20}$$

We note that $J_2'(r)$ is always equal to zero since $\frac{\mathrm{d}\lambda_2}{\mathrm{d}r} = \frac{\mathrm{d}\phi}{\mathrm{d}r} = 0$ at $r = 0$. With this fact and Eqs. (4b), (5b) and (6b) we concluded that the estimated value for $D(0)$ is definitely equal to the value of its initial guess and the estimated values for $D(r)$ will also deviate from the exact values near $r = 0$.

However, if we let $\frac{\mathrm{d}\lambda_2(0)}{\mathrm{d}r} = \frac{\mathrm{d}\lambda_2(\Delta r)}{\mathrm{d}r}$ and $\frac{\mathrm{d}\phi(0)}{\mathrm{d}r} = \frac{\mathrm{d}\phi(\Delta r)}{\mathrm{d}r}$, the singularity at $r = 0$ can be avoided in the present study and a reliable inverse solutions can be obtained. We will show this by using numerical experiments in Section 9.

7. Stopping criterion

If the problem contains no measurement errors, the traditional check condition can be specified as

$$J_1[Q(r)] < \eta_1 \tag{21a}$$

$$J_2[D(r)] < \eta_2 \tag{21b}$$

where η_1 and η_2 are the small-specified numbers. However, the measured temperature and irradiance data may contain measurement errors. Therefore, we do not expect the functional equations (3a) and (3b) to be equal to zero at the final iteration step.

Following the rigorous justification by Alifanov et al. [10], we use the discrepancy principle as the stopping criterion, i.e. we assume that the residuals for temperature and irradiance may be approximated by

$$|T(r,t) - Y(r,t)| \approx \sigma_1 \tag{22a}$$

$$|\phi(r) - \Phi(r)| \approx \sigma_2 \tag{22b}$$

where σ_1 and σ_2 are the standard deviations of the measurements, which are assumed to be constant.

By substituting Eqs. (22a) and (22b) into Eqs. (3a) and (3b), respectively, the following expressions are obtained for η_1 and η_2:

$$\eta_1 = \frac{1}{3}\sigma_1^2 t_f \tag{23a}$$

$$\eta_2 = \frac{1}{3}\sigma_2^2 \tag{23b}$$

Then, the stopping criterion is given by Eqs. (21a) and (21b) with η_1 and η_2 determined from Eqs. (23a) and (23b), respectively.

8. Computational procedure

The computational procedure for the solution of this inverse biotechnology problem may be summarized as follows:

First stage: Assign an initial guess for $Q^0(r)$.

Step 1 Solve the direct heat transfer problem given by Eq. (2a) for $T(r,t)$.
Step 2 Solve the adjoint problem given by Eq. (15) for $\lambda_1(r,t)$.
Step 3 Compute the gradient of the functional $J_1'[Q(r)]$ from Eq. (18).
Step 4 Compute the conjugate coefficients γ_1^n and the direction of descent $P_1^n(r)$ from Eqs. (6a) and (5a), respectively.
Step 5 Set $\Delta Q(r) = P_1^n(r)$ and solve the direct problem in variations given by Eq. (7) for $\Delta T(P_1^n)$.
Step 6 Compute the search step size β_1^n from Eq. (10).
Step 7 Compute the new estimation for $Q^{n+1}(r)$ from Eq. (4a).
Step 8 Examine the stopping criterion η_1. Continue if not satisfied.

Second stage: Assign an initial guess for $D^0(r)$.

Step 1 Solve the direct heat transfer problem given by Eq. (1a) for $\phi(r)$.
Step 2 Solve the adjoint problem given by Eq. (19) for $\lambda_2(r)$.
Step 3 Compute the gradient of the functional $J_2'[D(r)]$ from Eq. (20).

Step 4 Compute the conjugate coefficients γ_2^n and the direction of descent $P_2^n(r)$ from Eqs. (6b) and (5b), respectively.
Step 5 Set $\Delta D(r) = P_2^n(r)$ and solve the direct problem in variations given by Eq. (11) for $\Delta\phi(P_2^n)$.
Step 6 Compute the search step size β_2^n from Eq. (12).
Step 7 Compute the new estimation for $D^{n+1}(r)$ from Eq. (4b).
Step 8 Examine the stopping criterion η_2. Continue if not satisfied.

9. Results and discussion

The objective of this study is to show the validity of the CGM in simultaneously estimating the spatial-dependent optical absorption and diffusion coefficients, $\mu_a(r)$ and $D(r)$, for tissue with no prior information on the functional form of the unknown quantities.

Two numerical examples, with different functional form for $\mu_a(r)$ and $D(r)$, will be examined to illustrate the accuracy of the present algorithm in the inverse biotechnology problems based on the knowledge of measured temperature and irradiance distributions. As was mentioned previously, to estimate $\mu_a(r)$ we need to estimate $Q(r)$ first, for this reason the role of $\mu_a(r)$ is replaced by $Q(r)$.

One of the advantages of using the conjugate gradient method is that the initial guesses of the unknown functions $Q(r)$ and $D(r)$ can be chosen arbitrarily. In all the test cases considered here, the initial guesses of $Q(r)$ and $D(r)$ used to begin the iteration are taken as $Q^0(r) = D^0(r) = 1.0$.

In order to compare the results for situations involving random measurement errors, we assume normally distributed uncorrelated errors with zero mean and constant standard deviation. The simulated inexact measured temperature and irradiance $Y(r,t)$ and $\Phi(r)$, can be expressed as

$$Y = Y_{\text{exact}} + \omega\sigma_1 \tag{24a}$$

$$\Phi = \Phi_{\text{exact}} + \omega\sigma_2 \tag{24b}$$

where Y_{exact} and Φ_{exact} are the solutions of the direct problem with the exact values for $\mu_a(r)$ and $D(r)$; σ_1 and σ_2 are the standard deviations of the temperature and irradiance measurements, respectively; and ω is a random variable that generated by subroutine DRNNOR of the IMSL [11] and will be within −2.576 to 2.576 for a 99% confidence bound.

The procedures in obtaining Y_{exact} and Φ_{exact} are as follows:

(a) From Eq. (1a), use exact $\mu_a(r)$ and $D(r)$ to calculate irradiance $\phi(r)$, which is assigned as Φ_{exact}.
(b) Once $\phi(r)$ is calculated, from Eq. (2a) use $Q(r) = \mu_a(r)\phi(r)$ to calculate temperature $T(r,t)$, which is assigned as Y_{exact}.

We now present below two numerical experiments in determining $Q(r)$ (or $\mu_a(r)$) and $D(r)$ by the inverse analysis:

9.1. Numerical test case 1

The parameters for the direct problem are given as follows:

$$S = 100.0;\quad k(r) = 0.005;\quad C(r) = 4.5;$$
$$\phi(1) = 1.0;\ T(1,t) = 0.1;\quad T(r,0) = 0.0;\quad t_f = 1.0$$

Besides, the space and time increments used in numerical calculations are taken as $\Delta r = 0.01$ and $\Delta t = 0.001$ for a total time $t_f = 1.0$, respectively. Therefore a total of 202 unknown discreted coefficients are to be determined in this study.

The exact spatial-dependent optical absorption and diffusion coefficients, $\mu_a(r)$ and $D(r)$, for tissue are assumed as

$$\mu_a(r) = 5 + 2\cos(3\pi r);\quad 0 < r \leqslant 1 \tag{25a}$$

$$D(r) = 5 + 16r^2;\quad 0 < r \leqslant 1 \tag{25b}$$

One should note that in the present test case we use initial guess $Q^0(r) = D^0(r) = 1.0$, but now the exact values of $Q(1)$ and $D(0)$ are not equal to unity, therefore we concluded that the singularity near boundary $r = 0$ and 1 for the estimation of $D(r)$ and $Q(r)$ will be happened in the present study. However, if the modified conditions are used as mentioned previously, the estimation for $Q(1)$ and $D(0)$ can be improved significantly.

The inverse analysis is firstly performed in estimating $Q(r)$ by assuming exact measurements, $\sigma_1 = 0.0$. By setting $\eta_1 = 3\times10^{-9}$, after seven iterations the functional can be decreased to $J_1 = 2.56\times10^{-9}$. The measured and estimated temperatures, Y and T, are shown in Fig. 1 while the exact and estimated $Q(r)$ are shown in Fig. 2. It can be seen from Figs. 1 and 2 that there is a good agreement between the measured and estimated temperatures and the exact and estimated $Q(r)$.

The average errors for estimated temperature $T(r,t)$ and estimated $Q(r)$ are calculated as ERR1 = 0.024% and ERR2 = 0.036%, respectively, where the average errors for the estimated $T(r,t)$ and $Q(r)$ are defined as

$$\text{ERR1\%} = \left[\sum_{J=1}^{100}\sum_{I=1}^{101}\left|\frac{T(I,J) - Y(I,J)}{T(I,J)}\right|\right] \Big/ 10100 \times 100\% \tag{26a}$$

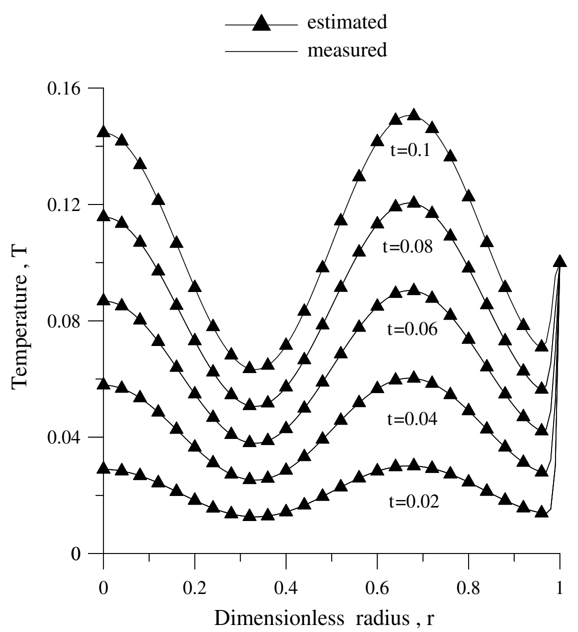

Fig. 1. The measured and estimated temperature distributions using exact measurements in test case 1.

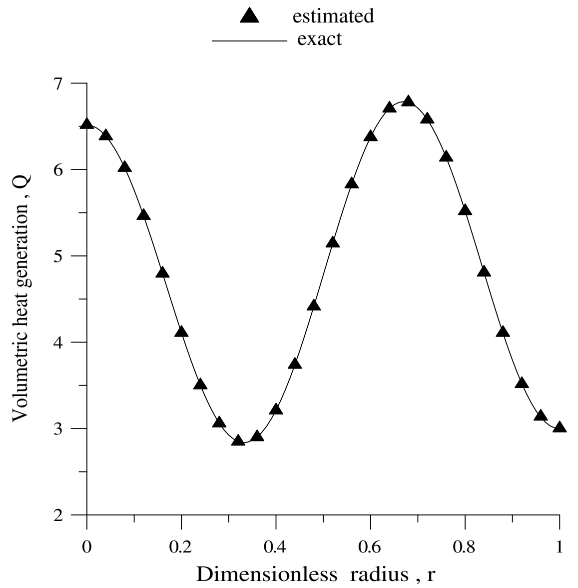

Fig. 2. The exact and estimated volumetric heat generation using exact measurements in test case 1.

$$\mathrm{ERR2\%} = \left[\sum_{I=1}^{101} \left| \frac{\widehat{Q}(I) - Q(I)}{Q(I)} \right| \right] \Big/ 101 \times 100\% \qquad (26b)$$

here I and J represent the index of discreted space and time, while $\widehat{Q}(I)$ denotes the estimated value.

Once $Q(r)$ is estimated, the inverse calculation in then proceeded to the second stage, i.e. the estimation of $D(r)$. By assuming exact measurements, $\sigma_2 = 0.0$ and by setting $\eta_2 = 1 \times 10^{-11}$, after 178 iterations the functional can be decreased to $J_2 = 8.77 \times 10^{-12}$. The measured and estimated irradiances, Φ and ϕ, are shown in Fig. 3 while the exact and estimated $D(r)$ are shown in Fig. 4.

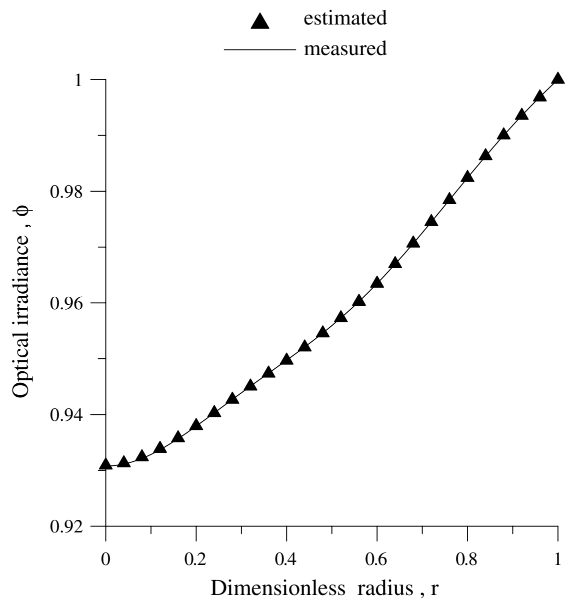

Fig. 3. The measured and estimated irradiance distributions using exact measurements in test case 1.

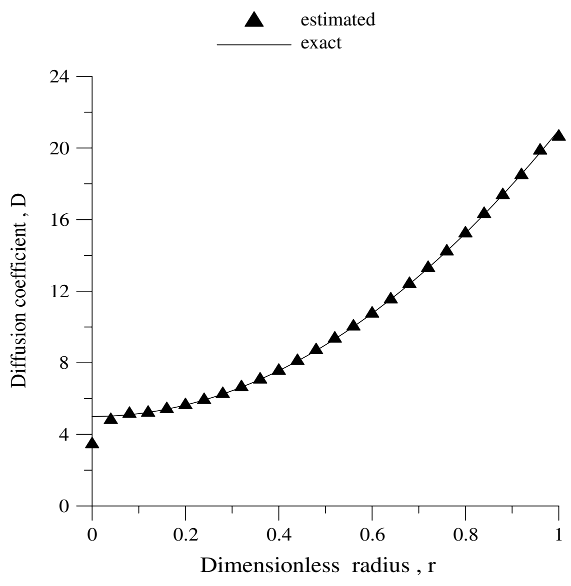

Fig. 4. The exact and estimated diffusion coefficient using exact measurements in test case 1.

It can be seen from Fig. 3 that there is a good agreement between the measured and estimated irradiance. Moreover, from Fig. 4 we learn that the estimations for $D(r)$ are very accurate except near $r = 0$ due to the singularity addressed previously.

The average errors for estimated irradiance $\phi(r)$ and estimated $D(r)$ are calculated as ERR3 = 0.00072% and ERR4 = 0.24%, respectively, where the average errors for the estimated $\phi(r,t)$ and $D(r)$ are defined as

$$\mathrm{ERR3\%} = \left[\sum_{I=1}^{101} \left| \frac{\phi(I) - \Phi(I)}{\phi(I)} \right| \right] \Big/ 101 \times 100\% \quad (26c)$$

$$\mathrm{ERR4\%} = \left[\sum_{I=1}^{101} \left| \frac{\widehat{D}(I) - D(I)}{D(I)} \right| \right] \Big/ 101 \times 100\% \quad (26d)$$

here I indicates the index of discreted space and $\widehat{D}(I)$ denotes the estimated value.

The inverse estimation of diffusion coefficient indicates that its value is not sensitive to the irradiance since ERR3 is very small, i.e. the difference between the measured and calculated irradiance is very small, but ERR4 is not that small. It is because that the role of diffusion coefficient in effecting the irradiance for steady state problem is insignificance.

Finally the optical absorption coefficient $\mu_a(r)$ can be obtained by using $\mu_a(r) = Q(r)/\phi(r)$ and the result is shown in Fig. 5. The average errors for estimated absorption coefficient $\mu_a(r)$ is calculated as ERR5 = 0.039%, where the average error ERR5 is defined as

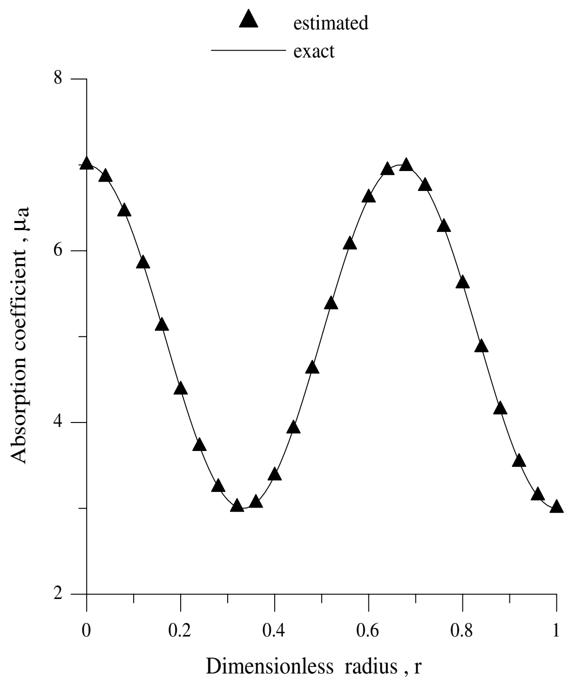

Fig. 5. The exact and estimated absorption coefficient using exact measurements in test case 1.

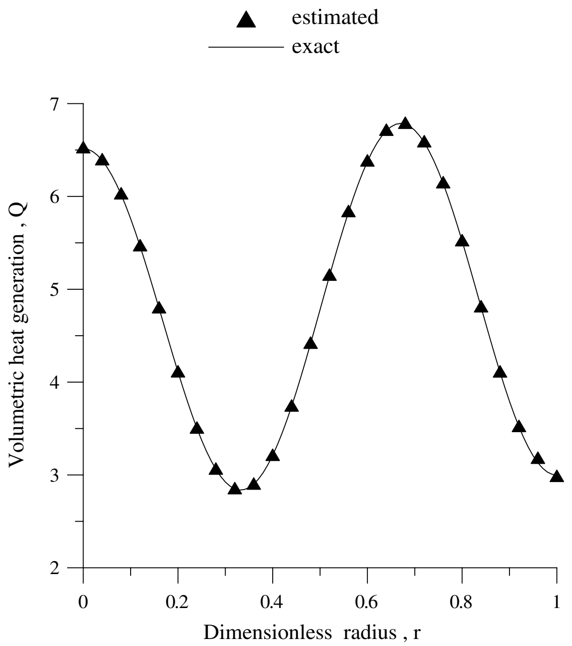

Fig. 6. The exact and estimated volumetric heat generation using inexact measurements in test case 1.

$$\mathrm{ERR5\%} = \left[\sum_{I=1}^{101} \left| \frac{\mu_a(I) - \hat{\mu}_a(I)}{\mu_a(I)} \right| \right] \Big/ 101 \times 100\% \quad (26e)$$

here I indicates the index of discreted space and $\hat{\mu}_a(I)$ denotes the estimated value.

Next, let us discuss the influence of the measurement errors on the inverse solutions. The measurement error for the temperature and irradiance are taken as $\sigma_1 = 5 \times 10^{-4}$ (about 1% of the average measured temperature) and $\sigma_2 = 9 \times 10^{-4}$ (about 0.1% of the average measured irradiance).

The stopping criteria can be obtained by discrepancy principle and given in Eq. (21). The number of iteration for $\sigma_1 = 5 \times 10^{-4}$ is 3 and for $\sigma_2 = 9 \times 10^{-4}$ is 18. The estimated $Q(r)$, $D(r)$ and $\mu_a(r)$ are shown in Figs. 6–8, respectively. The average errors for the estimated $Q(r)$, $D(r)$ and $\mu_a(r)$ are calculated as ERR2 = 0.29%, ERR4 = 5.47% and ERR5 = 0.33%, respectively. This implies that reliable inverse solutions can still be obtained when measurement errors are considered.

9.2. Numerical test case 2

The parameters for the direct problem, the space and time increments used in numerical test case 2 are taken the same as were used in numerical test case 1.

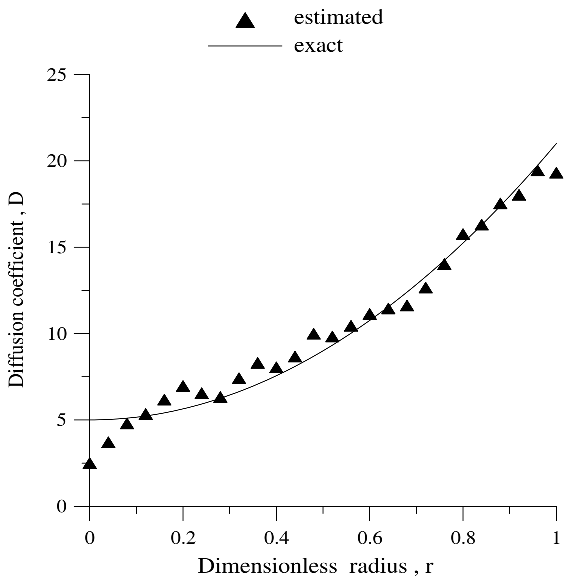

Fig. 7. The exact and estimated diffusion coefficient using inexact measurements in test case 1.

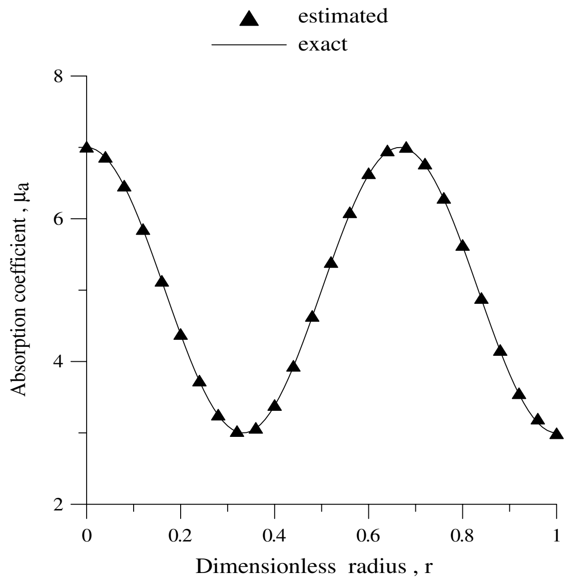

Fig. 8. The exact and estimated absorption coefficient using inexact measurements in test case 1.

The exact spatial-dependent optical absorption and diffusion coefficients, $\mu_a(r)$ and $D(r)$, for tissue are assumed as the following step functions

$$\mu_a(r) = \begin{cases} 2.0; & 0 \leqslant r < \frac{1}{3} \\ 5.0; & \frac{1}{3} \leqslant r < \frac{2}{3} \\ 8.0; & \frac{2}{3} \leqslant r \leqslant 1 \end{cases} \tag{27a}$$

$$D(r) = \begin{cases} 2.0; & 0 \leqslant r < \frac{1}{5} \\ 4.0; & \frac{1}{5} \leqslant r < \frac{2}{5} \\ 6.0; & \frac{2}{5} \leqslant r < \frac{3}{5} \\ 8.0; & \frac{3}{5} \leqslant r < \frac{4}{5} \\ 10.0; & \frac{4}{5} \leqslant r \leqslant 1 \end{cases} \tag{27b}$$

Test case 2 is a more rigorous examination since there exist discontinuities for both optical diffusion and absorption coefficients. It is expected that the inverse solutions are worse than test case 1.

When considering exact measurements for temperature and irradiance and following the similar procedures as performed in test case 1, for $\eta_1 = 3 \times 10^{-9}$ and $\eta_2 = 3 \times 10^{-10}$, after 10 and 213 iterations the functional can be decreased to $J_1 = 1.35 \times 10^{-9}$ and $J_2 = 2.97 \times 10^{-10}$. The inverse solutions are reported in Figs. 9 and 10 for the estimated optical diffusion coefficient and optical absorption coefficient, respectively. The average errors for ERR1, ERR2, ERR3, ERR4 and ERR5 are calculated as 0.022%, 0.045%, 0.0065%, 4.12% and 0.51%, respectively. Again, from Fig. 9 we learn that the singularity for the estimated $D(0)$ is improved significantly by using modified conditions. Next, when the measurement errors for temperature and irradiance are taken as $\sigma_1 = 6.24 \times 10^{-4}$ (about 1% of the average measured temperature) and $\sigma_2 = 4.52 \times 10^{-4}$ (about 0.05% of the average measured irradiance), the number of iteration to obtain the inverse solutions for $\sigma_1 = 6.24 \times 10^{-4}$ is 2 and for $\sigma_2 = 4.52 \times 10^{-4}$ is 41. The estimated $D(r)$ and $\mu_a(r)$ are shown in Figs. 11 and 12,

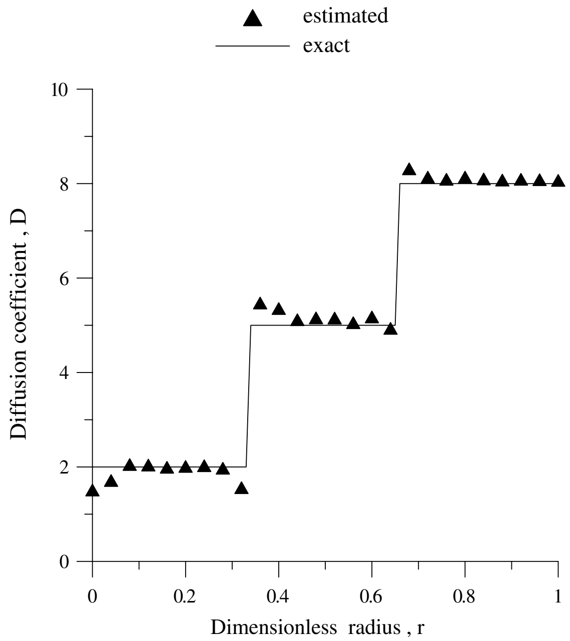

Fig. 9. The exact and estimated diffusion coefficient using exact measurements in test case 2.

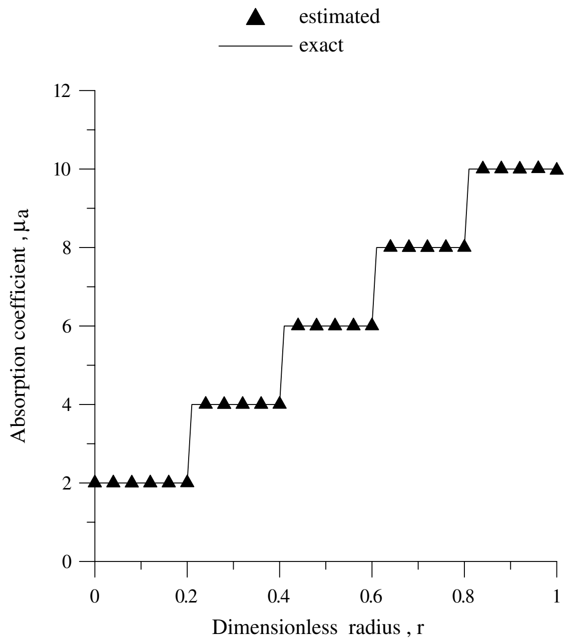

Fig. 10. The exact and estimated absorption coefficient using exact measurements in test case 2.

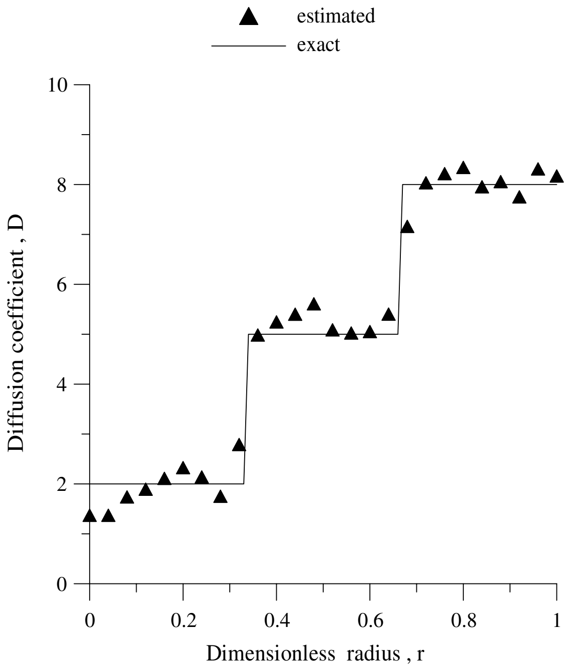

Fig. 11. The exact and estimated diffusion coefficient using inexact measurements in test case 2.

respectively. The average errors for the estimated $D(r)$ and $\mu_a(r)$ are calculated as ERR4 $= 9.26\%$ and ERR5 $=$ 1.64%, respectively.

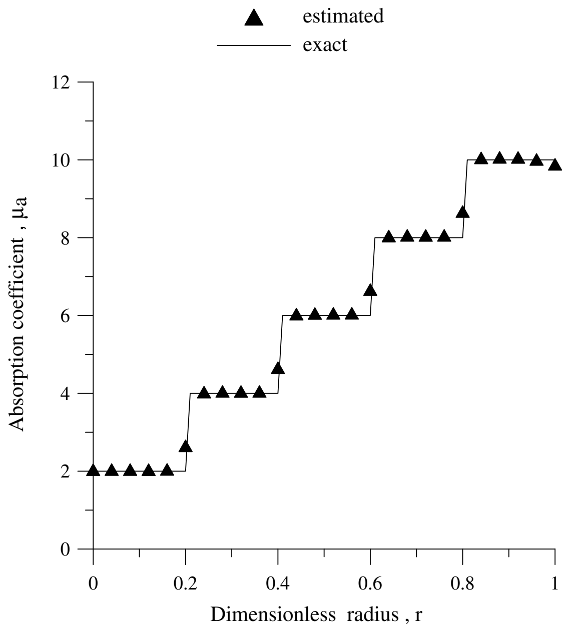

Fig. 12. The exact and estimated absorption coefficient using inexact measurements in test case 2.

From the above two test cases we learned that an inverse biotechnology problem in simultaneously estimating the optical diffusion and absorption coefficients of tissue is now completed. Reliable estimations can be obtained when using either exact or error measurements.

10. Conclusions

The CGM was successfully applied for the solution of the inverse biotechnology problem to estimate the unknown the spatial-dependent optical diffusion and absorption coefficients of tissue by utilizing simulated temperature and irradiance readings. Two numerical test cases involving different form of optical coefficients and measurement errors were considered. The results show that the inverse solutions obtained by CGM are still reliable as the measurement errors are increased.

Acknowledgements

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References

[1] K. Dowlatshahi, A.K. Bhattacharya, T. Matalon, B. Silver, J.W. Willams, Percutaneous interstitial laser therapy of

patient with recurrent hepatoma in a transplanted liver, Surgery 112 (1992) 603–606.
[2] Z. Amin, J.J. Donald, A. Masters, R. Kant, A.C. Steger, S.G. Bown, W.R. Lees, Hepatic metastases: Interstitial laser photocoagulation with real-time US monitoring and dynamic CT evaluation of treatment, Radiology 187 (1993) 339–347.
[3] A. Weinberg, E. Winger, The Physical Theory of Neutron Chain Reactors, University of Chicago Press, Chicago, 1958.
[4] O.M. Alifanov, Inverse Heat Transfer Problem, Springer-Verlag, Berlin, 1994.
[5] C.H. Huang, C.W. Chen, A boundary element based inverse-problem in estimating transient boundary conditions with conjugate gradient method, Int. J. Numer. Methods Eng. 42 (1998) 943–965.
[6] C.H. Huang, S.P. Wang, A three-dimensional inverse heat conduction problem in estimating surface heat flux by conjugate gradient method, Int. J. Heat Mass Transfer 42 (1999) 3387–3403.
[7] C.H. Huang, W.C. Chen, A three-dimensional inverse forced convection problem in estimating surface heat flux by conjugate gradient method, Int. J. Heat Mass Transfer 43 (2000) 3171–3181.
[8] C.H. Huang, S.C. Chin, A two-dimensional inverse problem in imaging the thermal conductivity of a non-homogeneous medium, Int. J. Heat Mass Transfer 43 (2000) 4061–4071.
[9] C.H. Huang, A nonlinear inverse vibration problem of estimating the external forces for a system with displacement-dependent parameters, J. Sound Vib. 248 (2001) 789–807.
[10] O.M. Alifanov, E.A. Artyukhin, S.V. Rumyantsev, Extreme Methods for Solving Ill-Posed Problems with Applications to Inverse Heat Transfer Problems, Begell House, Inc, New York, 1995.
[11] IMSL Library Edition 10.0. User's Manual: Math Library Version 1.0, IMSL, Houston, TX, 1987.