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Estimation of dimensionless parameters of Luikov's system for heat and mass transfer in capillary porous media

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Abstract

This work deals with the solution of inverse problems of parameter estimation involving heat and mass transfer in capillary porous media, as described by the linear one-dimensional Luikov's equations. Our main objective is to use the D-optimum criterion to design the experiment with respect to the magnitude of the applied heat flux, heating and final experimental times, as well as the number and locations of sensors. The present parameter estimation problem is solved with Levenberg–Marquardt's method of minimization of the ordinary least-squares norm, by using simulated temperature data containing random errors. Moisture content measured data is not considered available for the inverse analysis in order to avoid quite involved measurement techniques. We show that accurate estimates can be obtained for Luikov, Kossovitch and Biot numbers by using only temperature measurements in the inverse analysis. Also, the experimental time can be reduced if the body is heated during part of the total experimental time.

Keywords: Luikov's equations; Capillary-porous media; Heat and mass transfer; Inverse problem; Parameter estimation; Levenberg–Marquardt's method

1. Introduction

Heat and mass transfer in capillary porous media has practical applications in several different areas including, among others, drying and the study of moisture migration in soils and construction materials [1–3]. For the mathematical modeling of such phenomena, Luikov [1] has proposed his widely known formulation, based on a system of coupled partial differential equations, which takes into account the effects of the temperature gradient on the moisture migration.

The computation of temperature and moisture content fields in capillary porous media, from the knowledge of initial and boundary conditions, as well as of the thermophysical properties appearing in the formulation, constitutes a *Direct Problem* of heat and mass transfer. Several analytical, numerical and hybrid analytical-numerical techniques have been used in the past for the solution of direct problems formulated with Luikov's equations [1–11]. Appropriately formulated direct problems are mathematically classified as *well-posed*, that is, their solutions satisfy Hadamard's requirements of existence, uniqueness and stability with respect to the input data [12–17].

The numerical modeling of heat and mass transfer in a capillary porous medium requires the accurate knowledge of several thermophysical and boundary condition parameters that appear in the formulation. The identification of such parameters from the knowledge of temperature and/or moisture content measurements taken in the medium is an *Inverse Problem* of coupled heat and mass transfer [12–17]. Generally, inverse problems are mathematically classified as *ill-posed*, in the sense that their solutions do not satisfy Hadamard's requirement of stability under small perturbations in the input data [12–17]. Despite the ill-posed character, the solution of an inverse problem can be obtained through its reformulation in terms of a well-posed problem, such as a minimization problem associated with some kind of regularization (stabilization) technique. Different methods based on such an approach have been successfully used in the past for the estimation of parameters and functions, in linear and non-linear inverse problems. They include the Levenberg–Marquardt method of parameter estimation [12,

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Nomenclature

Q	dimensionless heat flux defined by Eq. (2c)
Lu	Luikov number defined by Eq. (2e)
Pn	Posnov number defined by Eq. (2f)
Ko	Kossovitch number defined by Eq. (2i)
Bi_q	dimensionless heat transfer coefficient defined by Eq. (2g)
Bi_m	dimensionless mass transfer coefficient defined by Eq. (2h)
X	dimensionless position defined by Eq. (2j)
$\mathbf{Y}$	vector of measured temperatures
$\mathbf{J}$	sensitivity matrix
J	sensitivity coefficients
$\mathbf{P}$	vector of unknown parameters
M	number of sensors
I	number of transient measurements taken per sensor
N	number of unknown parameters
S	ordinary least-squares norm defined by Eq. (15)

Greek symbols

θ	dimensionless temperature defined by Eq. (2a)
ϕ	dimensionless moisture content defined by Eq. (2b)
δ	thermogradient coefficient
ε	phase conversion factor
τ	dimensionless time defined by Eq. (2d)
τ_h	dimensionless heating time
τ_f	dimensionless final time of the experiment
σ	standard-deviation of the measurement errors

Subscripts

i	refers to the measurement time τ_i
m	refers to the sensor number
j	refers to the unknown parameters

Superscripts

k	iteration number

13,18–20] and the conjugate gradient method of parameter and function estimation [13,14,17].

Articles dealing with the solution of inverse heat transfer problems are quite common in the literature nowadays. However, it is interesting to note that only few articles are available on the solution of inverse problems of coupled heat and mass transfer [18,21–23]. A boundary inverse problem was addressed in reference [21], involving the estimation of the moisture flux at the outer surface of an annular region, by using the conjugate gradient method of function estimation. On the other hand, Refs. [18,22,23] dealt with the estimation of parameters appearing in Luikov's formulation, by utilizing the Levenberg–Marquardt method with temperature measurements. With the use of only temperature measurements in the parameter estimation procedure, very involved techniques for the measurement of moisture content, such as the use of gamma rays, can be avoided, resulting in simpler and faster experiments. The estimation of the moisture diffusivity, depending on temperature and moisture content, was examined by Kanevce et al. [22,23]. The physical problem considered in their works involved the drying of thin infinitely long samples of porous materials, heated by forced convection on both sides. In Ref. [18], the possibility of simultaneously estimating more than one parameter in Luikov's linear dimensionless formulation was investigated. The physical problem considered in this work [18] was different from that of Refs. [22,23]. It involved the drying of one-dimensional samples of porous materials, with one of the sides put into contact with a heater, while the other was open to surrounding air. Accurate estimates could be obtained for the Luikov, Kossovitch and Biot numbers [18].

In this paper, we extend the analysis of our previous work [18] and examine the effects of the heating process, more specifically the heat flux magnitude and the heating time period, on the accuracy of the estimated parameters. The D-optimum approach [12,13,17,18,24–27], based on the maximization of the determinant of Fisher's information matrix, is used for the experiment design, together with the analysis of the sensitivity coefficients. The associated direct problem is solved with the Generalized Integral Transform Technique [3,7–9]. The Levenberg–Marquardt method [12, 13,18–20] is used as the minimization procedure of the least-squares norm in order to estimate the parameters.

2. Direct problem

The physical problem involves a one-dimensional capillary porous medium, initially at uniform temperature and uniform moisture content. One of the boundaries, which is

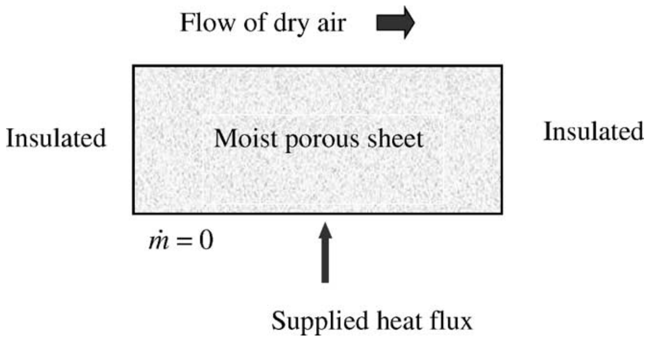

Fig. 1. Geometry for the drying of a moist porous medium.

impervious to moisture transfer, is in direct contact with a heater. The other boundary is in contact with the dry surrounding air, thus resulting in a convective boundary condition for both the temperature and the moisture content, as illustrated in Fig. 1. The linear system of equations proposed by Luikov [1] with associated initial and boundary conditions, for the modeling of such physical problem involving heat and mass transfer in a capillary porous media, can be written in dimensionless form as:

$$\frac{\partial\theta(X,\tau)}{\partial\tau} = \frac{\partial^2\theta(X,\tau)}{\partial X^2} - \varepsilon Ko\frac{\partial\phi(X,\tau)}{\partial\tau} \quad \text{in } 0 < X < 1, \quad \text{for } \tau > 0 \tag{1a}$$

$$\frac{\partial\phi(X,\tau)}{\partial\tau} = Lu\frac{\partial^2\phi(X,\tau)}{\partial X^2} - Lu\,Pn\frac{\partial^2\theta(X,\tau)}{\partial X^2} \quad \text{in } 0 < X < 1, \quad \text{for } \tau > 0 \tag{1b}$$

$$\theta(X,0) = 0, \quad \text{for } \tau = 0, \quad \text{in } 0 < X < 1 \tag{1c}$$

$$\phi(X,0) = 0, \quad \text{for } \tau = 0, \quad \text{in } 0 < X < 1 \tag{1d}$$

$$\frac{\partial\theta(0,\tau)}{\partial X} = -Q(\tau) \quad \text{at } X = 0, \quad \text{for } \tau > 0 \tag{1e}$$

$$\frac{\partial\phi(0,\tau)}{\partial X} - Pn\frac{\partial\theta(0,\tau)}{\partial X} = 0 \quad \text{at } X = 0, \quad \text{for } \tau > 0 \tag{1f}$$

$$\frac{\partial\theta(1,\tau)}{\partial X} + Bi_q\theta(1,\tau) = Bi_q - (1-\varepsilon)Ko\,Lu\,Bi_m\big[1-\phi(1,\tau)\big] \quad \text{at } X = 1, \quad \text{for } \tau > 0 \tag{1g}$$

$$\frac{\partial\phi(1,\tau)}{\partial X} + Bi_m^*\phi(1,\tau) = Bi_m^* - Pn\,Bi_q\big[\theta(1,\tau) - 1\big] \quad \text{at } X = 1, \quad \text{for } \tau > 0 \tag{1h}$$

where the following dimensionless groups were defined

$$\theta(X,\tau) = \frac{T(x,t) - T_o}{T_s - T_o} \tag{2a}$$

$$\phi(X,\tau) = \frac{u_o - u(x,t)}{u_o - u^*} \tag{2b}$$

$$Q(\tau) = \frac{q(\tau)l}{k(T_s - T_o)} \tag{2c}$$

$$\tau = \frac{at}{l^2} \tag{2d}$$

$$Lu = \frac{a_m}{a} \tag{2e}$$

$$Pn = \delta\frac{T_s - T_o}{u_o - u^*} \tag{2f}$$

$$Bi_q = \frac{hl}{k} \tag{2g}$$

$$Bi_m = \frac{h_m l}{k_m} \tag{2h}$$

$$Ko = \frac{r}{c}\frac{u_o - u^*}{T_s - T_o} \tag{2i}$$

$$X = \frac{x}{l} \tag{2j}$$

The properties of the porous medium appearing above include the thermal diffusivity (a), the moisture diffusivity (a_m), the thermal conductivity (k), the moisture conductivity (k_m) and the specific heat (c). Other physical quantities appearing in the dimensionless groups of Eqs. (2) are the heat transfer coefficient (h), the mass transfer coefficient (h_m), the thickness of porous medium (l), the prescribed heat flux ($q(\tau)$), the latent heat of evaporation of water (r), the temperature of the surrounding air (T_s), the uniform initial temperature in the medium (T_o), the moisture content of the surrounding air (u^*), the uniform initial moisture content in the medium (u_o), the thermogradient coefficient (δ) and the phase conversion factor (ε). Lu, Pn and Ko denote the Luikov, Possnov and Kossovitch numbers, respectively.

Problem (1) is referred to as a *Direct Problem* when initial and boundary conditions, as well as all parameters appearing in the formulation are known. The objective of the direct problem is to determine the dimensionless temperature and moisture content fields, $\theta(X,\tau)$ and $\phi(X,\tau)$, respectively, in the capillary porous media. The direct problem is solved here by applying the *Generalized Integral Transform Technique* as described next [3,7–9].

3. Method of solution for the direct problem

The Generalized Integral Transform Technique (GITT) is a powerful hybrid numerical-analytical approach, which has been successfully applied to obtain *benchmark* solutions for different classes of linear and non-linear diffusion/convection problems [3,7–9]. Such a technique, as applied to time dependent problems, includes the following basics steps:

(i) Choose an auxiliary eigenvalue problem;
(ii) Develop the appropriate transform/inverse formulae pair;
(iii) Integral transform the original problem by substituting the inverse formula into non-transformable terms or by using the integral balance approach;
(iv) Solve the resulting coupled system of ordinary differential equations in the time variable;
(v) Apply the inverse formula to the transformed field in order to obtain the solution for the original problem.

In order to overcome difficulties in the convergence of the solution in the neighborhood of boundaries containing non-homogeneities, the solution of the direct problem (1) is written in terms of analytical filtering solutions, $\theta_s(X;\tau)$ and $\phi_s(X;\tau)$, and filtered solutions, $\theta_h(X,\tau)$ and $\phi_h(X,\tau)$, as

$$\theta(X,\tau) = \theta_s(X;\tau) + \theta_h(X,\tau) \tag{3a}$$

$$\phi(X,\tau) = \phi_s(X;\tau) + \phi_h(X,\tau) \tag{3b}$$

The filtering solutions are obtained from the following steady-state problem, where τ appears as a parameter,

$$\alpha\frac{d^2\theta_s(X;\tau)}{dX^2} = \beta\frac{d^2\phi_s(X;\tau)}{dX^2} \quad \text{in } 0 < X < 1 \tag{4a}$$

$$\frac{d^2\phi_s(X;\tau)}{dX^2} = Pn\frac{d^2\theta_s(X;\tau)}{dX^2} \quad \text{in } 0 < X < 1 \tag{4b}$$

$$\frac{d\theta_s}{dX} = -Q(\tau) \quad \text{at } X = 0 \tag{4c}$$

$$\frac{d\phi_s}{dX} = -PnQ(\tau), \quad \text{at } X = 0 \tag{4d}$$

$$\frac{d\theta_s}{dX} + Bi_q\theta_s = Bi_q - (1-\varepsilon)Ko\,Lu\,Bi_m[1-\phi_s] \quad \text{at } X = 1 \tag{4e}$$

$$\frac{d\phi_s}{dX} + Bi_m^*\phi_s = Bi_m^* - Pn\,Bi_q[\theta_s - 1] \quad \text{at } X = 1 \tag{4f}$$

in the form

$$\theta_s(X;\tau) = 1 + Q(\tau)\left(1 + \frac{1}{Bi_q} - X\right) \tag{5a}$$

$$\phi_s(X;\tau) = 1 + PnQ(\tau)(1-X) \tag{5b}$$

where

$$\alpha = 1 + \varepsilon Ko\,Lu\,Pn \tag{6a}$$

$$\beta = \varepsilon Ko\,Lu \quad \text{and} \tag{6b}$$

$$Bi_m^* = Bi_m\big[1 - (1-\varepsilon)Pn\,Ko\,Lu\big] \tag{6c}$$

By substituting Eqs. (3a,b) into the direct problem given by Eqs. (1) and making use of the steady-state problem (4a–f), we obtain the following filtered problem

$$\frac{\partial\theta_h(X,\tau)}{\partial\tau} = \alpha\frac{\partial^2\theta_h(X,\tau)}{\partial X^2} - \beta\frac{\partial^2\phi_h(X,\tau)}{\partial X^2} - \frac{\partial\theta_s(X;\tau)}{\partial\tau} \quad \text{in } 0 < X < 1, \quad \text{for } \tau > 0 \tag{7a}$$

$$\frac{\partial\phi_h(X,\tau)}{\partial\tau} = Lu\frac{\partial^2\phi_h(X,\tau)}{\partial X^2} - Lu\,Pn\frac{\partial^2\theta_h(X,\tau)}{\partial X^2} - \frac{\partial\phi_s(X;\tau)}{\partial\tau} \quad \text{in } 0 < X < 1, \quad \text{for } \tau > 0 \tag{7b}$$

$$\theta_h(X,0) = -\theta_s(X;0) \quad \text{for } \tau = 0, \quad \text{in } 0 < X < 1 \tag{7c}$$

$$\phi_h(X,0) = -\phi_s(X;0) \quad \text{for } \tau = 0, \quad \text{in } 0 < X < 1 \tag{7d}$$

$$\frac{\partial\theta_h}{\partial X} = \frac{\partial\phi_h}{\partial X} = 0 \quad \text{at } X = 0, \quad \text{for } \tau > 0 \tag{7e,f}$$

$$\frac{\partial\theta_h}{\partial X} + Bi_q\theta_h = (1-\varepsilon)Ko\,Lu\,Bi_m\phi_h \quad \text{at } X = 1, \quad \text{for } \tau > 0 \tag{7g}$$

$$\frac{\partial\phi_h}{\partial X} + Bi_m^*\phi_h = -Pn\,Bi_q\theta_h \quad \text{at } X = 1, \quad \text{for } \tau > 0 \tag{7h}$$

The following eigenvalue problems are used in order to define the integral transform/inverse formula pairs for temperature and moisture content, respectively,

$$\frac{d^2\bar{\varphi}_i(X)}{dX^2} + \gamma_i^2\bar{\varphi}_i(X) = 0 \quad \text{in } 0 < X < 1 \tag{8a}$$

$$\frac{d\bar{\varphi}_i(0)}{dX} = 0 \tag{8b}$$

$$\frac{d\bar{\varphi}_i(1)}{dX} + Bi_q\bar{\varphi}_i(1) = 0 \tag{8c}$$

$$\frac{d^2\Gamma_i(X)}{dX^2} + \xi_i^2\overline{\Gamma}_i(X) = 0 \quad \text{in } 0 < X < 1 \tag{8d}$$

$$\frac{d\overline{\Gamma}_i(0)}{dX} = 0 \tag{8e}$$

$$\frac{d\overline{\Gamma}_i(1)}{dX} + Bi_m^*\overline{\Gamma}_i(1) = 0 \tag{8f}$$

with analytical solutions [2,28] given by

$$\bar{\varphi}_i(X) = \frac{\cos(\gamma_i X)}{\sqrt{N_1(\gamma_i)}} \tag{9a}$$

$$\overline{\Gamma}_i(X) = \frac{\cos(\xi_i X)}{\sqrt{N_2(\xi_i)}} \tag{9b}$$

and normalization integrals obtained as

$$N_1(\gamma_i) = \frac{1}{2}\left[1 + \frac{Bi_q}{\gamma_i^2 + Bi_q^2}\right] \tag{10a}$$

$$N_2(\xi_i) = \frac{1}{2}\left[1 + \frac{Bi_m^*}{\xi_i^2 + Bi_m^{*2}}\right] \tag{10b}$$

The eigenvalues can be computed from the solution of the following transcendental equations:

$$(\gamma_i)\tan(\gamma_i) = Bi_q \tag{11a}$$

$$(\xi_i)\tan(\xi_i) = Bi_m^* \tag{11b}$$

The integral transform/inverse formula pairs, for temperature and moisture content are respectively defined as

$$\bar{\theta}_i(\tau) = \int_{X=0}^{1} \bar{\varphi}_i(X)\theta_h(X,\tau)\,dX \tag{12a}$$

$$\theta_h(X,\tau) = \sum_{i=1}^{\infty}\bar{\varphi}_i(X)\bar{\theta}_i(\tau) \tag{12b}$$

$$\bar{\phi}_i(\tau) = \int_{X=0}^{1} \overline{\Gamma}_i(X)\phi_h(X,\tau)\,dX \tag{13a}$$

$$\phi_h(X,\tau) = \sum_{i=1}^{\infty}\overline{\Gamma}_i(X)\bar{\phi}_i(\tau) \tag{13b}$$

By integral transforming Eqs. (7a,b) with Eqs. (12b) and (13b) and performing some lengthy but straightforward manipulations, we obtain the following coupled system of ordinary differential equations for the transformed variables:

$$\frac{d\bar{\theta}_i(\tau)}{d\tau} + \alpha\gamma_i^2\bar{\theta}_i(\tau) - \beta\sum_{j=1}^{\infty}A_{ij}^*\bar{\phi}_j(\tau) = \bar{\varphi}_i(1)Ko\,Lu\big[(Bi_m - \varepsilon Bi_q)\phi_h(1,\tau) + \varepsilon Pn\,Bi_q\theta_h(1,\tau)\big] \tag{14a}$$

$$\frac{d\bar{\phi}_i(\tau)}{d\tau} + Lu\,\xi_i^2\bar{\phi}_i(\tau) - Lu\,Pn\sum_{j=1}^{\infty}B_{ij}^*\bar{\theta}_j(\tau) = -\overline{\Gamma}_i(1)Lu\,Pn\big[Bi_m^*\theta_h(1,\tau) + (1-\varepsilon)Ko\,Lu\,Bi_m\phi_h(1,\tau)\big] \tag{14b}$$

where

$$\theta_h(1,\tau) = -\frac{1}{Bi_q}\left[\sum_{j=1}^{\infty} \bar{f}_j \frac{d\bar{\theta}_j(\tau)}{d\tau} + Ko\sum_{j=1}^{\infty} \bar{f}_j^* \frac{d\bar{\phi}_j(\tau)}{d\tau}\right] \quad (14c)$$

$$\phi_h(1,\tau) = -\frac{1}{Lu\,Bi_m}\left[\sum_{j=1}^{\infty} \bar{f}_j^* \frac{d\bar{\phi}_j(\tau)}{d\tau}\right] \quad (14d)$$

$$\bar{f}_j = \int_{X=0}^{1} \bar{\varphi}_j(X)\,dX = \frac{1}{\sqrt{N_1(\gamma_j)}}\frac{\mathrm{sen}(\gamma_j)}{\gamma_j} \quad (14e)$$

$$\bar{f}_j^* = \int_{X=0}^{1} \bar{\Gamma}_j(X)\,dX = \frac{1}{\sqrt{N_2(\xi_j)}}\frac{\mathrm{sen}(\xi_j)}{\xi_j} \quad (14f)$$

$$A_{ij}^* = \int_{X=0}^{1} \bar{\varphi}_i(X)\bar{\Gamma}_j(X)\,dX \quad (14g)$$

$$B_{ij}^* = \int_{X=0}^{1} \bar{\varphi}_j(X)\bar{\Gamma}_i(X)\,dX \quad (14h)$$

This system is solved by using subroutines available in numerical libraries such as the IMSL [29], after being truncated to a sufficiently large order that provides convergence for the original variables towards the user prescribed accuracy target.

4. Inverse problem

For the *inverse problem* of interest here, the parameters $Lu, Pn, Ko, \varepsilon, Bi_q$ and Bi_m are regarded as unknown quantities. For the estimation of such parameters, we consider available the transient temperature measurements Y_{im} taken at the locations X_m, $m = 1, \ldots, M$. The subscript i above refers to the time at which the measurements are taken, that is, t_i, for $i = 1, \ldots, I$. We note that the temperature measurements may contain random errors, but all the other quantities appearing in the formulation of the direct problem are supposed to be known exactly.

Inverse problems are ill-posed [12–17]. Several methods of solution of inverse problems, such as the one used here, involve their reformulation in terms of well-posed minimization problems. By assuming additive, uncorrelated and normally distributed random errors, with constant standard deviation and zero mean, the solution of the present parameter estimation problem can be obtained through the minimization of the ordinary least-squares norm. Such a norm can be written as

$$S(\mathbf{P}) = [\mathbf{Y} - \theta(\mathbf{P})]^{\mathrm{T}}[\mathbf{Y} - \theta(\mathbf{P})] \quad (15)$$

where $\mathbf{P} = [Bi_q, Bi_m, Lu, Pn, Ko, \varepsilon,]$ denotes the vector of unknown parameters. The superscript T above denotes transpose and $[\mathbf{Y} - \theta(\mathbf{P})]^{\mathrm{T}}$ is given by

$$[\mathbf{Y} - \theta(\mathbf{P})]^{\mathrm{T}} \equiv [(\vec{Y}_1 - \vec{\theta}_1), (\vec{Y}_2 - \vec{\theta}_2), \ldots, (\vec{Y}_I - \vec{\theta}_I)] \quad (16a)$$

where $(\vec{Y}_i - \vec{\theta}_i)$ is a row vector containing the differences between the measured and estimated temperatures at the measurement positions X_m, $m = 1, \ldots, M$, at time t_i, that is,

$$(\vec{Y}_i - \vec{\theta}_i) = [Y_{i1} - \theta_{i1}, Y_{i2} - \theta_{i2}, \ldots, Y_{iM} - \theta_{iM}] \quad (16b)$$

The estimated temperatures θ_{im} are obtained from the solution of the direct problem, Eqs. (1), at the measurement location X_m and at time t_i, by using estimates for the unknown parameters P_j, $j = 1, \ldots, N$.

5. Method of solution for the inverse problem

The present inverse problem of parameter estimation is solved with the Levenberg–Marquardt method of minimization of the least-squares norm [12,13,18–20]. Such a method was first derived by Levenberg [19] in 1944, by modifying the ordinary least squares norm. Later, in 1963, Marquardt [20] derived basically the same technique by using a different approach. Marquardt's intention was to obtain a method that would tend to the Gauss method in the neighborhood of the minimum of the ordinary least squares norm, and would tend to the steepest descent method in the neighborhood of the initial guess used for the iterative procedure [12]. The iterative procedure of the Levenberg–Marquardt method is given by:

$$\mathbf{P}^{k+1} = \mathbf{P}^k + [(\mathbf{J}^k)^{\mathrm{T}}\mathbf{J}^k + \mu^k\Omega^k]^{-1}(\mathbf{J}^k)^{\mathrm{T}}[\mathbf{Y} - \theta(\mathbf{P}^k)] \quad (17)$$

where $\mathbf{J}^k$ is the *sensitivity matrix*, μ^k is a positive scalar named *damping parameter*, Ω^k is a *diagonal matrix* and the superscript k denotes the iteration number.

The purpose of the matrix term $\mu^k\Omega^k$ appearing in Eq. (17) is to damp oscillations and instabilities due to the ill-conditioned character of the problem, by making its components large as compared to those of $\mathbf{J}^{\mathrm{T}}\mathbf{J}$, if necessary. The damping parameter is made large in the beginning of the iterations, so that the matrix $\mathbf{J}^{\mathrm{T}}\mathbf{J}$ is not required to be non-singular and the Levenberg–Marquardt Method tends to the *Steepest Descent Method*, that is, a very small step is taken in the negative gradient direction. The parameter μ^k is then gradually reduced as the iteration procedure advances to the solution of the parameter estimation problem and then the Levenberg–Marquardt Method tends to the *Gauss Method* [12]. However, if the errors inherent to the measured data are amplified generating instabilities on the solution, as a result of the ill-posed character of the problem, the damping parameter is automatically increased. Such an automatic control of the damping parameter makes the Levenberg–Marquardt method a quite robust and stable estimation procedure, so that it does not require the use of the *Discrepancy Principle* in the stopping criterion to become stable, like the conjugate gradient method [13, 14]. Therefore, usual stopping criteria can be used for the Levenberg–Marquardt, such as

(i) $S(\mathbf{P}^{k+1}) < \varepsilon_1$ (18a)

(ii) $\left\| \left(\mathbf{J}^k\right)^{\mathrm{T}}\left[\mathbf{Y} - \mathbf{T}\left(\mathbf{P}^k\right)\right]\right\| < \varepsilon_2$ (18b)

(iii) $\left\|\mathbf{P}^{k+1} - \mathbf{P}^k\right\| < \varepsilon_3$ (18c)

where ε_1, ε_2 and ε_3 are user prescribed tolerances and $\|\cdot\|$ is the vector Euclidean norm.

The criterion given by Eq. (18a) tests if the least-squares norm is sufficiently small, which is expected to be in the neighborhood of the solution for the problem. Similarly, Eq. (18b) checks if the norm of the gradient of $S(\mathbf{P})$ is sufficiently small, since it is expected to vanish at the point where $S(\mathbf{P})$ is minimum. The last criterion given by Eq. (18c) results from the fact that changes in the vector of parameters are very small when the method has converged. Generally, these three stopping criteria need to be tested and the iterative procedure of the Levenberg–Marquardt method is stopped if any of them is satisfied. We note that, when the measurement errors start to cause oscillations on the inverse problem solution and the damping parameter μ^k is automatically increased by the Levenberg–Marquardt method, the increments on the parameters become very small, so that the iterative procedure is stopped through the criterion given by Eq. (18c).

The sensitivity matrix is defined as

$$\mathbf{J}(\mathbf{P}) \equiv \left[\frac{\partial \theta^{\mathrm{T}}(\mathbf{P})}{\partial \mathbf{P}}\right]^{\mathrm{T}} = \begin{bmatrix} \frac{\partial \vec{\theta}_1^{\mathrm{T}}}{\partial P_1} & \frac{\partial \vec{\theta}_1^{\mathrm{T}}}{\partial P_2} & \frac{\partial \vec{\theta}_1^{\mathrm{T}}}{\partial P_3} & \cdots & \frac{\partial \vec{\theta}_1^{\mathrm{T}}}{\partial P_N} \\ \frac{\partial \vec{\theta}_2^{\mathrm{T}}}{\partial P_1} & \frac{\partial \vec{\theta}_2^{\mathrm{T}}}{\partial P_2} & \frac{\partial \vec{\theta}_2^{\mathrm{T}}}{\partial P_3} & \cdots & \frac{\partial \vec{\theta}_2^{\mathrm{T}}}{\partial P_N} \\ \cdots & \cdots & \cdots & & \cdots \\ \frac{\partial \vec{\theta}_I^{\mathrm{T}}}{\partial P_1} & \frac{\partial \vec{\theta}_I^{\mathrm{T}}}{\partial P_2} & \frac{\partial \vec{\theta}_I^{\mathrm{T}}}{\partial P_3} & \cdots & \frac{\partial \vec{\theta}_I^{\mathrm{T}}}{\partial P_N} \end{bmatrix} \tag{19}$$

The elements of the sensitivity matrix are the sensitivity coefficients. They are defined as the first derivative of the estimated temperatures with respect to each of the unknown parameters P_j, $j = 1, \ldots, N$. The sensitivity coefficients are required to be large in magnitude, so that the estimated parameters are not very sensitive to the measurement errors. Also, the columns of the sensitivity matrix are required to be linearly independent, in order to have the matrix $\mathbf{J}^{\mathrm{T}}\mathbf{J}$ invertible, that is, the determinant of $\mathbf{J}^{\mathrm{T}}\mathbf{J}$ cannot be zero or even very small. Such a requirement over the determinant of $\mathbf{J}^{\mathrm{T}}\mathbf{J}$ is better understood by taking into account a statistical analysis, as described below.

6. Statistical analysis

After the minimization of the least squares norm given by Eq. (15), a *statistical analysis* can be performed in order to obtain confidence intervals and a confidence region for the estimated parameters [12]. *Confidence intervals* at the 99% confidence level are obtained as:

$$\widehat{P}_j - 2.576\sigma_{\widehat{P}_j} \leqslant \widehat{P}_j \leqslant \widehat{P}_j + 2.576\sigma_{\widehat{P}_j} \quad j = 1, \ldots, N \tag{20a}$$

where $\widehat{P}_j$ are the values estimated for the unknown parameters, P_j, for $j = 1, \ldots, N$, and $\sigma_{\widehat{P}_j}$ are the standard deviations obtained from the covariance matrix of the estimated parameters.

The *Confidence Region* can be computed from

$$\left(\widehat{\mathbf{P}} - \mathbf{P}\right)^{\mathrm{T}}\mathbf{V}^{-1}\left(\widehat{\mathbf{P}} - \mathbf{P}\right) \leqslant \chi_N^2 \tag{20b}$$

where χ_N^2 is the chi-square distribution for N degrees of freedom, for a given confidence level and $\mathbf{V}$ is the covariance matrix of the estimated parameters given by [12]:

$$\mathbf{V} = \left(\mathbf{J}^{\mathrm{T}}\mathbf{J}\right)^{-1}\sigma^2 \tag{21}$$

7. Experimental design

The design of optimum experiments is of capital importance in parameter and in function estimations. It basically consists in examining *a priori* some kind of measure of the accuracy of the estimated quantities in order to choose experimental variables, such as the number and location of sensors, experimental duration, etc., so that minimum variance estimates are obtained *via* the inverse analysis. Optimum experiments can be designed by minimizing the hypervolume of the confidence region of the estimated parameters. The minimization of the hypervolume of the confidence region given by Eq. (20b) can be obtained by maximizing the determinant of $\mathbf{V}^{-1}$, in the so-called *D-optimum design* [12, 13,17,18,24–27]. Since the covariance matrix $\mathbf{V}$ is given by Eq. (21), we can then design optimum experiments by maximizing the determinant of the matrix $\mathbf{J}^{\mathrm{T}}\mathbf{J}$, also referred to as the Fisher Information Matrix [24].

For cases involving a single sensor, each element $\mathbf{F}_{m,n}$, $m, n = 1, \ldots, N$, of the matrix $\mathbf{F} \equiv \mathbf{J}^{\mathrm{T}}\mathbf{J}$ is given by:

$$\mathbf{F}_{m,n} \equiv \left[\mathbf{J}^{\mathrm{T}}\mathbf{J}\right]_{m,n} = \sum_{i=1}^{I}\left(\frac{\partial \theta_i}{\partial P_m}\right)\left(\frac{\partial \theta_i}{\partial P_n}\right) \quad \text{for } m, n = 1, \ldots, N \tag{22}$$

where I is the number of transient measurements and N is the number of unknown parameters. If we take into account restrictions, such as a large but fixed number of transient measurements of M sensors, we can choose to maximize the determinant of an alternative form of $\mathbf{F}$, here denoted as $\mathbf{F}_I$ [12], the elements of which are given by

$$[\mathbf{F}_I]_{m,n} = \frac{1}{M\tau_f}\sum_{s=1}^{M}\int_{\tau=0}^{\tau_f}\left(P_m\frac{\partial T_s}{\partial P_m}\right)\left(P_n\frac{\partial T_s}{\partial P_n}\right)\mathrm{d}\tau \quad \text{for } m, n = 1, \ldots, N \tag{23}$$

where τ_f is the final experimental time.

8. Results and discussion

The present parameter estimation problem is classified as non-linear, because the sensitivity coefficients are functions of the unknown parameters. As a result, the analysis of the sensitivity coefficients and of the determinant of the matrix $\mathbf{J}^T\mathbf{J}$ presented below is not global, that is, it is dependent on the values chosen in advance for the unknown parameters. Let us consider in this paper a test-case involving the following values for the dimensionless variables [2,4,5,7]: $Bi_q = 2.5$, $Bi_m = 2.5$, $Lu = 0.4$, $Pn = 0.6$, $Ko = 5$ and $\varepsilon = 0.2$. By following the same approach of references [25–27], we consider the applied heat flux to be in the form of a step function in time, that is,

$$Q(\tau) = \begin{cases} Q_0, & \text{for } 0 < \tau \leqslant \tau_h \\ 0, & \text{for } \tau > \tau_h \end{cases} \tag{24}$$

where Q_0 is the magnitude of the dimensionless heat flux applied during the heating period $0 < \tau \leqslant \tau_h$. Because the heat flux given by Eq. (24) is a piecewise constant function, the solution technique for the direct problem, as described above, needs to be applied sequentially for the heating period ($0 < \tau \leqslant \tau_h$) and then for the postheating period ($\tau > \tau_h$). Also, we note in this case that $\partial\theta_s/\partial\tau = \partial\phi_s/\partial\tau = 0$ for $0 < \tau < \tau_h$ and for $\tau > \tau_h$.

Fig. 2(a) and (b) present the temperature and moisture content variations at several points inside the body, respectively, for $\tau_h = \tau_f$ and $Q_0 = 0.9$. As a result of the evaporation and moisture transfer to the surrounding air, the moisture content is smaller (larger $\phi(X,\tau)$) near the open boundary for up to $\tau = 2$. For larger times, the moisture content near the heated boundary becomes smaller than that near the open boundary, as a result of the moisture flow from the regions at higher temperatures.

We present in Fig. 3(a)–(c) the relative sensitivity coefficients for temperature, for positions $X = 0, 0.4$ and 1, respectively, with respect to the different parameters appearing in Luikov's formulation. Similarly to Fig. 2(a) and (b), we considered for Fig. 3(a)–(c) $\tau_h = \tau_f$ and $Q_0 = 0.9$. The relative sensitivity coefficient is obtained by multiplying the sensitivity coefficient by the value of the parameter that it is referred to. Therefore, the relative sensitivity coefficients can be compared to the magnitude of the measured temperatures and, as a result, it is easier to detect relative small magnitudes and linear dependence. The sensitivity coefficients were computed here by finite differences, by using a forward approximation for the first derivatives [12,13]. Fig. 3(a)–(c) show that the relative sensitivity coefficients are very little affected by the sensor location. Therefore, the temperatures in the body are equally sensitive to variations on the parameters and the sensors can be located at any point in the region. An analysis of Fig. 3(a)–(c) reveals a strong linear dependence of the sensitivity coefficients with respect to Bi_m and Lu. Thus, the simultaneous estimation of Bi_m and Lu is impossible if only temperature measurements are used in the estimation procedure. Also, the relative sensitivity coefficients with respect to Pn and ε are quite small. Hence, temperature measurements do not provide useful information for the estimation of Pn and ε.

From the foregoing analysis of Fig. 3(a)–(c), it appears possible to estimate simultaneously Bi_q, Lu and Ko. The relative sensitivity coefficients of such parameters are not linearly-dependent and they attain values of about the same order of magnitude of the temperatures in the region, as can be noticed in Fig. 2(a). Therefore, the results presented hereafter are based on the estimation of such three parameters.

Fig. 4 presents the time variation of the determinant of the matrix $\mathbf{F}_I$, the elements of which are given by Eq. (23). Fig. 4 was obtained with the measurements of a single sensor located at $X = 0$ and for different heating times, by

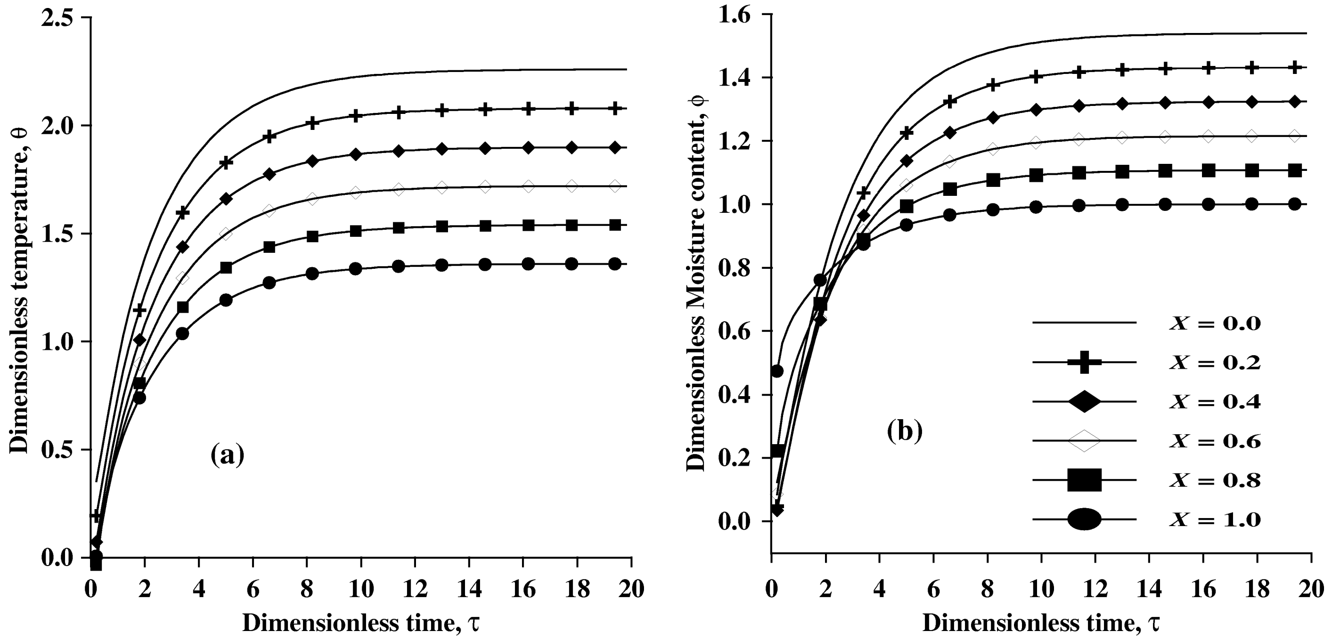

Fig. 2. Temperature (a) and moisture content (b) variations inside the body for $Q_0 = 0.9$.

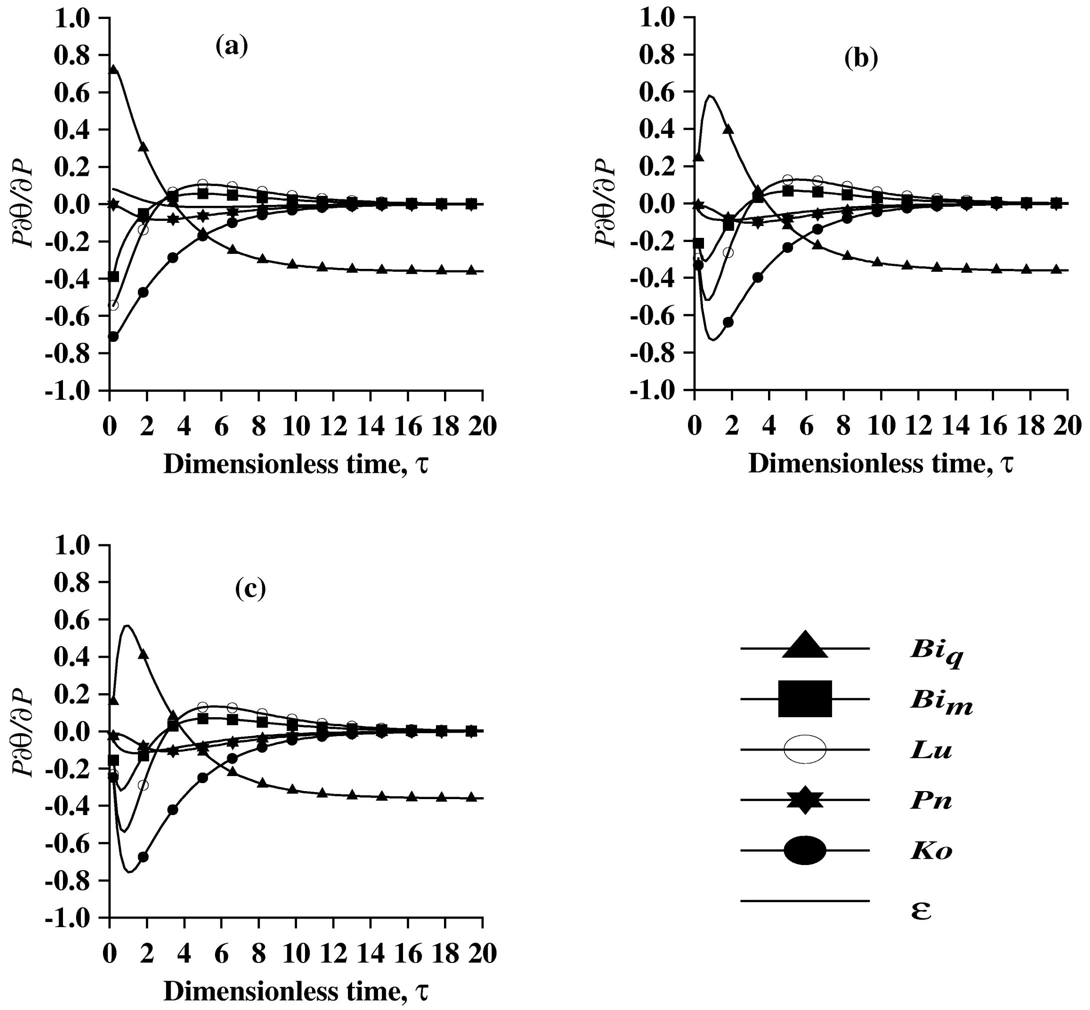

Fig. 3. Relative sensitivity coefficients for temperature at different positions for $Q_0 = 0.9$: (a) $X = 1$, (b) $X = 0.4$ and (c) $X = 0$.

considering $Q_0 = 0.9$. We note that we do not take into consideration for the present analysis the restriction of the maximum temperature in the region [12,13,25–27]. Such is the case because the temperatures in the region may become negative (i.e., the temperature drops below the initial value) for small times, as a result of evaporation, and then become positive for larger times, when the moisture changes are controlled by the moisture flow instead of evaporation. Fig. 4 shows that, for heating times smaller than $\tau_h = 8$, $\det(\mathbf{F}_I)$ undergoes a sudden increase at the time that the heating is stopped and then decreases after reaching a maximum value. Such an increase in $\det(\mathbf{F}_I)$ results from a sudden change in the shape of the sensitivity coefficients when the heating is stopped, as illustrated in Fig. 5 for $\tau_h = 4$ and for a sensor at $X = 0$. After the heating is stopped, the temperature and the moisture content in the region tend to the equilibrium with the surrounding air and the sensitivity coefficients eventually become null. Consequently, $\det(\mathbf{F}_I)$ decreases after passing through a maximum value. For heating times $\tau_h \geqslant 8$, the sensitivity coefficients tend to zero so fast when the heating is stopped that $\det(\mathbf{F}_I)$ does not experience any increase. Actually, in such cases $\det(\mathbf{F}_I)$

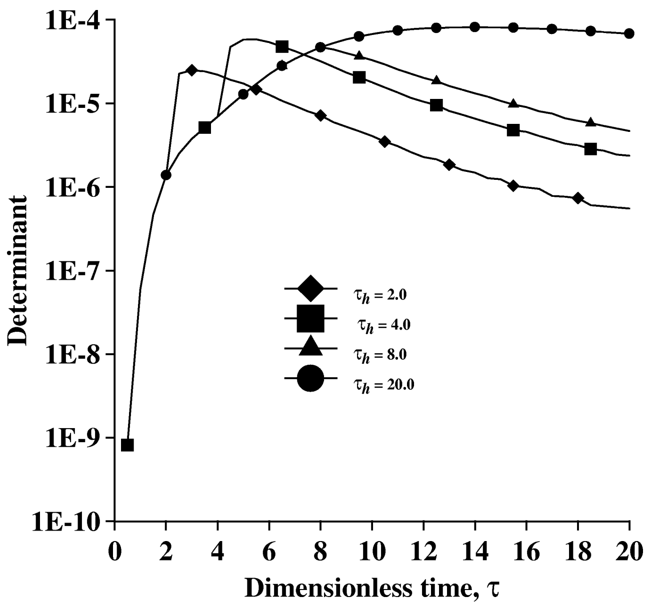

Fig. 4. Transient variation of $\det(\mathbf{F}_I)$ for different heating times obtained with the measurements of a single sensor located at $X = 0$ for $Q_0 = 0.9$.

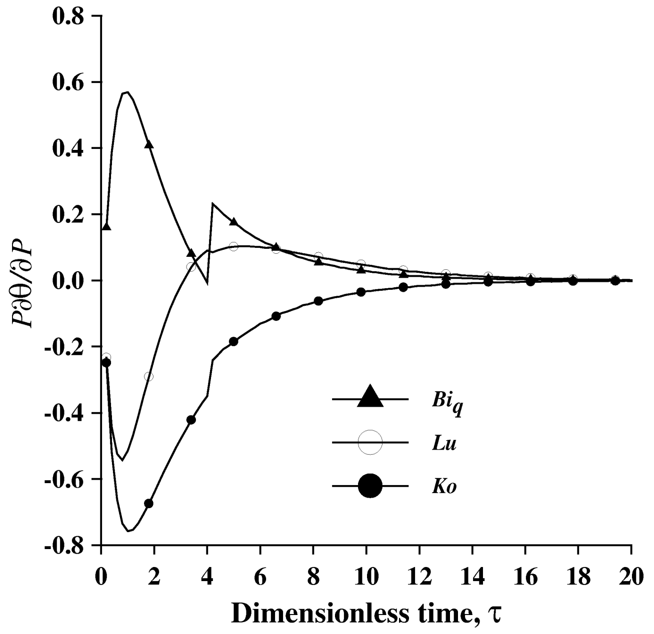

Fig. 5. Relative sensitivity coefficients for $\tau_h = 4$, $Q_0 = 0.9$ and $X = 0$.

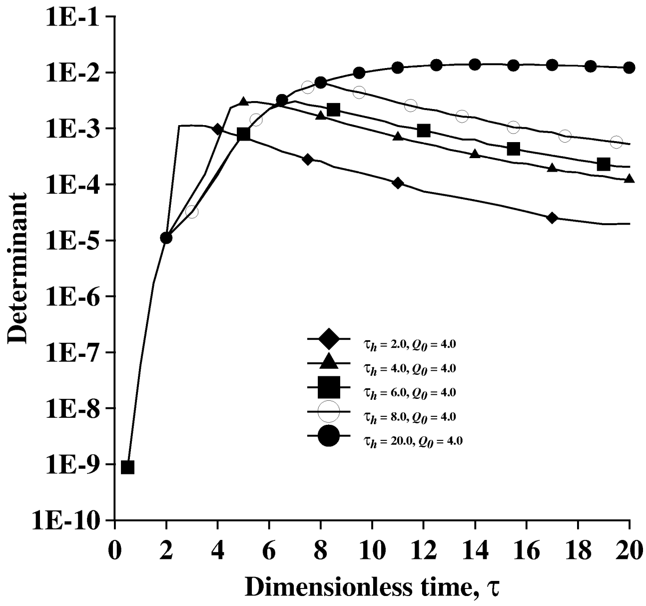

Fig. 6. Transient variation of $\det(\mathbf{F}_I)$ for different heating times and $Q_0 = 4$ obtained with the measurements of a single sensor located at $X = 0$.

attain values smaller than those obtained with continuous heating, as depicted in Fig. 4.

An analysis of Fig. 4 reveals the very interesting fact that the maximum value of $\det(\mathbf{F}_I)$ for $\tau_h = 4$ is about the same as the one obtained with continuos heating. However, the maximum value of $\det(\mathbf{F}_I)$ for $\tau_h = 4$ occurs at the final experimental time of $\tau_f = 5.5$, instead of $\tau_f = 10$ for continuous heating. Therefore, for the present test-case involving the values for the dimensionless variables referenced above, the use of $\tau_h = 4$ and $\tau_f = 5.5$ may result in estimates as accurate as those obtained with continuos heating, but in half of the experimental duration.

We now examine the effects of the magnitude of the applied heat flux Q_0 on the values of $\det(\mathbf{F}_I)$. Fig. 6 shows the transient variation of $\det(\mathbf{F}_I)$ for different heating times and for $Q_0 = 4$. A comparison of Figs. 4 and 6 reveals a general increase in the values of $\det(\mathbf{F}_I)$ when larger heat fluxes are used in the experiment. This is a result of the larger magnitudes of the sensitivity coefficients when the heat flux is increased, as illustrated in Fig. 7, which presents the relative sensitivity coefficients with respect to Bi_q, Lu and Ko for $\tau_h = \tau_f$, $Q_0 = 4$ and $X = 0$. We notice in Fig. 6 a sudden increase in $\det(\mathbf{F}_I)$ when the heating is stopped, for $\tau_h < 6$. However, such an increase is not sufficient for $\det(\mathbf{F}_I)$ to reach the same values obtained in the steady-state with continuous heating, as for the case involving $Q_0 = 0.9$ shown in Fig. 4. Therefore, it is not expected that the use of $\tau_h = 4$ and $\tau_f = 5.5$ result in parameters as accurate as those obtained with $\tau_h = \tau_f = 10$. On the other hand, the duration of the experiment can be reduced to $\tau_f = 5.5$ and parameters more accurate than those obtained with continuous heating can be estimated for such a final time, if we consider $\tau_h = 4$.

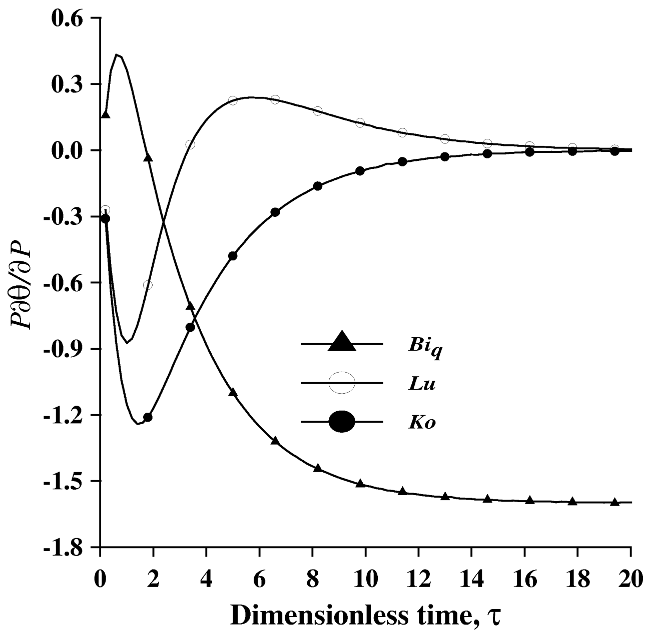

Fig. 7. Relative sensitivity coefficients for $\tau_h = \tau_f$ at $X = 0$, for $Q_0 = 4$.

The foregoing analysis reveals an increase in the determinant of $\mathbf{F}_I$ when heat fluxes of larger magnitudes are used in the experiments. However, the magnitude of the heat flux cannot be chosen arbitrarily, because the maximum temperature in the region can become quite large. Also, the analysis above indicates that the use of heating times smaller than the final times can result in faster experiments.

Let us now consider the estimation of Lu, Ko and Bi_q, by using 100 transient temperature readings of a single sensor located at $X = 0$. Measurements with different levels of random error were considered for the analysis, includ-

Table 1
Estimated parameters and normalized confidence intervals

Test-case	Experimental conditions	Parameter	Exact	Estimated $\sigma = 0$	Estimated $\sigma = 0.01Y_{\max}$	Normalized standard deviation
1	$Q_0 = 4$	Bi_q	2.5	2.5	2.511	0.0023
	$\tau_h = 4.0$	Lu	0.4	0.4	0.411	0.0056
	$\tau_f = 5.5$	Ko	5.0	5.0	4.990	0.0087
2	$Q_0 = 4$	Bi_q	2.5	2.5	2.499	0.0016
	$\tau_h = 10.0$	Lu	0.4	0.4	0.397	0.0032
	$\tau_f = 10.0$	Ko	5.0	5.0	4.997	0.0083
3	$Q_0 = 0.9$	Bi_q	2.5	2.5	2.495	0.0072
	$\tau_h = 4.0$	Lu	0.4	0.4	0.400	0.0073
	$\tau_f = 5.5$	Ko	5.0	5.0	4.990	0.0129

ing $\sigma = 0$ (errorless measurements) and $\sigma = 0.01Y_{\max}$, where $Y_{\max}$ is the maximum measured temperature. For the estimation of the unknown parameters, we utilized the Levenberg–Marquardt method [12,13,18–20] of minimization of the least-squares norm. The subroutine DBCLSJ of the IMSL [29] based on such method was used in the present work. The initial guesses used in the iterative procedure of the Levenberg–Marquardt method, were taken as $Lu^0 = 0.04$, $Ko^0 = 10$ and $Bi_q^0 = 0.25$. The results shown below, obtained with measurements with random error, were averaged over 10 runs of the program in order to reduce the bias introduced by the random number generator utilized.

Table 1 presents the results obtained for the estimated parameters with three different test-cases. In test-cases 1 and 2 we considered $Q_0 = 4$. These test-cases differ by their heating and final times. In test-case 1, they were taken, respectively, as $\tau_h = 4.0$ and $\tau_f = 5.5$, while in test-case 2 they were taken as $\tau_h = \tau_f = 10$. Such values for the heating and final times were chosen based on the analysis of Fig. 6. Test-case 1 corresponds to a small duration of the experiment and the heating time is assumed smaller than the final time in order to enhance the accuracy of the estimated parameters, as discussed above. Test-case 2 deals with the use of continuous heating and measurements taken up to the steady-state, when the determinant of $\mathbf{F}_I$ reaches its maximum value for $Q_0 = 4$. Test-case 3 involves the use of a smaller applied heat flux, $Q_0 = 0.9$. The heating and final times were taken as $\tau_h = 4.0$ and $\tau_f = 5.5$, respectively. Such values were chosen based on the analysis of Fig. 4, because they permit the estimation of parameters as accurate as those obtained with experiments run up to the steady-state for $Q_0 = 0.9$, but in almost half of the experimental time. Table 1 also presents the normalized standard deviations obtained for the parameters for each test-case. Such normalized standard-deviations were computed by dividing the original standard-deviations, obtained from the diagonals of the covariance matrix **V**, by the maximum measured temperature. The use of the normalized standard-deviations is required for the present analysis because the different test-cases involved measurements with different standard deviations given by $0.01Y_{\max}$.

Table 1 shows that the parameters were exactly recovered when errorless measurements were used in the inverse analysis in any of the test-cases. Also, it shows that quite good estimates were obtained by using measurements with random errors with $\sigma = 0.01Y_{\max}$. As expected, the normalized standard deviations follow the trend observed in Figs. 4 and 6 for the determinant of the matrix $\mathbf{F}_I$. The smallest and largest standard deviations were obtained with the experimental conditions of test-cases 2 and 3, respectively, which corresponded to the largest and smallest values of $\det(\mathbf{F}_I)$, respectively. We also notice in table 1 that, despite having a smaller value of $\det(\mathbf{F}_I)$, the use of $\tau_h = 4.0$ and $\tau_f = 5.5$ in test-case 1 resulted in estimates of accuracy comparable to those obtained for test-case 2. Therefore, the final experimental time can be reduced without significant losses in accuracy for the estimated parameters.

9. Conclusions

In this paper we presented the solution for an inverse problem of parameter estimation in a one-dimensional capillary porous media, by using Luikov's model for the heat and mass transfer processes. The associated direct problem was solved with the Generalized Integral Transform Technique. The present parameter estimation problem was solved by using the Levenberg–Marquardt method of minimization of the least-squares norm.

An analysis of the sensitivity coefficients and of the determinant of the information matrix shows that it is possible to estimate simultaneously the Luikov number, the Kossovitch number and the Biot number, by using only temperature measurements. For the case under picture, the temperatures at any point in the medium are equally sensitive to variations in the unknown parameters. Hence, the sensor position is not relevant for the inverse analysis. The effects of the heat flux magnitude and of the heating time on the accuracy of the estimated parameters were examined in the paper. We show that more accurate estimates can be obtained by increasing the magnitude of the applied heat flux and, for small heat fluxes, by using a heating time smaller than the final experimental time.

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