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An inverse problem of parameter estimation for heat and mass transfer in capillary porous media

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Abstract

This work deals with the solution of an inverse problem of parameter estimation involving heat and mass transfer in capillary porous media, as described by the dimensionless linear Luikov's equations. The physical problem under picture involves the drying of a moist porous one-dimensional medium. The main objective of this paper is to simultaneously estimate the dimensionless parameters appearing in the formulation of the physical problem by using transient temperature and moisture content measurements taken inside the medium. The inverse problem is solved by using the Levenberg–Marquardt method of minimization of the least-squares norm with simulated measurements.

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

1. Introduction

The phenomena of coupled heat and mass transfer in capillary porous media has been drawing the attention of research groups for a long time, because of its importance in several practical applications that are still quite relevant nowadays, such as drying and moisture migration in soils and construction materials. For the mathematical modeling of such phenomena, Luikov [1] has proposed a model based on a system of coupled diffusion 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 [1–3]. Such type of direct problem, based on Luikov's theory, was solved analytically through different approaches, including the *classical integral transform technique* [2]. Lobo et al. [4] found that the associated eigenvalue problem, required for the solution with this technique, had complex eigenvalues that were not accounted for in previous works. The effects on the solution of including one pair of conjugate complex eigenvalues were critically addressed by Lobo et al. [4], while the inclusion of complex eigenvalues of higher order were discussed in Ref. [5]. The use of the *generalized integral transform technique* (GITT), with simpler eigenvalue problems involving analytical eigenfunctions, can avoid the calculation of complex eigenvalues for Luikov's formulation. For more details on the use of such hybrid numerical–analytical technique, the reader is referred to [6–8]. We note that numerical techniques have also been used for the solution of Luikov's system of equations [9–11].

Appropriately formulated direct problems are mathematically classified as *well-posed*, that is, their solutions satisfy the requirements of existence, uniqueness and stability with respect to the input data [12–17]. On the other hand, the simultaneous estimation of thermophysical and boundary condition parameters that

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Nomenclature

Bi_m	dimensionless mass transfer coefficient defined by Eq. (2h)
Bi_q	dimensionless heat transfer coefficient defined by Eq. (2g)
C	measured moisture content
$\mathbf{E}$	vector with estimated values for temperature and moisture content
I	number of transient measurements taken per sensor
J	sensitivity coefficients
$\mathbf{J}$	sensitivity matrix
Ko	Kossovitch number defined by Eq. (2i)
L	number of unknown parameters
Lu	Luikov number defined by Eq. (2e)
M	number of temperature sensors
$\mathbf{M}$	vector with temperature and moisture content measured data
N	number of moisture content sensors
$\mathbf{P}$	vector of unknown parameters
Pn	Posnov number defined by Eq. (2f)
Q	dimensionless heat flux defined by Eq. (2c)
S	weighted least-squares norm defined by Eq. (3)
$\mathbf{W}$	weighting matrix given by Eq. (4c)
X	dimensionless position defined by Eq. (2j)
Y	measured temperature

Greek symbols

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

Subscripts

i	refers to the measurement time τ_i
l	refers to the unknown parameters
n	refers to the moisture content sensor number
m	refers to the temperature sensor number

Superscripts

k	iteration number
T	transpose

appear in Luikov's formulation, by using 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*, that is, their solutions may not satisfy the requirements of existence, uniqueness and 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 [12–28].

Recently, several articles dealing with the solution of inverse problems of coupled heat and mass transfer appeared in the literature [18–20,23–28]. Boundary inverse problems were solved in Refs. [26,27] by using the conjugate gradient method of function estimation. A parameter estimation problem was solved in Ref. [28], involving the identification of the initial condition, the boundary mass transfer coefficient and of two parameters appearing in the definition of the mass diffusion coefficient during drying. In [28], the energy conservation equation was written by using a lumped approach and Fick's second law described the moisture diffusion process, with a diffusion coefficient dependent on temperature and moisture content. Refs. [18–20,23–25] dealt with the estimation of parameters appearing in Luikov's formulation, by utilizing the Levenberg–Marquardt method of minimization of the least-squares norm with temperature measurements. The estimation of moisture diffusivity as a function of temperature and moisture content was examined by Kanevce et al. [23,24]. Later, they examined the estimation of other parameters appearing in the formulation [25]. In Ref. [18], the Kossovitch, Luikov and heat transfer Biot numbers were simultaneously estimated by using only temperature measurements in Luikov's linear dimensionless formulation. The effects of lateral heat losses on the accuracy of such estimated dimensionless numbers were examined in [19] and, recently, the D-optimum experimental design [12–14] was applied for the selection of the heating procedure, in order to reduce the confidence intervals of the estimated parameters [20]. We note that the physical problem considered in [23–25,28] involved the drying of thin infinitely long samples of porous materials, heated by forced convection on both sides. On the other hand, the physical problem considered in [18–20] 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 the surrounding air.

In this paper, we extend the analysis of our previous works [18–20] and examine the effects of utilizing measurements of moisture content, in addition to temperature measurements, for estimating simultaneously all parameters appearing in Luikov's linear dimensionless formulation. The sensitivity coefficients and the determinant of the information matrix are examined in order to design the experiment and to detect linear dependence among the unknown parameters. The associated direct problem is solved with the GITT [3,6–8]. The Levenberg–Marquardt method [12,13,18–25] is applied as the minimization procedure of the least-squares norm, in order to estimate the parameters. Simulated temperature and moisture content measurements containing random errors are used in the inverse analysis, as described below.

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 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:

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

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

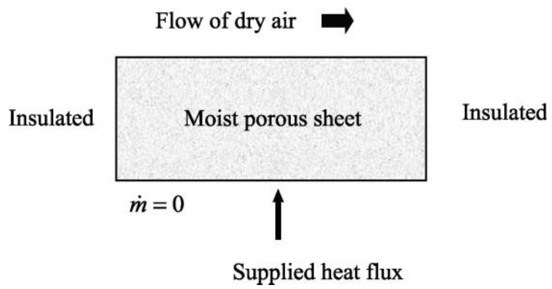

Fig. 1. Geometry for the drying of a moist porous medium.

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

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

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

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

where the following dimensionless groups were defined

$$\theta(X,\tau) = \frac{T(x,t) - T_0}{T_s - T_0}, \quad \phi(X,\tau) = \frac{u_0 - u(x,t)}{u_0 - u^*}, \quad Q = \frac{ql}{k(T_s - T_0)}, \quad \tau = \frac{at}{l^2} \tag{2a–d}$$

$$Lu = \frac{a_m}{a}, \quad Pn = \delta\frac{T_s - T_0}{u_0 - u^*}, \quad Bi_q = \frac{hl}{k}, \quad Bi_m = \frac{h_m l}{k_m}, \quad Ko = \frac{r(u_0 - u^*)}{c(T_s - T_0)}, \quad X = \frac{x}{l} \tag{2e–j}$$

$$Bi_m^* = Bi_m[1 - (1-\varepsilon)PnKoLu] \tag{2k}$$

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), the latent heat of evaporation of water (r), the temperature of the surrounding air (T_s), the uniform initial temperature in the medium (T_0), the moisture content of the surrounding air (u^*), the uniform initial moisture content in the medium (u_0), the thermogradient coefficient (δ) and the phase conversion factor (ε). *Lu*, *Pn* and *Ko* denote the Luikov, Posnov 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 was solved here by applying the GITT [3,6–8,18–20]. The 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 [3,6–8]. 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; and (v) apply the inverse formula to the transformed field in order to obtain the solution for the original problem. For the sake of brevity, we omit details of GITT as applied to the present problem, but they can be readily found in Refs. [3,6–8,18–20].

3. Inverse problem

For the *inverse problem* of interest here, the parameters Lu, Pn, Ko, ε, 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, $m = 1, \ldots, M$, as well as the moisture content measurements C_{in} taken at the locations X_n^*, $n = 1, \ldots, N$. The subscript i above refers to the time when the measurements are taken, that is, t_i, for $i = 1, \ldots, I$. We note that the measurements may contain random errors, but all the other quantities appearing in the formulation of the direct problem are supposed to be known exactly. Also, most likely the standard deviation of the temperature measurements is different from that of the moisture content measurements.

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. We assume the measurement errors to be additive, uncorrelated and normally distributed, with known standard deviation and zero mean. Since the standard deviation of the measurements is not constant, despite being assumed as known, the solution of the present inverse problem is obtained through the minimization of the weighted least-squares norm in order to obtain minimum variance estimates [12]. Such a norm can be written as

$$S(\mathbf{P}) = [\mathbf{M} - \mathbf{E}(\mathbf{P})]^{\mathrm{T}}\mathbf{W}[\mathbf{M} - \mathbf{E}(\mathbf{P})] \tag{3}$$

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

$$[\mathbf{M} - \mathbf{E}(\mathbf{P})]^{\mathrm{T}} \equiv [(\vec{M}_1 - \vec{E}_1), (\vec{M}_2 - \vec{E}_2), \ldots, (\vec{M}_I - \vec{E}_I)] \tag{4a}$$

where $(\vec{M}_i - \vec{E}_i)$ is a row vector containing the differences between measured and estimated temperatures and moisture contents at the measurement positions X_m, $m = 1, \ldots, M$, and X_n^*, $n = 1, \ldots, N$, respectively, at time t_i, that is,

$$(\vec{M}_i - \vec{E}_i) = [Y_{i1} - \theta_{i1}, Y_{i2} - \theta_{i2}, \ldots, Y_{iM} - \theta_{iM}, C_{i1} - \phi_{i1}, C_{i2} - \phi_{i2}, \ldots, C_{iN} - \phi_{iN}] \tag{4b}$$

The estimated temperatures and moisture content are obtained from the solution of the direct problem, Eqs. (1), at the respective measurement locations, by using estimates for the unknown parameters P_l, $l = 1, \ldots, L$.

The weighting matrix $\mathbf{W}$ is a diagonal matrix with elements given by the inverse of the variances of the measurements [12,13], that is,

$$\mathbf{W} = \begin{bmatrix} \frac{1}{\sigma_{11}^2} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & & & & & & & & & \vdots \\ \vdots & & \frac{1}{\sigma_{1M}^2} & & & & & & & & \vdots \\ \vdots & & & \frac{1}{\sigma_{11}^{*2}} & & & & & & & \vdots \\ \vdots & & & & \ddots & & & & & & \vdots \\ \vdots & & & & & \frac{1}{\sigma_{1N}^{*2}} & & & & & \vdots \\ \vdots & & & & & & \ddots & & & & \vdots \\ \vdots & & & & & & & \frac{1}{\sigma_{I1}^2} & & & \vdots \\ \vdots & & & & & & & \ddots & & & \vdots \\ \vdots & & & & & & & & \frac{1}{\sigma_{IM}^2} & & \vdots \\ \vdots & & & & & & & & & \frac{1}{\sigma_{I1}^{*2}} & \vdots \\ \vdots & & & & & & & & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \frac{1}{\sigma_{IN}^{*2}} \end{bmatrix} \tag{4c}$$

4. 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 [12,13,18–25]. Such a method was first derived by Levenberg [21] in 1944, by modifying the ordinary least-squares norm. Later, in 1963, Marquardt [22] 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:

$$\mathbf{P}^{k+1} = \mathbf{P}^k + [(\mathbf{J}^k)^{\mathrm{T}}\mathbf{W}\mathbf{J}^k + \mu^k\mathbf{\Omega}^k]^{-1}(\mathbf{J}^k)^{\mathrm{T}}\mathbf{W}[\mathbf{M} - \mathbf{E}(\mathbf{P}^k)] \tag{5}$$

where $\mathbf{J}^k$ is the *sensitivity matrix*, μ^k is a positive scalar named *damping parameter*, $\mathbf{\Omega}^k$ is a *diagonal matrix* and the superscript k denotes the iteration number. The purpose of the matrix term $\mu^k\ \mathbf{\Omega}^k$ appearing in Eq. (5) 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 $\mathbf{J}^T\mathbf{WJ}$, if necessary. The damping parameter is made large in the beginning of the iterations, so that the matrix $\mathbf{J}^T\mathbf{WJ}$ 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

$$\text{(i)} \quad S(\mathbf{P}^{k+1}) < \varepsilon_1 \tag{6a}$$

$$\text{(ii)} \quad \|(\mathbf{J}^k)^T[\mathbf{Y} - \mathbf{T}(\mathbf{P}^k)]\| < \varepsilon_2 \tag{6b}$$

$$\text{(iii)} \quad \|\mathbf{P}^{k+1} - \mathbf{P}^k\| < \varepsilon_3 \tag{6c}$$

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

The criterion given by Eq. (6a) tests if the least-squares norm is sufficiently small, which is expected in the neighborhood of the solution for the problem. Similarly, Eq. (6b) 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. (6c) 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. (6c).

The sensitivity matrix is defined as

$$\mathbf{J}(\mathbf{P}) \equiv \left[\frac{\partial \mathbf{E}^T(\mathbf{P})}{\partial \mathbf{P}}\right]^T = \begin{bmatrix} \frac{\partial \vec{E}_1^T}{\partial P_1} & \frac{\partial \vec{E}_1^T}{\partial P_2} & \frac{\partial \vec{E}_1^T}{\partial P_3} & \cdots & \frac{\partial \vec{E}_1^T}{\partial P_L} \\ \frac{\partial \vec{E}_2^T}{\partial P_1} & \frac{\partial \vec{E}_2^T}{\partial P_2} & \frac{\partial \vec{E}_2^T}{\partial P_3} & \cdots & \frac{\partial \vec{E}_2^T}{\partial P_L} \\ \vdots & \vdots & \vdots & & \vdots \\ \frac{\partial \vec{E}_I^T}{\partial P_1} & \frac{\partial \vec{E}_I^T}{\partial P_2} & \frac{\partial \vec{E}_I^T}{\partial P_3} & \cdots & \frac{\partial \vec{E}_I^T}{\partial P_L} \end{bmatrix} \tag{7a}$$

where

$$\frac{\partial \vec{E}_i^T}{\partial P_l} = \begin{bmatrix} \frac{\partial \theta_{i1}}{\partial P_l} \\ \frac{\partial \theta_{i2}}{\partial P_l} \\ \vdots \\ \frac{\partial \theta_{iM}}{\partial P_l} \\ \frac{\partial \phi_{i1}}{\partial P_l} \\ \frac{\partial \phi_{i2}}{\partial P_l} \\ \vdots \\ \frac{\partial \phi_{iN}}{\partial P_l} \end{bmatrix}, \quad \text{for } i = 1, \ldots, I \text{ and } l = 1, 2, \ldots, L \tag{7b}$$

The elements of the sensitivity matrix are the sensitivity coefficients. They are defined as the first derivative of the estimated quantities with respect to each of the unknown parameters P_l, $l = 1, \ldots, L$. The sensitivity coefficients are required to be large in magnitude, so that the estimated parameters are not very sensitive to measurement errors. Also, the columns of the sensitivity matrix are required to be linearly independent in order to have the matrix $\mathbf{J}^T\mathbf{WJ}$ invertible. In problems involving parameters with different orders of magnitude, the sensitivity coefficients with respect to the various parameters may also differ by several orders of magnitude, creating difficulties in their comparison and identification of linear dependence. These difficulties can be alleviated through the analysis of the *normalized sensitivity coefficients*, which are obtained by multiplying the original sensitivity coefficients by the parameters that they are referred to. Note that the normalized sensitivity coefficients have the units of the measured variable, either temperature or moisture content; hence, they are compared as having the magnitude of the measured variable as a basis.

5. Statistical analysis

After the minimization of the least-squares norm given by Eq. (3), 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:

$$\hat{P}_l - 2.576\sigma_{\hat{P}_l} \leqslant P_l \leqslant \hat{P}_l + 2.576\sigma_{\hat{P}_l}, \quad l = 1, \ldots, L \tag{8}$$

where $\hat{P}_l$ are the values estimated for the unknown parameters, P_l, for $l = 1, \ldots, L$, and $\sigma_{\hat{P}_l}$ are the standard deviations obtained from the covariance matrix of the estimated parameters.

The *confidence region* can be computed from [12]:

$$(\hat{\mathbf{P}} - \mathbf{P})^T\mathbf{V}^{-1}(\hat{\mathbf{P}} - \mathbf{P}) \leqslant \chi_L^2 \tag{9}$$

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

$$\mathbf{V} = (\mathbf{J}^{\mathrm{T}}\mathbf{W}\mathbf{J})^{-1} \tag{10}$$

We note that Eq. (10) is exact for linear estimation problems and is approximately used for non-linear parameter estimation problems such as the one under picture in this paper, where the sensitivity coefficients are functions of the unknown parameters.

6. 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. (9) can be obtained by maximizing the determinant of $\mathbf{V}^{-1}$, in the so-called *D-optimum design* [12–14,17].

For the design of optimum experiments, let us consider the weighting matrix $\mathbf{W}$ as the identity matrix. Therefore, the elements $\mathbf{F}_{r,s}$, r, $s = 1, \ldots, L$, of the so-called information matrix $\mathbf{F} \equiv \mathbf{J}^{\mathrm{T}}\mathbf{J}$, are given by:

$$\mathbf{F}_{r,s} \equiv [\mathbf{J}^{\mathrm{T}}\mathbf{J}]_{r,s} = \sum_{i=1}^{I}\left[\sum_{m=1}^{M}\left(\frac{\partial\theta_{im}}{\partial P_r}\frac{\partial\theta_{im}}{\partial P_s}\right) + \sum_{n=1}^{N}\left(\frac{\partial\phi_{in}}{\partial P_r}\frac{\partial\phi_{in}}{\partial P_s}\right)\right], \quad \text{for } r,s = 1,\ldots,L \tag{11}$$

where I is the number of transient measurements and L is the number of unknown parameters.

We note that for non-linear estimation problems the analyses of the sensitivity coefficients and of the determinant of $\mathbf{F}$ are not global, because these quantities are functions of the unknown parameters. Therefore, a priori estimated values for the parameters are required for the design of optimum experiments. In practical situations involving non-linear estimation problems, the optimum design of the experiment is performed in an iterative manner. Low-accuracy estimates for the unknown parameters, which can be obtained from previous experiments or from literature data, are used in the initial experimental design. As more accurate estimates are obtained with new experiments, the experimental design is improved and the accuracy of the estimated parameters is further enhanced.

7. Results and discussion

For the design of optimum experiments and for the solution of the present inverse problem of parameter

Table 1
Test-cases examined

Physical variables	Wood			Ceramics
	Test-case 1	Test-case 2	Test-case 3	Test-case 4
l (m)	0.05	0.05	0.05	0.05
ρ_0 (kg/m^3)	370	370	370	2000
h_q (W/m^2 K)	22.5	1.6	22.5	17
h_m (kg/m^2 s °M)	2.5×10^{-6}	6.0×10^{-8}	2.5×10^{-6}	1.6×10^{-5}
k_q (W/m K)	0.65	0.65	0.65	0.34
k_m (kg/m s °M)	2.2×10^{-8}	2.2×10^{-8}	2.2×10^{-8}	2.4×10^{-7}
δ (°M/K)	2.0	2.0	2.0	0.56
c_q (J/kg K)	2500	2500	2500	607
c_m (kg/kg °M)	10^{-2}	10^{-2}	10^{-2}	1.8×10^{-3}
λ (J/kg)	2.5×10^{6}	2.5×10^{6}	2.5×10^{6}	2.5×10^{6}
T_0 (°C)	24	24	24	24
T_s (°C)	26	26	36	30
u_0 (°M)	86	86	86	80
u^* (°M)	8	8	8	40
$\boldsymbol{Bi_q}$	**1.7**	**0.1**	**1.7**	**2.5**
$\boldsymbol{Bi_m}$	**5.7**	**0.1**	**5.7**	**2.5**
Lu	**0.008**	**0.008**	**0.008**	**0.2**
Pn	**0.05**	**0.05**	**0.3**	**0.084**
Ko	**390**	**390**	**65**	**49**
$\boldsymbol{\varepsilon}$	**0.2**	**0.2**	**0.2**	**0.2**

estimation, we examine four test-cases of practical interest, involving different materials and different boundary conditions on the surface of the body in contact with the surrounding air. Table 1 summarizes the four test-cases examined in this work. Test-cases 1–3 deal with the drying of wood, while test-case 4 deals with the drying of ceramics. The physical properties presented in Table 1 were obtained from Ref. [9] for wood and from Ref. [11] for ceramics. Note in Table 1 that for all test-cases the thickness of the sample was taken as 0.05 m and the initial temperature as 24 °C.

In test-cases 1–3, dealing with the drying of wood, we analyzed the effects of the air conditions on the determinant of the information matrix. Test-case 1 involved heat and mass transfer coefficients at the boundary $X = 1$ of the order of those for forced convection ($h_q = 22.5$ W/m^2 °C and $h_m = 2.5 \times 10^{-6}$ kg/m^2 s °M), with the surrounding air slightly heated as compared to the initial temperature for the medium ($T_0 = 24$ °C and $T_s = 26$ °C). Such air temperature was the same considered for test-case 2, but the heat and mass transfer coefficients for this test-case were of the order of those for natural convection ($h_q = 1.6$ W/m^2 °C and $h_m = 6 \times 10^{-8}$ kg/m^2 s °M). For test-case 3, the heat and mass transfer coefficients utilized were the same as for test-case 1, but the air temperature was taken as 36 °C instead of 26 °C. Test-case 4 involved the drying of ceramics, with heat and mass transfer coefficients of the order of those for forced convection ($h_q = 17$ W/m^2 °C and $h_m = 1.6 \times 10^{-5}$ kg/m^2 s °M) with air slightly heated ($T_s = 30$ °C).

Fig. 2a and b present the temperature and moisture content variations with time, respectively, for different positions along the medium, for test-case 1. We can notice in Fig. 2a a large decrease in the temperature for small times, as a result of the moisture vaporization. For larger times, temperatures in the region become positive when vaporization effects are less important and the temperature distribution is governed by diffusion.

The normalized sensitivity coefficients for temperature and moisture content measurements are presented in Figs. 3 and 4, respectively, at different locations inside the medium, for test-case 1. Fig. 3 shows that the temperature sensitivity coefficients with respect to Bi_m and Lu are proportional, i.e., linearly dependent. The temperature sensitivity coefficients with respect to Pn and ε are practically null, while the others attain values comparable to the measured temperatures (see also Fig. 2a). The temperature sensitivity coefficients with respect to Ko and Bi_q are not linearly dependent with respect to the others. Note in Fig. 3 that the temperature sensitivity coefficients are basically not affected by the sensor position. Let us now consider the analysis of the moisture content sensitivity coefficients presented in Fig. 4. Such a figure shows that the moisture content sensitivity coefficients with respect to Ko, Bi_q, Pn and ε are practically

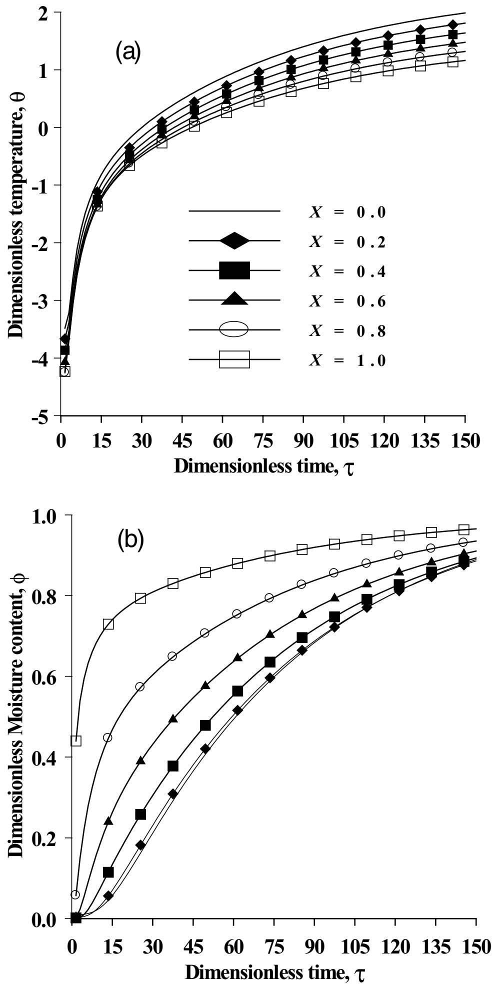

Fig. 2. Temperature (a) and moisture content (b) variations inside the body for test-case 1.

null for all measurement positions. The sensitivity coefficients with respect to Bi_m and Lu attain magnitudes of the same order of the measured moisture content (see Fig. 2b), but they are linearly dependent, except for $X = 0$. An analysis of Figs. 3 and 4 reveals the difficulty involved in the simultaneous estimation of the dimensionless parameters appearing in Luikov's linear formulation. Both temperature and moisture content measurements do not provide useful information for the estimation of Pn and ε, because their sensitivity coefficients are practically null. Also, there is a general tendency of linear dependence for the sensitivity coefficients with respect to Bi_m and Lu, independently of the type of measurement considered. However, these sensitivity coefficients attain values of the order of the measured variables and the constant of proportionality between them is different for temperature and moisture content

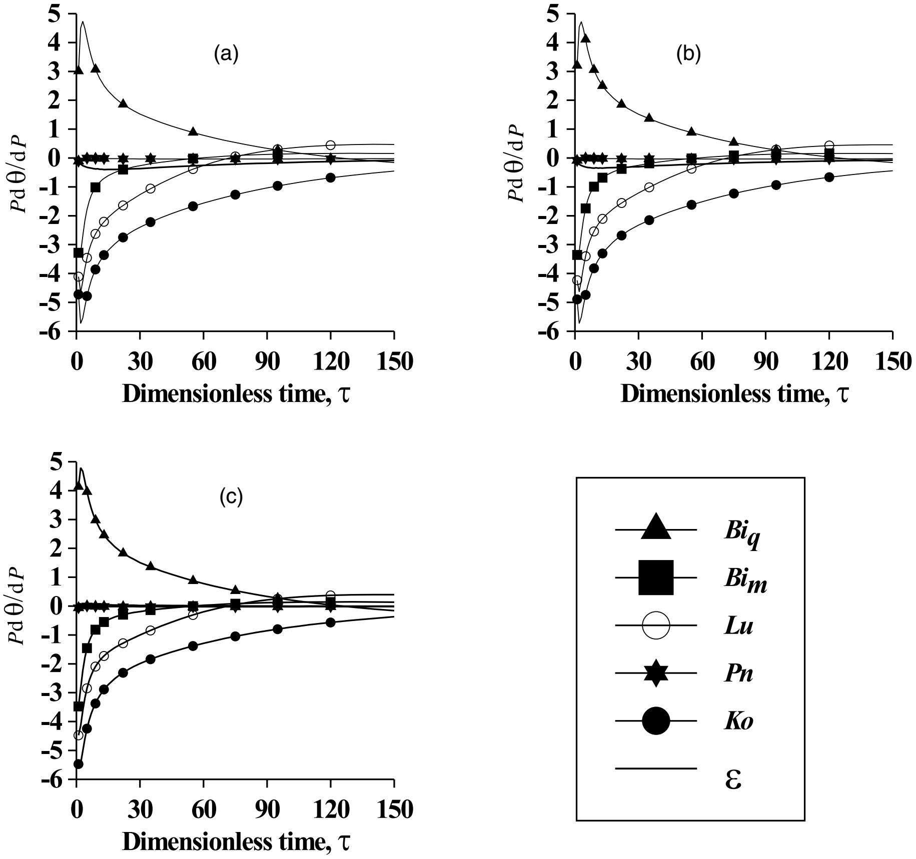

Fig. 3. Normalized temperature sensitivity coefficients for test-case 1 for (a) $X = 0$, (b) $X = 0.4$ and (c) $X = 1$.

measurements; hence, the columns of the sensitivity matrix do not become linearly dependent.

The determinant of the information matrix is presented in Fig. 5 for test-case 1, by considering different numbers of temperature and moisture content sensors available for the analysis. The moisture content sensors were located inside the medium starting from the boundary at $X = 0$, because at this position the sensitivity coefficients with respect to Bi_m and Lu are not linearly dependent, as shown by Fig. 4. The temperature sensors were located inside the medium starting from the boundary at $X = 1$, although the temperatures at different sensor locations are equally sensitive to variations in the parameters, as shown by Fig. 3. For the results presented in Fig. 5, we considered available one measurement per sensor per unity of dimensionless time. Also, the curves in Fig. 5 were based on six unknown parameters, that is, $\mathbf{P}^{\mathrm{T}} = [Bi_q, Bi_m, Lu, Pn, Ko, \varepsilon]$. We can notice in Fig. 5, for each curve referent to the different number of sensors, a large increase in the determinant of the information matrix for small times and that the rate of increase of the determinant is reduced for times greater than 80. Therefore, a final time equal to 80 appears to be suitable for test-case 1, because very little improvement on the accuracy of the estimated parameters is expected for larger times. We note that the determinant increases when more sensors are utilized, because more information is available for the inverse analysis.

Fig. 6 presents the determinant of the information matrix for test-case 2, where the heat and mass transfer coefficients at the boundary $X = 1$ corresponded to natural convection conditions. The frequency of measurements and the number of unknown parameters are the same as those considered for Fig. 5. A comparison of Figs. 5 and 6 show a large reduction of the determinant of the information matrix, when the heat and mass transfer coefficients are decreased. This is basically due to the reduction observed in the magnitudes of the moisture content sensitivity coefficients and because of a strong tendency towards linear dependence of the sensitivity coefficients for several parameters, when natural convection boundary conditions are imposed. Therefore, Figs. 5 and 6 show that forced convection boundary conditions should be preferred for the body surface open to the surrounding air at $X = 1$.

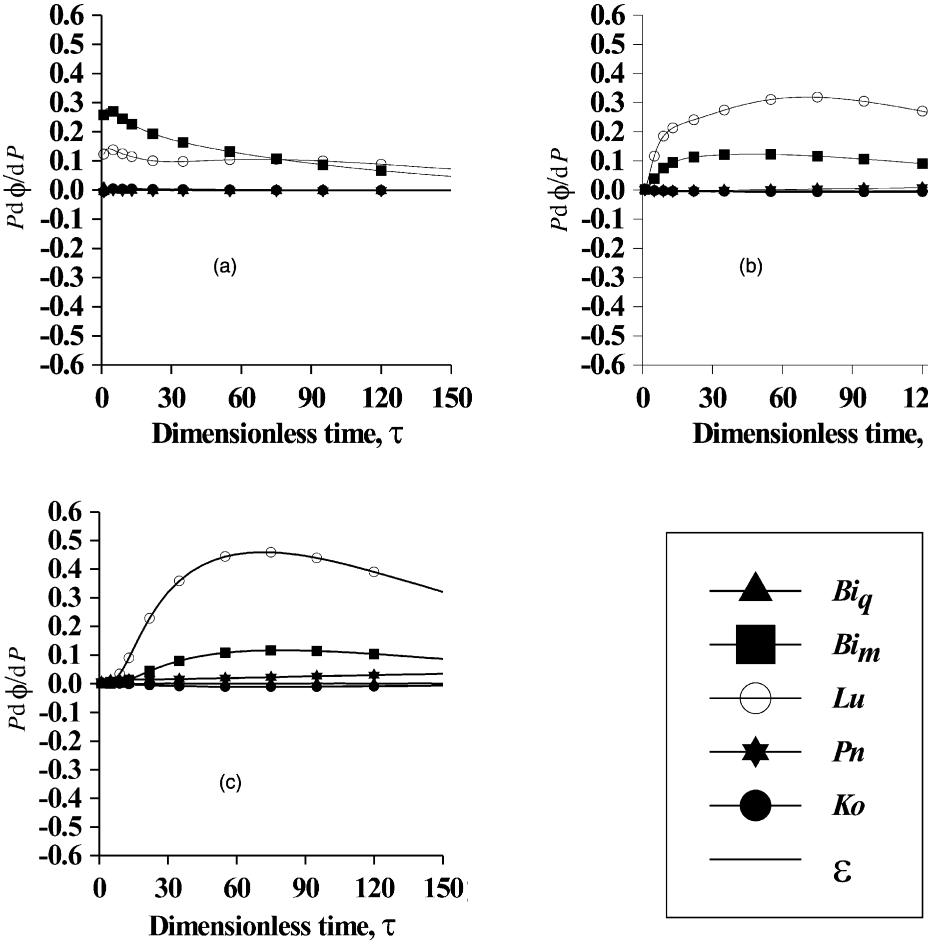

Fig. 4. Normalized moisture content sensitivity coefficients for test-case 1 for (a) $X = 0$, (b) $X = 0.4$ and (c) $X = 1$.

The determinant of the information matrix for test-case 3 is presented in Fig. 7. Such as for test-case 2, the frequency of measurements and the number of unknown parameters are the same as those considered for Fig. 5. We can notice in Fig. 7 that the increase of the temperature of the surrounding air has the same effect of reducing the determinant of the information matrix, as the use of natural convection boundary conditions. Therefore, a comparison of Figs. 5–7 reveals that forced convection of slightly heated surrounding air should be preferred for the boundary conditions at the open boundary of the body at $X = 1$, in order to improve the accuracy of the estimated parameters.

It is interesting to note that similar results, with respect to the boundary conditions and the surrounding air temperature, were observed by Kanevce et al. [24] for the estimation of the mass diffusion coefficient as a function of temperature and moisture diffusivity. The use of larger heat and mass transfer coefficients and smaller temperatures of the surrounding air resulted in larger values for the determinant of the information matrix, despite the fact that the physical problem involved the heating of the sample by convection on both of its sides [24].

Let us now take into picture the analysis of test-case 4 involving the drying of ceramics. Based on the foregoing analysis of test-cases 1–3, the boundary condition at the open boundary of the body at $X = 1$ for test-case 4 involved forced convection of slightly heated air, as can be noticed in Table 1. Fig. 8 presents the determinant of the information matrix for test-case 4, for six unknown parameters, that is, $\mathbf{P}^T = [Bi_q, Bi_m, Lu, Pn, Ko, \varepsilon]$ and for a frequency of one measurement per sensor per unity of dimensionless time. A comparison of Figs. 5 and 8 show larger values for the determinant of the information matrix for ceramics than for wood. As a result, more accurate estimates are expected for the estimation of the dimensionless parameters appearing in Luikov's formulation for ceramics. The sensitivity coefficients for test-case 4 are not presented here for the

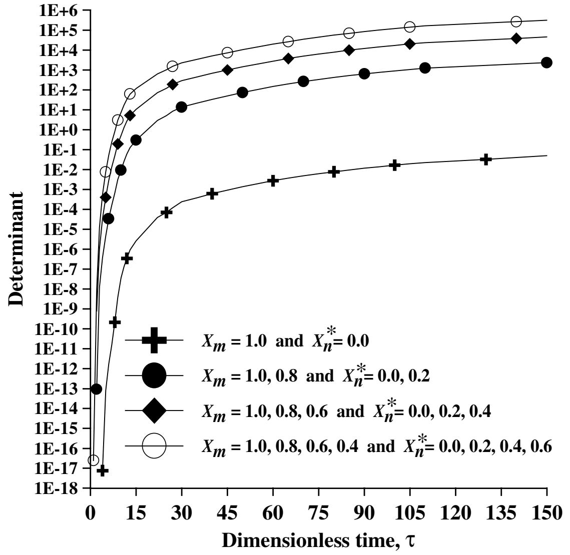

Fig. 5. Determinant of the information matrix for different number of sensors for test-case 1.

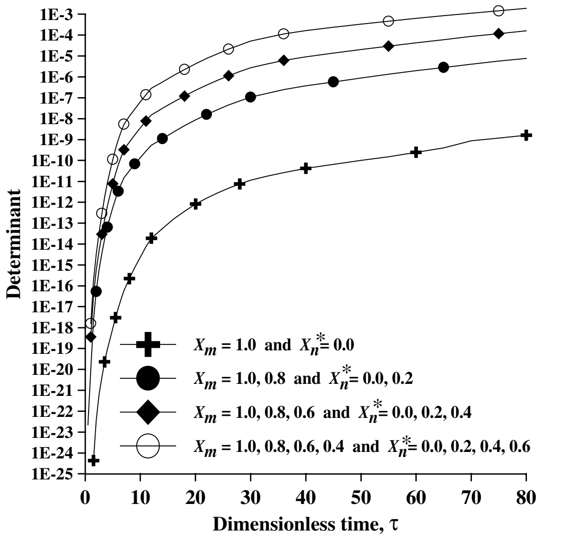

Fig. 7. Determinant of the information matrix for different number of sensors for test-case 3.

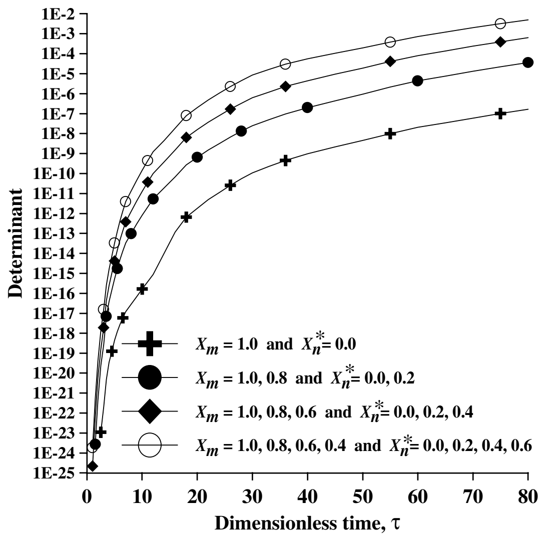

Fig. 6. Determinant of the information matrix for different number of sensors for test-case 2.

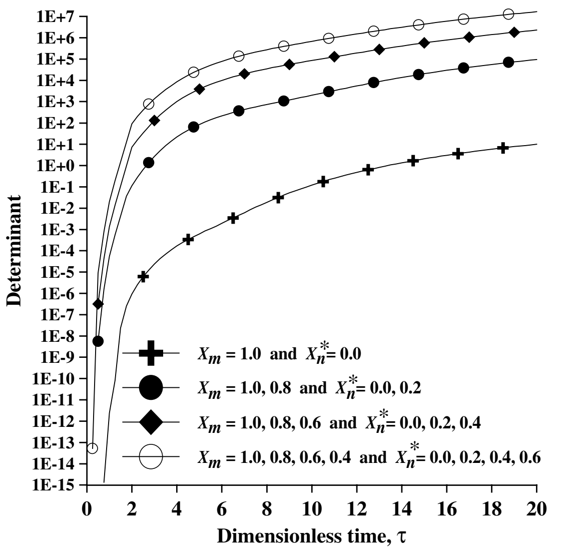

Fig. 8. Determinant of the information matrix for different number of sensors for test-case 4.

sake of brevity, but qualitatively they are quite similar to those for test-case 1, presented in Figs. 3 and 4. Therefore, temperature and moisture content sensitivity coefficients with respect to Pn and ε are also rather small for test-case 4, so that the measurements do not provide useful information for the estimation of such parameters.

The foregoing analysis reveals that, for the cases examined, only the parameters Bi_q, Bi_m, Lu and Ko can be simultaneously estimated by using both temperature and moisture content measurements. Therefore, only such four parameters are considered as unknown quantities for the inverse analysis presented below, based on the Levenberg–Marquardt method of minimization of the least-squares norm, by using simulated transient measurements. The parameters Pn and ε are then considered to be known exactly; but we note that this is not a strong hypothesis, since their sensitivity

Table 2
Results obtained for the estimation of parameters in test-case 4

Parameters	Exact	Estimated $\sigma = 0$	Estimated $\sigma = 0.01M_{\max}$	Confidence intervals
Bi_q	2.5	2.500	2.508	(2.505, 2.510)
Bi_m	2.5	2.500	2.487	(2.456, 2.519)
Lu	0.2	0.200	0.200	(0.146, 0.255)
Ko	49	49.000	49.123	(48.669, 49.578)

coefficients are practically null and the measurements are not affected by their values.

We present below in Table 2 the results obtained for the estimation of Bi_q, Bi_m, Lu and Ko for test-case 4. For the inverse analysis, we considered simulated temperature measurements to be available at $X_m = 0.9$, 0.7, 0.5 and 0.0, and moisture content measurements at $X_n^* = 0.1$, 0.2, 0.3 and 0.4. Based on the analysis of Fig. 8, the final dimensionless time was taken as 10, since the determinant of the information matrix increases very little for larger times. For the physical case under picture, such dimensionless time corresponds to 25 h. Measurements were assumed available in a frequency of one reading per sensor every 20 min. In order to examine the accuracy of the Levenberg–Marquardt method, as applied to the present parameter estimation approach, we used simulated measurements containing random measurement errors with standard deviation $\sigma = \sigma^* = 0$ (errorless measurements), as well as $\sigma = 0.01\ Y_{\max}$ and $\sigma^* = 0.01\ C_{\max}$, where $Y_{\max}$ and $C_{\max}$ denote the maximum measured temperature and moisture content, respectively. The initial guesses for the unknown parameters, required for the iterative procedure of the Levenberg–Marquardt method, were taken as $Bi_q^0 = 1.0$, $Bi_m^0 = 5.0$, $Lu^0 = 0.02$ and $Ko^0 = 4.9$. Table 2 shows that the values were exactly recovered when errorless measurements were used in the inverse analysis. Similarly, quite accurate estimates were obtained when the measurements with random errors were taken into account, even for initial guesses as far as one order of magnitude from the exact parameters.

8. Conclusions

In this paper we presented the solution for an inverse problem of parameter estimation in a one-dimensional capillary porous media, by using the dimensionless Luikov's model for the heat and mass transfer process. The associated direct problem was solved with the GITT. The present parameter estimation problem was solved by using the Levenberg–Marquardt method of minimization of the least-squares norm. Temperature and moisture content measurements are assumed available for the inverse problem. Since temperature measurements may contain errors with standard deviation different from the moisture content measurements, the weighted least-squares norm is used as the objective function in order to obtain minimum variance estimates.

For the cases examined in this work, involving the drying of wood and ceramics, 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 numbers for heat and mass transfer. The Posnov number and the phase change conversion factor cannot be estimated, because their sensitivity coefficients are practically null. Results obtained by using simulated measurements with random errors illustrate the accuracy of the present approach for the simultaneous identification of parameters in Luikov's dimensionless linear formulation.

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