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INVERSE ANALYSIS IN MOIST CAPILLARY POROUS MEDIA

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Abstract*. This work deals with the solution of inverse problems of parameter estimation in drying in capillary porous media. The physical problem considered here is described by the linear one-dimensional Luikov's equations. The associated direct problem is solved analytically by the Classical Integral Transform Technique. An analysis of the sensitivity coefficients and the use of the D-optimum criterion permit the design of the experiment with respect to the final experimental time, number and locations of sensors and the number of parameters that can be estimated. The present parameter estimation problem is solved with Levenberg–Marquardt's method of minimization of the ordinary least-squares norm, by using simulated experimental data with random errors.*

Keywords: Luikov's equations, Heat and mass transfer, Drying, Inverse problem, Levenberg – Marquardt's method.

1. INTRODUCTION

The phenomena of 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 (Luikov, 1966, Mikhailov and Özisik, 1984, Ribeiro and Lobo, 1998). For the mathematical modeling of such phenomena, Luikov (1966) 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 the temperature and the 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. Such type of direct problem, based on Luikov's theory, was solved analytically through the use of the *Classical Integral Transform Technique* (Mikhailov and Özisik, 1984). Later, Lobo et al (1987) found that the associated eigenvalue problem 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 (1987), while the inclusion of complex eigenvalues of higher order were discussed by Guigon et al (1999). The use of the *Generalized Integral Transform Technique*, with simpler eigenvalue problems involving analytical eigenfunctions, can avoid the calculation of complex eigenvalues for the drying problem based on Luikov's formulation. For more details on the use of such hybrid numerical-analytical technique, the reader is referred to the works of Ribeiro et al (1993), Cotta (1993), Ribeiro and Cotta (1995) and Ribeiro and Lobo (1998). We note that numerical techniques such as finite differences have also been used in the past for the solution of Luikov's system of equations (Lobo et al, 1995, Lobo, 1997).

The numerical modeling of drying in capillary porous media requires the accurate knowledge of several thermophysical and boundary condition parameters that appear in the formulation. The use of *inverse analysis* techniques permits the estimation of such parameters, from the knowledge of temperature and moisture content measurements taken in the media (Beck and Arnold, 1977, Orlande et al, 1995, Mejias et al, 1999, Dantas and Orlande, 1996, Özisik and Orlande, 1999).

In this paper we present the solution of the inverse problem of estimating several thermophysical and boundary condition parameters, appearing in Luikov's formulation for the drying of a one-dimensional capillary porous media. Such parameters include the Luikov number, the Posnov number, the Kossovitch number, the phase change criterion, and the Biot numbers for heat and mass transfer at one of the boundaries. The present inverse problem of parameter estimation is solved by using the Levenberg-Marquardt method of minimization of the least-squares norm (Beck and Arnold, 1977, Özisik and Orlande, 1999). Simulated temperature measurements are used here in order to verify the accuracy of the present parameter estimation approach.

2. DIRECT PROBLEM

The physical problem under picture 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 put in contact with a heater. The other boundary is put 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 (1966), for the modeling of such physical problem involving the drying of a capillary porous medium, can be written in dimensionless form as (Luikov, 1966, Mikhailov and Özisik, 1984, Cotta, 1993, Ribeiro, 1993, Ribeiro and Lobo, 1998):

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

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

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

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

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

$$-\frac{\partial\phi(1,\tau)}{\partial X}+Pn\frac{\partial\theta(1,\tau)}{\partial X}+Bi_m[(1-\phi(1,\tau)]=0, \qquad \text{at } X=1, \text{ for } \tau>0 \qquad (1h)$$

The various dimensionless groups appearing above are defined as

$$\theta(X,\tau)=\frac{T(x,t)-T_o}{T_s-T_o}, \quad \phi(X,\tau)=\frac{u_o-u(x,t)}{u_o-u^*}, \quad Q=\frac{ql}{k(T_s-T_o)}, \quad \tau=\frac{at}{l^2}, \qquad (2.a\text{-}d)$$

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

where a is the thermal diffusivity of the porous medium, a_m is the moisture diffusivity in the porous medium, c is the specific heat of porous medium, h is the heat transfer coefficient, h_m is the mass transfer coefficient, k is the thermal conductivity, k_m is the moisture conductivity, l is the sheet thickness, q is the prescribed heat flux, r is the latent heat of evaporation of water, T_s is the temperature of the surrounding air, T_o is the uniform initial temperature in the medium, u^* is the moisture content of the surrounding air, u_o is the uniform initial moisture content in the medium, δ is the thermogradient coefficient and ε is the phase conversion factor. *Lu*, *Pn* and *Ko* are denoted as the Luikov, Posnov and Kossovitch numbers, respectively.

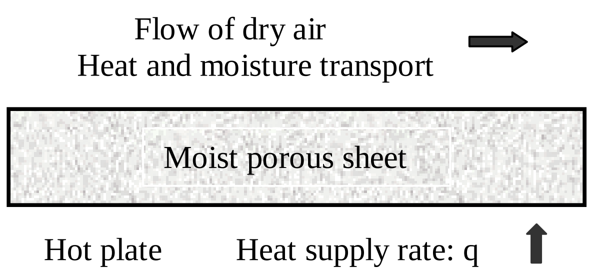

Figure 1 - Geometry for the drying of a moist porous medium

The above 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.

3. 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 measurement locations X_m, m=1,…,M, as well as the transient measurements of the moisture content C_{in} taken at the measurement locations X_n, n=1,…,N. The subscript i above refers to the time when the measurements are taken, that is, t_i , for i=1,…,I. We note that the temperature and moisture content 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 generally ill-posed (Hadamard, 1923, Beck and Arnold, 1977, Özisik and Orlande, 1999), as a result of the errors inherent to the measurements used in the analysis. The accurate solution of inverse problems generally 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

$$S(P)=\sum_{i=1}^{I}\{\sum_{m=1}^{M}[Y_{im}-\theta_{im}]^2+\sum_{n=1}^{N}[C_{in}-\phi_{in}]^2\} \tag{3.a}$$

or

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

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

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

where $\left(\vec{M}_i-\vec{E}_i\right)$, i=1,...,I is a row vector containing the differences between the measured and estimated potentials at the measurement positions X_m, m=1,...,M for temperature and X_n, n=1,...,N for moisture at time t_i, that is,

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

The estimated potentials θ_{im}, m=1,…,M and ϕ_{in}, n=1,…,N, are obtained from the solution of the direct problem, Eqs. (1), for temperature at the measurement location X_m, and for moisture content at the measurement location X_n , respectively, at time t_i.

The present inverse problem of parameter estimation is solved with the Levenberg-Marquardt method (Beck and Arnold, 1977, Özisik and Orlande, 1999). The iterative procedure of such method is given by

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

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

The purpose of the matrix term $\mu^k\,\Omega^k$, included in equation (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 $\mathbf{J}^T\mathbf{J}$ if necessary. The damping parameter is made large in the beginning of the iterations, since the problem is generally *ill-conditioned* in the region around the initial guess used for the iterative procedure, which can be quite far from the exact parameters. With such an approach, the matrix $\mathbf{J}^T\mathbf{J}$ is not required to be non-singular in the beginning of iterations 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* (Beck and Arnold, 1977, Özisik and Orlande, 1999).

The sensitivity matrix is defined as

$$\boldsymbol{J}(\boldsymbol{P}) \equiv \left[\frac{\partial \boldsymbol{E}^T(\boldsymbol{P})}{\partial \boldsymbol{P}}\right]^T = \begin{bmatrix} \frac{\partial \vec{E}_1^T}{\partial P_1} & \frac{\partial \vec{E}_1^T}{\partial P_2} & \frac{\partial \vec{E}_1^T}{\partial P_3} & \cdots & \frac{\partial \vec{E}_1^T}{\partial P_N} \\ \frac{\partial \vec{E}_2^T}{\partial P_1} & \frac{\partial \vec{E}_2^T}{\partial P_2} & \frac{\partial \vec{E}_2^T}{\partial P_3} & \cdots & \frac{\partial \vec{E}_2^T}{\partial P_N} \\ \vdots & \vdots & \vdots & & \vdots \\ \frac{\partial \vec{E}_I^T}{\partial P_1} & \frac{\partial \vec{E}_I^T}{\partial P_2} & \frac{\partial \vec{E}_I^T}{\partial P_3} & \cdots & \frac{\partial \vec{E}_I^T}{\partial P_N} \end{bmatrix} \tag{6}$$

The elements of the sensitivity matrix are denoted as the sensitivity coefficients. They are defined as the first derivative of the estimated potential with respect to the unknown parameters. The sensitivity coefficients are required to be large in magnitude in order to estimate parameters 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 $\mathbf{J}^T\mathbf{J}$ invertible, that is, the determinant of $\mathbf{J}^T\mathbf{J}$ cannot be zero or even very small. Such a requirement over the determinant of $\mathbf{J}^T\mathbf{J}$ is better understood by taking into account a statistical analysis, as described below.

After the minimization of the least squares norm given by Eq. (3.b), a *statistical analysis* can be performed in order to obtain confidence intervals and a confidence region for the estimated parameters. *Confidence intervals* at the 99% confidence level are obtained as (Beck and Arnold, 1977, Özisik and Orlande, 1999):

$$\hat{P}_j - 2.576\,\sigma_{\hat{P}_j} \le P_j \le \hat{P}_j 2.576\,\sigma_{\hat{P}_j} \tag{7.a}$$

where $\hat{P}$ are the values estimated for the unknown parameters.

The *Confidence Region* can be computed as

$$(\hat{\boldsymbol{P}} - \boldsymbol{P})^T \boldsymbol{V}^{-1} (\hat{\boldsymbol{P}} - \boldsymbol{P}) \le \chi_N^2 \tag{7.b}$$

where χ_N^2 is the chi-square distribution for N degrees of freedom (number of unknown parameters), for a given confidence level and **V** is the covariance matrix of the estimated parameters given by

$$\boldsymbol{V} = (\boldsymbol{J}^T \boldsymbol{J})^{-1} \sigma^2 \tag{8}$$

An analysis of Eq. (7.b) reveals that some measure of the matrix $\boldsymbol{V}^{-1}$ needs to be maximized in order to minimize the hypervolume of the confidence region and, as a result, obtain minimum variance estimates. Since the covariance matrix is given by Eq. (8), we can choose to maximize the determinant of the matrix $\boldsymbol{J}^T\boldsymbol{J}$ by using the so called *D-optimum criterion* (Beck and Arnold, 1977, Özisik and Orlande, 1999), in order to design the experiment with respect to its duration and to the number and location of sensors.

RESULTS AND DISCUSSION

The present parameter estimation problem is classified as nonlinear, 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 $\boldsymbol{J}^T\boldsymbol{J}$ is not global, that is, it is dependent on values chosen in advance for the unknown parameters. The same values studied by Mikhailov and Özisik (1984) were used in the analysis presented below. They are $\varepsilon = 0.2$, $Lu = 0.4$, $Pn = 0.6$, $Ko = 5.0$, $Bi_q = Bi_m = 2.5$ and $Q = 0.9$.

For the solution of the direct problem given by equations (1), we considered the Classical Integral Transform Technique (Mikhailov and Özisik, 1984). The solution was obtained by taking into account as many eigenvalues (including the complex ones) as required for its convergence to a user prescribed tolerance of 10^{-6}. The full eigenvalues spectra is accurately computed though the Generalized Integral Transform Technique as applied to the solution of coupled eigenvalue problems (Guigon et al, 1999). The sensitivity coefficients were computed by finite differences, by using a forward approximation for the first derivatives.

We present in figure 2 the relative sensitivity coefficients for temperature and moisture content, for the positions X=0, 0.5 and 1, with respect to the different unknown parameters. 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 potentials and, as a result, it is easier to detect relative small magnitudes and linear dependency.

An analysis of the temperature sensitivity coefficients shown in figure 2 reveals a strong linear dependence of the sensitivity coefficients with respect to *Biq*, *Bim* and *Lu*, for each measurement location. Similar behavior is observed with the temperature sensitivity coefficients for *Ko* and ε. Therefore, it appears that the simultaneous estimation of *Biq*, *Bim* and *Lu* is impossible if only temperature measurements of a single sensor are used in the analysis. Such is also the case for the simultaneous estimation of *Ko* and ε. The temperature sensitivity coefficients with respect to Pn and ε are very small, as compared to the other sensitivity coefficients. Hence, temperature measurements do not provide useful information for the estimation of Pn and ε. The magnitudes of the other temperature sensitivity coefficients generally increase as the measurement location moves towards X=1.

We note in figure 2 that the moisture content sensitivity coefficients with respect to *Ko* and ε are almost identical for the three measurement locations tested. As a result, the simultaneous estimation of such parameters by using only moisture content measurements does not appear to be possible. The other moisture content sensitivity coefficients do not appear to be linearly-dependent for the position X=0. However, as the measurement position for the moisture content moves towards X=1, we note a general decrease in the magnitudes of the sensitivity coefficients and a tendency for the linear dependence of the sensitivity coefficients with respect to Bim and Lu. The other moisture content sensitivity coefficients are practically null at X=1.

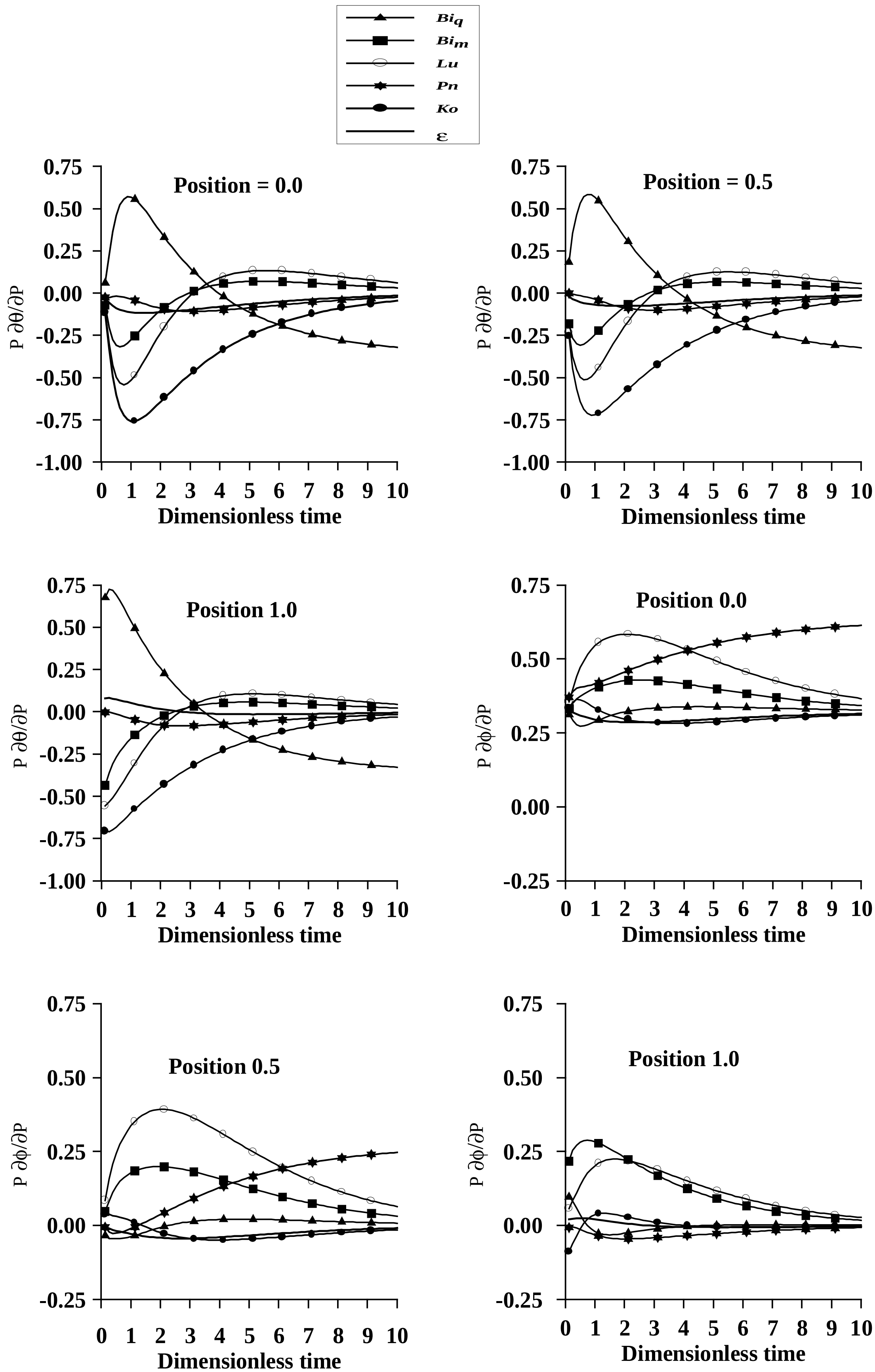

Figure 2 – Sensitivity coefficients for temperature and moisture content at different positions

The foregoing analysis of the sensitivity coefficients reveals that the most significant temperature measurements for the estimation of the unknown parameters, should be taken near the boundary X=1. On the other hand, the most significant moisture content measurements should be taken near the boundary X=0. Also, due to the linear dependence of several sensitivity coefficients, it is not possible to simultaneously estimate all the six unknown parameters if only temperature measurements or only moisture content measurements are used in the inverse analysis. It is interesting to note that, although the temperature and moisture content sensitivity coefficients with respect to *Ko* and ε are linearly dependent, their simultaneous estimation might be possible. Such is the case because for each row of the sensitivity matrix, the elements (sensitivity coefficients) with respect to *Ko* and ε are proportional; but the proportionality constant changes from the row containing temperature sensitivity coefficients to the rows containing moisture content sensitivity coefficients. As a result, the columns of the sensitivity matrix are not linear dependent if both temperature and moisture content measurements are used in the analysis.

Figure 3 presents the variation of the determinant of the matrix $\boldsymbol{J}^T\boldsymbol{J}$ for different number of sensors. The temperature sensors were located near the boundary X=1, while the moisture content measurements were taken near the boundary X=0, as a result of the analysis of the sensitivity coefficients discussed above. Figure 3 shows that, as expected, det$(\boldsymbol{J}^T\boldsymbol{J})$ increases as more sensors are used in the analysis. Such is the case because more information becomes available as more sensors are used for the estimation of the six unknown parameters and, hence, more accurate estimates can be obtained. After a very large increase in det($\boldsymbol{J}^T\boldsymbol{J}$) for small times, the rate of increase of det$(\boldsymbol{J}^T\boldsymbol{J})$ is reduced for larger times and basically det($\boldsymbol{J}^T\boldsymbol{J}$) becomes constant for times greater than 10.

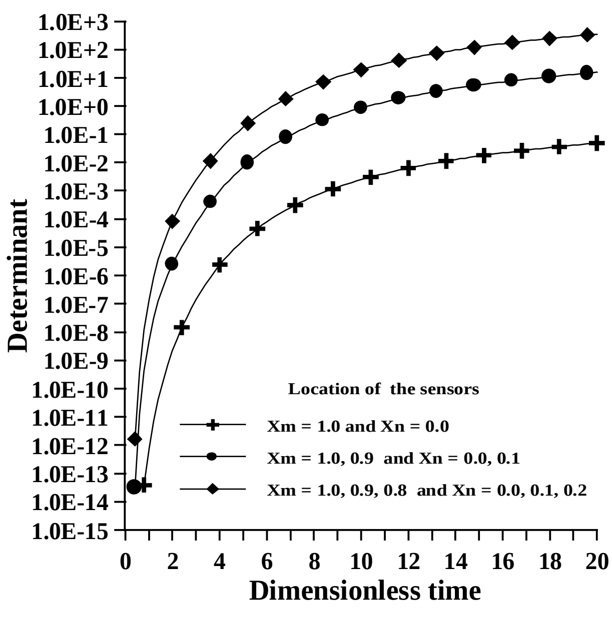

Figure 3 – Transient variation of det($\boldsymbol{J}^T\boldsymbol{J}$) for different number of sensors.

For the results presented below, involving the estimation of the six unknown parameters by using simulated measurements, we considered available the transient readings of three temperature sensors located at X=1, 0.9 and 0.8, and three moisture content sensors located at X=0, 0.1 and 0.2. The final experimental time was taken as t_f=10, since det($\boldsymbol{J}^T\boldsymbol{J}$) does increase significantly for larger times. During the time period $0 < t \leq 10$, we considered available 80 transient measurements per sensor.

The simulated experimental data was obtained from the solution of the direct problem given by equations (1) at the measurement locations, by using prescribed values for the unknown parameters. The data generated in such manner is considered as errorless. In order to simulate measurements containing random errors (M), we added to such errorless measurements (M_{exa}) an error term in the form

$$M = M_{exa} + \omega\sigma \tag{9}$$

where ω is a random variable with normal distribution, zero mean and unitary standard deviation and σ is the standard-deviation of the measurements. We note that M represents temperature as well as moisture content measurements.

For the estimation of the unknown parameters, we utilized the Levenberg-Marquardt method of minimization of the least-squares norm, as described above. The subroutine DBCLSJ of the IMSL Library (1987), based on such method was used in the present work.

Table 1 illustrates the results obtained for the estimated parameters by using measurements with different levels of random error, including σ=0 (errorless measurements) and $\sigma=0.01\ M_{max}$, where M_{max} is the maximum value of the measured temperatures and moisture content. The initial guesses used in the iterative procedure of the Levenberg-Marquardt method, were taken as $Lu^0 = 1.0$, $Pn^0 = 0.06$, $Ko^0 = 3.0$, $Bi_q^0 = 1.5$, $Bi_m^0 = 3.5$ and $\varepsilon^0 = 0.02$. An analysis of Table 1 reveals that accurate estimates can be obtained for the six parameters of interest for Luikov's formulation of the physical problem under picture in this paper.

Table 1. Estimated parameters obtained with the Levenberg- Marquardt method

Parameters	Exact	Estimated $\sigma=0$	Estimated $\sigma=0.01\ M_{max}$
Bi_q	2.5	2.5000	2.5088
Bi_m	2.5	2.5000	2.5100
Lu	0.4	0.4000	0.3996
Pn	0.6	0.6000	0.6010
Ko	5.0	5.0000	5.0062
ε	0.2	0.2000	0.1988

CONCLUSIONS

In this paper we presented the solution of an inverse problem of parameter estimation in drying. The one-dimensional physical problem considered here was formulated with Luikov's model of heat and mass transfer in capillary porous media. The resulting direct problem was solved with the Classical Integral Transform Technique by using as many eigenvalues, including the complex ones, as required for convergence.

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 matrix $\boldsymbol{J}^T\boldsymbol{J}$ shows that it is necessary to take temperature and moisture content measurements in order to estimate simultaneously the Luikov number, the Posnov number, the Kossovitch number, the phase change criterion and the Biot numbers for heat and mass transfer. Also, the number and location for the sensors, as well as the duration of the experiment can be estimated from such an analysis.

The use of simulated temperature measurements containing random errors shows that accurate estimates can be obtained for the unknown parameters with the present approach.

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