

Estimation of thermophysical properties of moist materials under different drying conditions

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(Received 2 February 2003; in final form 23 February 2005)

This article deals with the solution for the inverse problem of simultaneously estimating moisture content and temperature-dependent moisture diffusivity, together with thermal conductivity, heat capacity, density, and phase conversion factor of a drying body as well as boundary condition coefficients, by using only temperature measurements. Two different physical problems, convective and contact drying, are examined and compared. The present parameter estimation problem is solved with the Levenberg–Marquardt method of minimization of the least-squares norm, by using simulated experimental data. The temperature responses during the drying are obtained with a numerical solution of the non-linear one-dimensional Luikov's equations. As a representative drying body, a mixture of bentonite and quartz sand with known thermophysical properties has been chosen. Analyses of the sensitivity coefficients and of the determinant of the information matrix are presented.

Keywords: Moisture diffusivity; Convective and contact drying; Inverse approach

1. Introduction

Drying of hygroscopic capillary-porous bodies is a complex process of simultaneous heat and moisture transport within the material and from its surface to the surroundings, caused by a number of mechanisms. There are several different methods of mathematically modeling the drying process. In the approach proposed by Luikov [1], the drying body's moisture content and temperature field are expressed by a system of two coupled partial differential equations. The system of equations incorporates coefficients that must be determined experimentally.

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The main problem is the determination of the moisture diffusivity connected with the difficulty of moisture content measurements. Local moisture content measurements are practically unfeasible, especially for small drying objects. Standard drying curve measurements (body mean moisture content during drying) are complex and have low accuracy.

Dantas *et al.* [2–4] and Kanevce *et al.* [5–8] recently analyzed the application of inverse analysis approaches to the estimation of thermophysical properties of drying bodies. The main idea of the applied methods was to take advantage of the relation between the heat and mass (moisture) transport processes within the drying body and from its surface to the surrounding media. Then, the estimation of the thermophysical properties of the drying body could be performed on the basis of accurate and easy-to-perform thermocouple temperature measurements, by using an inverse analysis approach. Kanevce *et al.* [5–8] analyzed this idea by using the temperature response of a body exposed to convective drying, while Dantas *et al.* [2–4] examined contact drying experiments.

The objective of this article is to compare these two kinds of experiments for the estimation of the thermophysical properties of a drying body. In order to perform this analysis, the sensitivity coefficients and the determinant of the information matrix were calculated.

2. A mathematical model of drying

Two different physical problems, convective and contact drying, are analyzed here. In the convective drying experiment (see figure 1) the boundaries of the drying body are in contact with the drying air, thus resulting in a convective boundary condition for both the temperature and the moisture content. In the contact drying experiment (see figure 2), one of the boundaries of the one-dimensional body is in contact with a heater. That boundary is impervious to moisture transfer. The other boundary is in contact with the dry air, thus resulting in a convective boundary condition.

An infinite flat plate of the capillary porous material with negligible shrinkage has been considered in both the experiments examined here.

The system of equations for energy balance and moisture transport can be expressed [1] as

$$c\rho_s \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \varepsilon\rho_s \Delta H \frac{\partial X}{\partial t} \quad (1)$$

$$\frac{\partial X}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial X}{\partial x} + D\delta \frac{\partial T}{\partial x} \right) \quad (2)$$

where $T(x, t)$ and $X(x, t)$ are the unsteady temperature and moisture content fields, respectively. From previous experimental and numerical examinations of the transient moisture and temperature profiles [9] it was concluded that, for practical calculations, the influence of the thermogradient coefficient, δ , is small and can be ignored. It was also concluded that the system of coupled partial differential equations

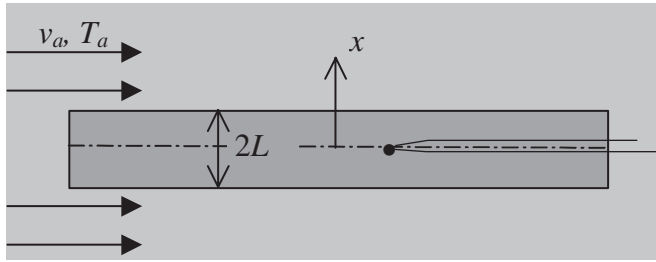


Figure 1. Scheme of the convective drying experiment.

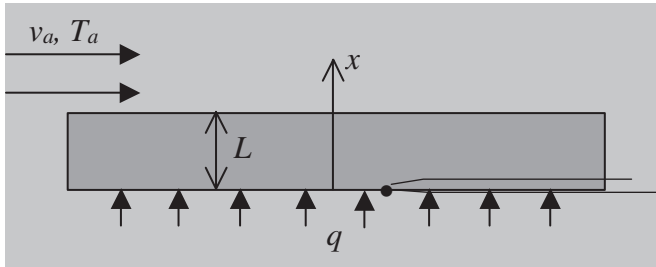


Figure 2. Scheme of the contact drying experiment.

can be used by treating the transport coefficients as constants, except for the moisture diffusivity, D . Consequently, the resulting system of equations for temperature and moisture content prediction becomes

$$\frac{\partial T}{\partial t} = \frac{k}{c\rho_s} \frac{\partial^2 T}{\partial x^2} + \frac{\varepsilon \Delta H}{c} \frac{\partial X}{\partial t} \quad (3)$$

$$\frac{\partial X}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial X}{\partial x} \right) \quad (4)$$

As initial conditions, uniform temperature and moisture content profiles are assumed, that is,

$$T(x, 0) = T_0, \quad X(x, 0) = X_0, \quad \text{for } t = 0 \quad (5)$$

The convective boundary conditions on the body surface at $x=L$ are given by:

$$\begin{aligned} -k \left(\frac{\partial T}{\partial x} \right)_{x=L} + j_q - \Delta H(1 - \varepsilon)j_m &= 0 \\ D\rho_s \left(\frac{\partial X}{\partial x} \right)_{x=L} + D\delta\rho_s \left(\frac{\partial T}{\partial x} \right)_{x=L} + j_m &= 0 \end{aligned} \quad (6)$$

where the convective heat flux, $j_q(t)$, and mass flux, $j_m(t)$, can be written, respectively as:

$$\begin{aligned} j_q &= h(T_a - T_{x=L}) \\ j_m &= h_D(C_{x=L} - C_a) \end{aligned} \quad (7)$$

The water vapor concentration in the drying air, C_a , is calculated by

$$C_a = \varphi p_s(T_a)/461.9(T_a + 273) \quad (8)$$

The water vapor concentration of the air in equilibrium with the surface of the body exposed to convection is calculated by

$$C_{x=L} = \frac{a(T_{x=L}, X_{x=L}) p_s(T_{x=L})}{461.9(T_{x=L} + 273)} \quad (9)$$

The water activity, a , or the equilibrium relative humidity of the air in contact with the convection surface at temperature $T_{x=L}$ and moisture content $X_{x=L}$ is calculated from experimental water sorption isotherms.

In the case of the convective drying experiment the problem is symmetrical, and the boundary conditions on the mid-plane of the plate ($x=0$) are given by

$$\left(\frac{\partial T}{\partial x}\right)_{x=0} = 0, \quad \left(\frac{\partial X}{\partial x}\right)_{x=0} = 0 \quad (10a)$$

In the case of the contact drying experiment the boundary conditions at the surface $x=0$, in contact with the heater that provides the heat flux q , are

$$-k\left(\frac{\partial T}{\partial x}\right)_{x=0} = q, \quad \left(\frac{\partial X}{\partial x}\right)_{x=0} = 0 \quad (10b)$$

3. Parameter estimation

The estimation methodology used is based on the minimization of the ordinary least square norm

$$E(\mathbf{P}) = [\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T[\mathbf{Y} - \mathbf{T}(\mathbf{P})] \quad (11)$$

Here, $\mathbf{Y}^T = [Y_1, Y_2, \dots, Y_{imax}]$ is the vector of measured temperatures, $\mathbf{T}^T(\mathbf{P}) = [T_1(\mathbf{P}), T_2(\mathbf{P}), \dots, T_{imax}(\mathbf{P})]$ is the vector of estimated temperatures at time t_i ($i=1, 2, \dots, imax$), $\mathbf{P}^T = [P_1, P_2, \dots, P_N]$ is the vector of unknown parameters, $imax$ is the total number of measurements, and N is the total number of unknown parameters ($imax \geq N$).

A version of Levenberg–Marquardt’s method was applied for the solution of the present parameter estimation problem [10–12]. This method is quite stable, powerful, straightforward, and has been applied to a variety of inverse problems. It belongs

to a general class of damped least square methods [11]. The solution for vector \mathbf{P} is achieved with the following iterative procedure

$$\mathbf{P}^{r+1} = \mathbf{P}^r + [(\mathbf{J}^r)^T \mathbf{J}^r + \mu^r \mathbf{I}]^{-1} (\mathbf{J}^r)^T [\mathbf{Y} - \mathbf{T}(\mathbf{P}^r)] \tag{12}$$

where the superscript r denotes the number of iterations and the sensitivity matrix is given by:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial T_1}{\partial P_1} & \dots & \frac{\partial T_1}{\partial P_N} \\ \frac{\partial T_{1,max}}{\partial P_1} & \dots & \frac{\partial T_{1,max}}{\partial P_N} \end{bmatrix} \tag{13}$$

Near the initial guess used for the iterative procedure of the Levenberg–Marquardt method the problem can be ill-conditioned, so that a large damping parameter is commonly initially chosen, thus making the term $\mu \mathbf{I}$ large as compared to the term $\mathbf{J}^T \mathbf{J}$. The term $\mu \mathbf{I}$ damps instabilities due to ill-conditioned character of the problem. Hence, the matrix $\mathbf{J}^T \mathbf{J}$ is not required to be non-singular at the beginning of iterations, but the procedure tends towards a slow-convergent steepest descent method. As the iteration process approaches the converged solution, the damping parameter decreases and the Levenberg–Marquardt method tends towards the Gauss’ method. The iterative procedure of the Levenberg–Marquardt method is stopped if either the ordinary least squares norm, $E(\mathbf{P})$, the norm of the gradient of $E(\mathbf{P})$, or the changes in the vector of parameters become sufficiently small [12].

4. Results and discussion

For the direct problem solution, the system of equations (3) and (4) with initial conditions given by equations (5) and boundary conditions given by equations (6) and (10a) or (10b), has been solved numerically for a model material [5], involving a mixture of bentonite and quartz sand, with the following experimentally determined thermophysical properties [9]: $\rho_s = 1738 \text{ kg m}^{-3}$, $\Delta H = 2.31 \times 10^6 \text{ J kg}^{-1}$, $c = 1550 \text{ J K}^{-1} \text{ kg}_{\text{db}}^{-1}$, $k = 2.06 \text{ W m}^{-1} \text{ K}^{-1}$, and $\varepsilon = 0.5$.

The experimentally obtained desorption isotherms of the model material are given by the following empirical equation [9]

$$a = 1 - \exp(-1.5 \times 10^6 (T + 273)^{-0.91} X^{(-0.005(T+273)+3.91)}) \tag{14}$$

where the water activity, a , represents the relative humidity of the air in equilibrium with the drying object at temperature, T , and moisture content, X .

The following empirical expression can describe the experimentally obtained relationship for the moisture diffusivity of this material

$$D = D_X X^{-2} \left(\frac{T + 273}{303} \right)^{D_T} \tag{15}$$

where $D_X = 9.0 \times 10^{-12} \text{ m}^2 \text{ s}^{-1}$ and $D_T = 10$.

In the inverse problem investigated here, the values of D_X , D_T , ρ_s , c , k , ε , h , and h_D are regarded as unknown for the convective drying experiment. For the contact drying experiment there is one additional unknown parameter, the applied heat flux, q . All other quantities appearing in the direct problem formulation were assumed to be exactly known.

For the estimation of these unknown parameters, the transient readings of a single temperature sensor, located at the position $x=0$, were considered available for the inverse analysis. Simulated experimental data were used in this work. Such data were obtained from the numerical solution of the direct problem presented above, by treating the values and expressions for the material properties as known. In order to simulate real measurements, normally distributed errors with zero mean and constant standard deviation, σ , were added to the numerical temperature responses.

4.1. Convective drying experiment

The vector of unknown parameters in the case of the convective drying experiment is

$$\mathbf{P}^T = [D_X, D_T, \rho_s, c, k, \varepsilon, h, h_D] \quad (16)$$

The possibility of simultaneously estimating the moisture content and temperature-dependent moisture diffusivity together with other thermophysical properties of the model material, as well as the heat and mass transfer coefficients in the convective drying experiment, by using only temperature measurements, was already investigated in [8]. Here, we will outline the main conclusions and results.

Following the conclusions of other published works [6,7] the selected drying air bulk temperature, speed, and relative humidity were taken as $T_a = 80^\circ\text{C}$, $V_a = 10 \text{ m s}^{-1}$, and $\varphi = 0.12$, respectively.

The analysis of the sensitivity coefficients has been carried out for a plate of thickness $2L = 6 \text{ mm}$, with an initial moisture content of $X(x, 0) = 0.20 \text{ kg kg}_{\text{db}}^{-1}$ and initial temperature $T(x, 0) = 20^\circ\text{C}$. Figure 3 shows the relative sensitivity coefficients $P_j \partial T_i / \partial P_j$, with respect to all the unknown parameters, $j = 1, 2, \dots, 8$.

The temperature sensitivity coefficient with respect to the phase conversion factor, ε , is very small. This indicates that ε cannot be estimated in this case. The relative sensitivity coefficients with respect to the dry material density, ρ_s , and the convection heat transfer coefficient, h , are linearly dependent. This makes it impossible to simultaneously estimate ρ_s and h . Due to these reasons and to the fact that the density of the dry material can be relatively easily determined by a separate experiment, the density of the dry material was assumed as known for the inverse analysis.

The relative sensitivity coefficient with respect to the thermal conductivity, k , is very small, except for the moment when the body moisture content is nearly equal to its equilibrium value. This is also a moment when a small evaporation rate and fast body temperature increase occur. Temperature measurements of a single thermocouple do not make it possible to estimate the thermal conductivity, if the initial guess is higher than the exact value of the parameter. In the cases when the initial guess for thermal conductivity is smaller than the exact value, the estimation of the thermal conductivity by a single thermocouple temperature response of a thin drying plate is possible.

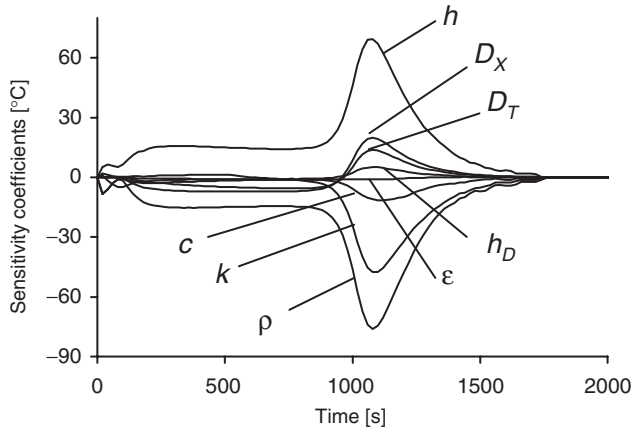


Figure 3. Relative sensitivity coefficients for the convective drying experiment.

An analysis of the determinant of the information matrix $\mathbf{J}^T\mathbf{J}$ with normalized elements confirms the previous conclusions. Figure 4 presents transient variations of the determinant of the information matrix if five, (D_X, D_T, c, h, h_D) , six, $(D_X, D_T, c, h, h_D, \rho_s)$, seven, $(D_X, D_T, c, h, h_D, \rho_s, k)$, and eight, $(D_X, D_T, c, h, h_D, \rho_s, k, \epsilon)$ parameters are simultaneously considered as unknowns.

Based on the foregoing analyses of the sensitivity coefficients and of the determinant of the information matrix, we now consider as unknown parameters for the inverse problem the moisture diffusivity parameters, D_X and D_T , the specific heat, c , the convection heat transfer coefficient, h , and the convection mass transfer coefficient, h_D . For the solution of such a parameter estimation problem with the Levenberg–Marquardt method, we use simulated measurements of a single thermocouple, with different levels of random errors, including $\sigma = 0$ (errorless measurements), 0.2, and 0.5°C , respectively. Table 1 shows the parameters estimated for these different levels of random errors. For comparison, the exact values for the parameters are also shown in this table. The obtained results show good agreement between the estimated and exact values for the parameters. For measurements with a standard deviation of 0.5°C , the maximum relative error between the estimated and exact values is 4.4% for h_D , but for the other parameters the error is smaller than 1%.

4.2. Contact drying experiment

The vector of unknown parameters in the case of the contact drying experiment is

$$\mathbf{P}^T = [D_x, D_T, \rho_s, c, k, \epsilon, h, h_D, q] \tag{17}$$

The analysis of the sensitivity coefficients has been carried out for an infinite flat plate with an initial moisture content of $X(x, 0) = 0.20 \text{ kg kg}_{\text{db}}^{-1}$ and initial temperature of $T(x, 0) = 20.0^\circ\text{C}$. The possibility of simultaneously estimating the moisture content and temperature-dependent moisture diffusivity together with other thermophysical properties of the model material, as well as the heat and mass transfer coefficients

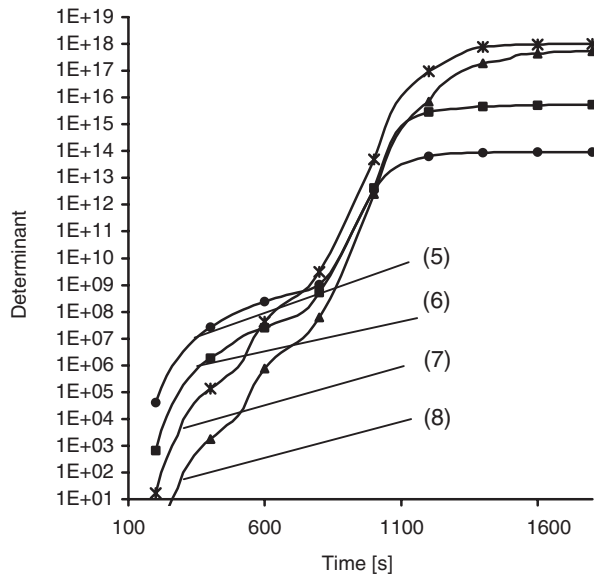


Figure 4. Determinant of the information matrix for the convective drying experiment.

Table 1. Estimated parameters in the convective drying experiment.

Parameters	Exact values	Estimated values			Relative errors for $\sigma=0.5$ [%]
		$\sigma=0^\circ\text{C}$	$\sigma=0.2^\circ\text{C}$	$\sigma=0.5^\circ\text{C}$	
$D_X \times 10^{12} [\text{m}^2 \text{s}^{-1}]$	9.00	8.99	9.04	9.06	0.7
D_T	10.0	10.0	9.999	10.1	1.0
$c [\text{J K}^{-1} \text{kg}^{-1}]$	1550	1551	1550	1551	0.1
$h [\text{W m}^{-2} \text{K}^{-1}]$	83.1	83.1	83.2	83.3	0.2
$h_D \times 10^2 [\text{m s}^{-1}]$	9.29	9.29	9.12	8.88	4.4

and the applied heat flux, has been investigated for a variety of boundary conditions and dimensions of the drying body.

The drying air bulk temperature, T_a , was varied between 20 and 80°C, the drying air velocity, V_a , between 3 and 10 m s⁻¹, the applied heat flux, q , between 1000 and 5000 W m⁻², and the plate thickness L , between 3 and 6 mm. The relative humidity of the drying air was $\varphi = 0.12$. The best combination of the relative temperature sensitivity coefficients with respect to all the unknown parameters, was obtained with $T_a = 20^\circ\text{C}$, $V_a = 10 \text{ m s}^{-1}$, $q = 3000 \text{ W m}^{-2}$, and $L = 3 \text{ mm}$.

Figure 5 shows the relative sensitivity coefficients $P_j \partial T_i / \partial P_j$ with respect to all unknown parameters. It can be seen that the relative sensitivity coefficients with respect to the applied heat flux, the dry material density, and the convection heat transfer coefficient are much larger than the other sensitivity coefficients. Due to the same reasons underlined in the case of convective drying experiment, the phase conversion factor and the dry material density were taken as known quantities for the cases examined below.

Figure 6 presents the transient the variation of the determinant of the information matrix if nine, $(D_X, D_T, c, \rho_s, k, \varepsilon, h, h_D, q)$, seven, $(D_X, D_T, c, k, h, h_D, q)$, six,

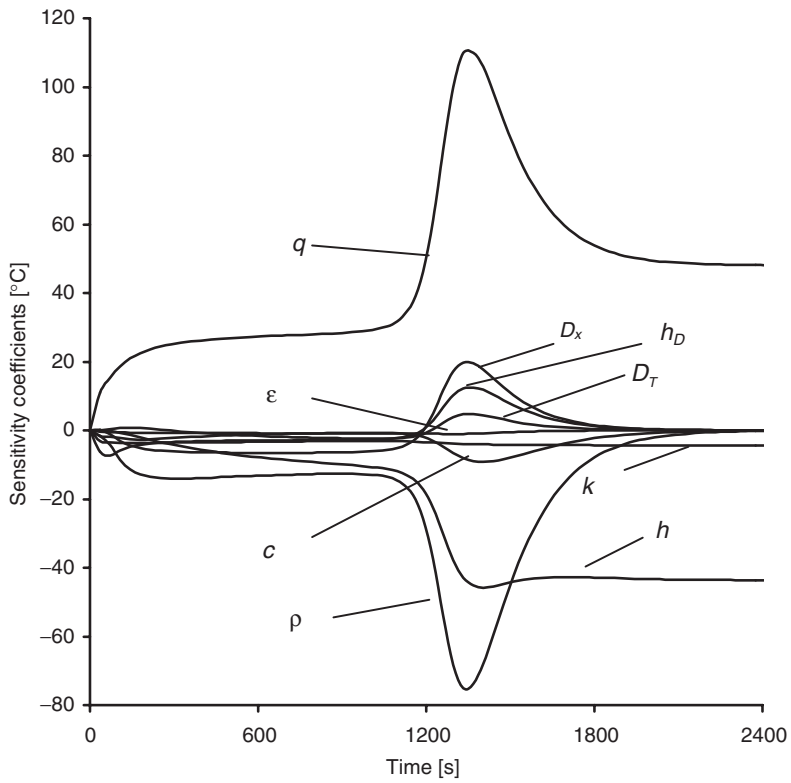


Figure 5. Relative sensitivity coefficients for the contact drying experiment.

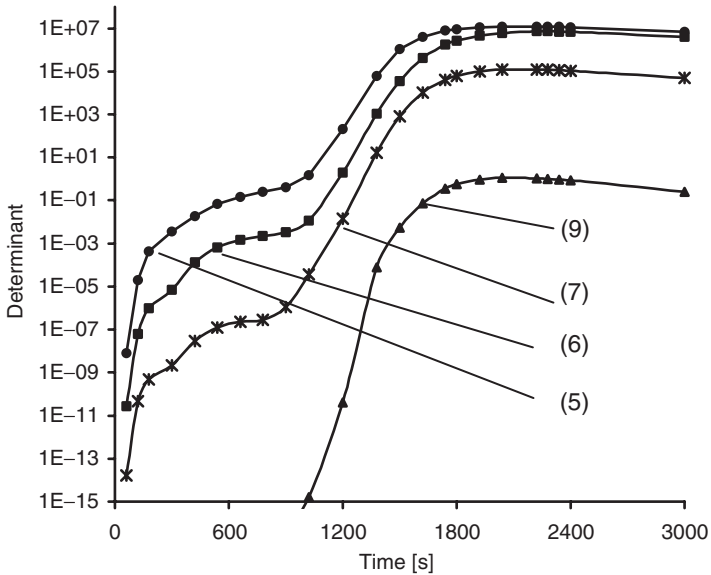


Figure 6. Determinant of the information matrix for the contact drying experiment.

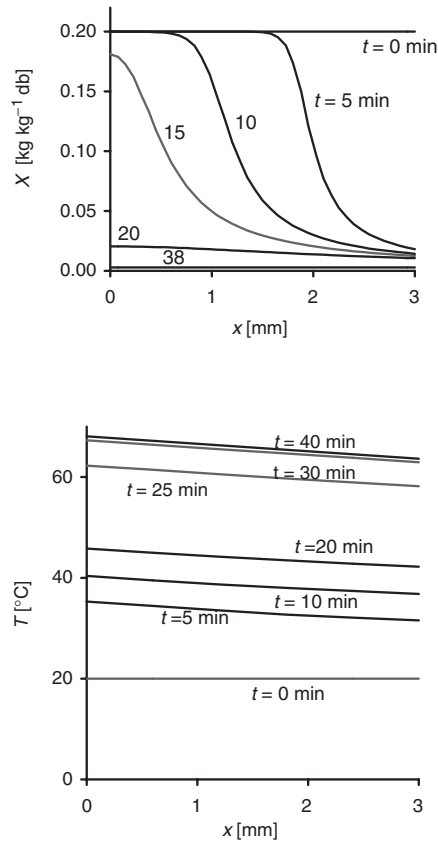


Figure 7. Transient moisture content and temperature profiles in the case of the contact drying experiment.

(D_X, D_T, c, h, h_D, q) , and five, (D_X, D_T, h, h_D, q) parameters are simultaneously considered as unknown. Elements of the information matrix were defined for a large but fixed number of transient temperature measurements (501 in these cases) [12]. The maximum determinant of the information matrix corresponds to the drying time when equilibrium moisture content and temperature profiles have been reached as can be seen in figures 7 and 8.

Table 2 shows the estimated parameters for $\sigma = 0.5$, for five, six, and seven unknown parameters. For comparison, the values of exact parameters and the values estimated with errorless ($\sigma = 0$) temperature data are shown in this table. Table 2 also shows the initial guesses used for the Levenberg–Marquardt method, as well as the relative errors for the case involving the estimation of seven unknown parameters. Estimated values of similar accuracy have been obtained with other initial guesses. If the dry material density and the phase conversion factor are considered as known, the remaining seven $(D_X, D_T, c, k, h, h_D, q)$ parameters can be simultaneously estimated with the relative errors within 2.9%. The accuracy of computing the parameters in the case when six (D_X, D_T, c, h, h_D, q) parameters were simultaneously estimated was within 2%. In the case of simultaneous estimation of the moisture diffusivity and the boundary condition parameters, (D_X, D_T, h, h_D, q) , the relative errors of the computed parameters were within 1%.

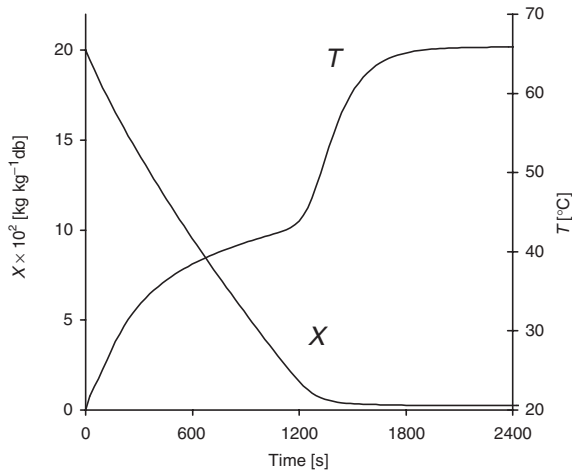


Figure 8. Volume-averaged moisture content and temperature changes during the contact drying experiment.

Table 2. Estimated parameters in the contact drying experiment.

Parameters	Exact values	Initial guesses	Estimated values				Relative errors for $\sigma=0.5$ [%]
			$\sigma=0$	$\sigma=0.5$	$\sigma=0.5$	$\sigma=0.5$	
$D_X \times 10^{12} \text{ [m}^2 \text{ s}^{-1}\text{]}$	9.00	11.00	9.00	9.049	9.063	9.041	0.5
$D_T \text{ [-]}$	10.0	12.0	10.0	9.904	9.806	9.874	1.3
$c \text{ [J K}^{-1} \text{ kg}^{-1}\text{]}$	1550	1300	1550	–	1533	1531	1.2
$K \text{ [W m}^{-1} \text{ K}^{-1}\text{]}$	2.06	2.70	2.06	–	–	2.12	3.1
$h \text{ [W m}^{-2} \text{ K}^{-1}\text{]}$	68.7	80.0	68.70	68.697	68.64	68.59	0.2
$h_D \times 10^2 \text{ [m s}^{-1}\text{]}$	6.94	8.00	6.94	6.90	6.89	6.82	1.7
$q \text{ [W m}^{-2}\text{]}$	3000	3500	3000	3000	2997	3003	0.1

5. Conclusions

The use of two types of experiments, convective and contact drying, for the solution of the inverse problem of simultaneous estimation of thermophysical properties of a drying body together with the boundary conditions parameters, by using only temperature measurements, has been analyzed in this article.

Values of two moisture diffusivity parameters, the dry material density, the thermal conductivity, the specific heat, the phase conversion factor, the convection heat transfer coefficient, and the mass transfer coefficient were regarded as unknown quantities in the convective drying experiment. In the contact drying experiment an additional unknown parameter, the applied heat flux, was taken into account. In the convective drying experiment, based on a single thermocouple transient response, it was possible to estimate simultaneously five of the eight unknown parameters: the two moisture diffusivity parameters, the specific heat, the convection heat transfer coefficient, and the mass transfer coefficient. In the contact drying experiment it was possible to estimate simultaneously seven of the nine unknown parameters: the two moisture diffusivity parameters, the specific heat, the thermal conductivity, the convection heat transfer coefficient, the mass transfer coefficient, and the applied heat flux.

The application of the convective or contact drying experiment for the estimation of the thermophysical properties of the drying body primarily depends on the available experimental setup; but the use of the contact drying experiment allows for the estimation of the thermal conductivity together with the other parameters.

Nomenclature

a	Water activity
c	Specific heat, $\text{J K}^{-1}\text{kg}_{\text{db}}^{-1}$
C	Concentration of water vapor, kg m^{-3}
D	Moisture diffusivity, $\text{m}^2 \text{s}^{-1}$
h	Heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$
h_D	Mass transfer coefficient, m s^{-1}
ΔH	Latent heat of vaporization, J kg^{-1}
\mathbf{I}	Identity matrix
j_m	Boundary mass flux, $\text{kg m}^{-2} \text{s}^{-1}$
j_q	Boundary heat flux, W m^{-2}
\mathbf{J}	Sensitivity matrix
κ	Thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$
L	Flat plate thickness, m
p_s	Saturation pressure, Pa
\mathbf{P}	Vector of unknown parameters
q	Applied heat flux, W m^{-2}
t	Time, s
T	Temperature, $^{\circ}\text{C}$
\mathbf{T}	Vector of estimated temperatures, $^{\circ}\text{C}$
V	Velocity, m s^{-1}
x	Spatial coordinate, m
X	Moisture content (dry basis), $\text{kg kg}_{\text{db}}^{-1}$
\mathbf{Y}	Vector of measured temperatures, $^{\circ}\text{C}$
δ	Thermo-gradient coefficient, 1K^{-1}
ε	Phase conversion factor
σ	Standard deviation
μ	Damping parameter
ρ	Density, kg m^{-3}
φ	Relative humidity

Subscripts

a	Drying air
s	Dry solid

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