APPLICATION OF INVERSE CONCEPTS TO DRYING

by

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This paper deals with the application of inverse approaches to estimation of drying body parameters. Simultaneous estimation of the thermophysical properties of a drying body as well as the heat and mass transfer coefficients, by using only temperature measurements, is analysed. A mathematical model of the drying process has been developed, where the moisture content and temperature fields in the drying body are expressed by a system of two coupled partial differential equations. For the estimation of the unknown parameters, the transient readings of a single temperature sensor located in an infinite flat plate, exposed to convective drying, have been used. The Levenberg-Marquardt method and a hybrid optimization method of minimization of the least-squares norm are used to solve the present parameter estimation problem. An analysis of the influence of the drying air velocity, drying air temperature, drying body dimension, and drying time on the thermophysical properties estimation, that enables the design of the proper experiments by using the so-called D-optimum criterion was conducted. In order to perform this analysis, the sensitivity coefficients and the sensitivity matrix determinant were calculated for the characteristic drying regimes and the drying body dimensions.

Key words: *inverse approach, drying, thermophysical properties, heat and mass transfer coefficients*

Introduction

Inverse approach to parameter estimation in the last few decades has become widely used in various scientific disciplines. Kanevce, Kanevce, and Dulikravich [1-5] and Dantas, Orlande, and Cotta [6-8] recently analysed application of inverse approaches to estimation of drying body parameters.

There are several methods for describing the complex simultaneous heat and moisture transport processes within drying material. In the approach proposed by Luikov [9], the drying body moisture content and temperature field are expressed by a system of two coupled partial differential equations. The system of equations incorporates coefficients that are functions of temperature and moisture content, and must be determined experimentally. All the coefficients, except for the moisture diffusivity, can be relatively easily determined by experiments. The main problem in the moisture diffusivity determination by classical or inverse methods is the difficulty of moisture content measurements.

The main idea of the present method is to make use of the interrelation between the heat and mass (moisture) transport processes within the drying body and from its surface to the surroundings. Then, the moisture diffusivity can be estimated on the basis of accurate and easy to perform single thermocouple temperature measurements by using an inverse approach.

The objective of this paper is an analysis of the possibility of simultaneous estimation of several thermophysical properties of a drying body and the heat and mass transfer coefficients. In order to perform this analysis, the sensitivity coefficients and the sensitivity matrix determinant were calculated. The proposed method of simultaneous estimation of several thermophysical properties of the drying body and the related heat and mass transfer coefficients using the transient readings of a single temperature sensor was tested for a model material. It was a mixture of bentonite and quartz sand with known thermophysical properties and negligible shrinkage effect.

Physical problem and mathematical formulation

The physical problem involves an infinite flat plate of thickness $2L$ initially at uniform temperature and uniform moisture content (fig. 1). The surfaces 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. The problem is symmetrical relative to the mid-plane of the plate.

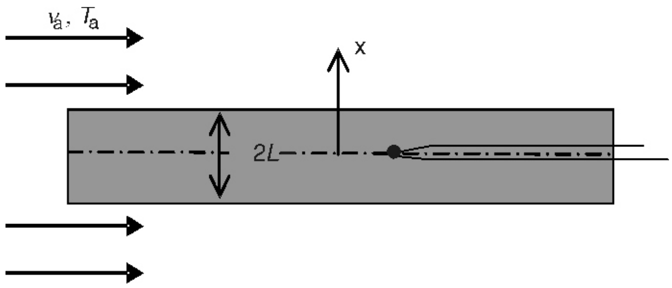

Figure 1. Scheme of the drying experiment

In this case of an infinite flat plate, if the shrinkage of the material can be neglected (ρ_s = const), the unsteady temperature field, $T(x, t)$, and moisture content field, $X(x, t)$, in the drying body are expressed by the following system of coupled nonlinear partial differential equations for energy and moisture transport:

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

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

Here, t, x, c, k, ΔH, ε, δ, D, and ρ_s are time, distance from the mid-plane of the plate, specific heat, thermal conductivity, latent heat of vaporization, ratio of water evaporation rate to the reduction rate of the moisture content, thermo-gradient coefficient, moisture diffusivity, and density of dry solid, respectively.

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

$$t = 0 \qquad T(x,\, 0) = T_0, \qquad X(x,\, 0) = X_0 \tag{3}$$

The temperature and the moisture content boundary conditions on the surfaces of the drying body in contact with the drying air are:

$$\begin{aligned} -k \left(\frac{\partial T}{\partial x}\right)_{x=L} + j_q - \Delta H(1-\varepsilon) j_m = 0 \\ -D\rho_s \left(\frac{\partial X}{\partial x}\right)_{x=L} - D\delta\rho_s \left(\frac{\partial T}{\partial x}\right)_{x=L} + j_m = 0 \end{aligned} \tag{4}$$

The convective heat flux, $j_q(t)$, and mass flux, $j_m(t)$, on these surfaces are:

$$\begin{aligned} j_q = h(T_a - T_{x=L}) \\ j_m = h_D (C_{x=L} - C_a) \end{aligned} \tag{5}$$

where h is the heat transfer, and h_D is the mass transfer coefficient, T_a is the temperature of the drying air, and $T_{x=L}$ is the temperature on the surface of the drying body. The water vapor concentration in the drying air, C_a, is calculated from:

$$C_a = \frac{\varphi p_s (T_a)}{461.9(T_a + 273)} \tag{6}$$

where φ is the relative humidity of the drying air and p_s is the saturation pressure. The water vapor concentration of the air in equilibrium with the surface of the body exposed to convection is calculated from:

$$C_{x=L} = \frac{a(T_{x=L}, X_{x=L}) p_s (T_{x=L})}{461.9(T_{x=L} + 273)} \tag{7}$$

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.

The boundary conditions on the mid-plane of the drying plate are:

$$\left.\frac{\partial T}{\partial x}\right|_{x=0} = 0, \quad \left.\frac{\partial X}{\partial x}\right|_{x=0} = 0 \tag{8}$$

The problem defined by eqs. (1-8) 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 temperature and moisture content fields in the drying body.

Estimation of parameters

For the inverse problem of interest here, the moisture diffusivity together with other thermophysical properties of the drying body as well as the heat and mass transfer coefficients are regarded as unknown parameters.

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

$$\mathrm{E}(\mathbf{P}) = [\mathbf{Y} - \mathbf{T}(\mathbf{P})]^{\mathrm{T}}[\mathbf{Y} - \mathbf{T}(\mathbf{P})] \tag{9}$$

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

A hybrid optimisation algorithm OPTRAN [10] and the Levenberg-Marquardt method [11, 12] have been utilized for the minimization of E(**P**) representing the solution of the present parameter estimation problem.

The Levenberg-Marquardt method is a quite stable, powerful, and straightforward gradient search minimization algorithm that has been applied to a variety of inverse problems. It belongs to a general class of damped least square methods. The solution for vector **P** is achieved using the following iterative procedure:

$$\mathbf{P}^{r+1} = \mathbf{P}^r + [(\mathbf{J}^r)^{\mathrm{T}}\mathbf{J}^r + \mu^r\mathbf{I}]^{-1}(\mathbf{J}^r)^{\mathrm{T}}[\mathbf{Y} - \mathbf{T}(\mathbf{P}^r)] \tag{10}$$

where r is the number of iterations, **I** is identity matrix, μ is the damping parameter, and **J** is the sensitivity matrix defined as:

$$\mathbf{J} = \begin{bmatrix} \dfrac{\partial T_1}{\partial P_1} & \cdots & \dfrac{\partial T_1}{\partial P_N} \\ \vdots & & \\ \dfrac{\partial T_{i\max}}{\partial P_1} & \cdots & \dfrac{\partial T_{i\max}}{\partial P_N} \end{bmatrix} \tag{11}$$

Near the initial guess, the problem is generally ill-conditioned so that large damping parameters are chosen thus making term $\mu\mathbf{I}$ large as compared to term $\mathbf{J}^T\mathbf{J}$. The term $\mu\mathbf{I}$ damps instabilities due to the ill-conditioned character of the problem. So, the matrix $\mathbf{J}^T\mathbf{J}$ is not required to be non-singular at the beginning of iterations and 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 a Gauss method. In fact, this method is a compromise between the steepest descent and Gauss method by choosing μ so as to follow the Gauss method to as large an extent as possible, while retaining a bias towards the steepest descent direction to prevent instabilities. The presented iterative procedure terminates if the norm of gradient of E(**P**) is sufficiently small, if the ratio of the norm of the gradient of E(**P**) to E(**P**) is small enough, or if the changes in the vector of parameters are very small.

An alternative to the Levenberg-Marquardt algorithm is the hybrid optimisation program OPTRAN [10]. OPTRAN incorporates six of the most popular optimisation algorithms: the Davidon-Fletcher-Powell gradient search [13], sequential quadratic programming (SQP) algorithm [14], Pshenichny-Danilin quasi-Newtonian algorithm [15], a modified Nelder-Mead (NM) simplex algorithm [16], a genetic algorithm (GA) [17], and a differential evolution (DE) algorithm [18]. Each algorithm provides a unique approach to optimisation with varying degrees of convergence, reliability and robustness at different stages during the iterative optimisation procedure. The hybrid optimiser OPTRAN includes a set of rules and switching criteria to automatically switch back and forth among the different algorithms as the iterative process proceeds in order to avoid local minima and accelerate convergence towards a global minimum.

The population matrix was updated every iteration with new designs and ranked according to the value of the objective function, in this case the ordinary least square norm. As the optimisation process proceeded, the population evolved towards its global minimum. The optimisation problem was completed when one of several stopping criteria was achieved:

– the maximum number of iterations or objective function evaluations was exceeded,
– the best design in the population was equivalent to a target design, or
– the optimisation program tried all six algorithms, but failed to produce a non-negligible decrease in the objective function.

The last criterion usually indicated that a global minimum had been found.

Results and discussions

The proposed method of simultaneous estimation of the thermophysical properties of a drying body as well as the heat and mass transfer coefficients, by using only temperature measurements, was tested for a model material, involving a mixture of bentonite and quartz sand. From the experimental and numerical examinations of the transient moisture and temperature profiles [19] it was concluded that for practical calculations, the influence of the thermodiffusion is small and can be ignored. Consequently, δ was utilized in this paper. It was also concluded that in this case, the system of two partial differential eqs. (1) and (2) can be used by treating all the coefficients except for the moisture diffusivity as constants. The appropriate mean values for the model material are [19]:

– density of the dry solid , ρ_s = 1738 kg/m^3,
– heat capacity, c = 1550 J/Kkg (db),
– thermal conductivity, k = 2.06 W/Km,
– latent heat of vaporization, $\Delta H = 2.31 \cdot 10^6$ J/kg,
– phase conversion factor, ε = 0.5, and
– thermo-gradient coefficient, δ = 0.

The following expression can describe the experimentally obtained relationship for the moisture diffusivity [20]:

$$D = 9.0 \cdot 10^{-12} X^{-2} \left(\frac{T-273}{303}\right)^{10} \tag{12}$$

The experimentally obtained desorption isotherms of the model material [19] are presented by the empirical equation:

$$a = 1 - \exp[-1.5 \cdot 10^{6} (T-273)^{-0.91} X^{0.005(T-273)+3.91}] \tag{13}$$

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.

For the direct problem solution, the system of eqs. (1) and (2) with the initial conditions (3) and the boundary conditions (4) and (8) was solved numerically with the experimentally determined thermophysical properties. An explicit finite-difference procedure was used.

For the inverse problem investigated here, values of the moisture diffusivity, D, density of the dry solid, ρ_s, heat capacity, c, thermal conductivity, k, phase conversion factor, ε, heat transfer coefficient, h and mass transfer coefficient, h_D, are regarded as unknown.

Here the moisture diffusivity of the model material has been represented by the following function of temperature and moisture content:

$$D = D_X X^{-2} \left(\frac{T-273}{303}\right)^{D_T} \tag{14}$$

where D_X and D_T are constants.

Thus, the vector of unknown parameters is:

$$\mathbf{P}^{\mathrm{T}} = [D_X, D_T, \rho_s, c, k, \varepsilon, h, h_D] \tag{15}$$

For the estimation of these unknown parameters, the transient readings of a single temperature sensor located in the mid-plane of the sample was considered (fig. 1).

The relative sensitivity coefficient, $P_m\partial T_i/\ P_m$, $i = 1, 2, ..., i\max$, $m = 1, 2, \ldots, N$, analysis was carried out in order to define the influence of the drying air velocity and temperature and drying body dimension [2-5]. Following the conclusions of these previous works the selected drying air bulk temperature, speed, and relative humidity were $T_a = 80$ °C, $v_{a,} = 10$ m/s and $\varphi = 0.12$, respectively, and the plate thickness, $2L = 4$ mm. The initial moisture content was $X(x, 0) = 0.20$ kg/kg and initial temperature $T(x, 0) = 20$ °C. Figure 2 shows the relative sensitivity coefficients for temperature with respect to all unknown parameters, $m = 1, 2, \ldots, 8$.

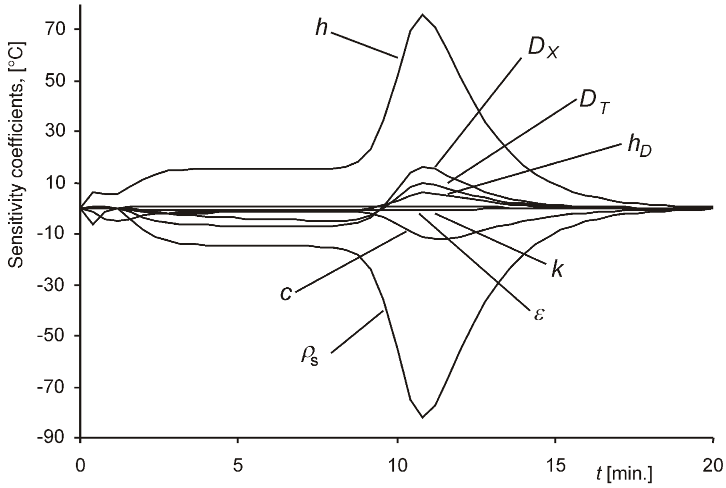

Figure 2. Relative sensitivity coefficients

It can be seen that the relative sensitivity coefficients with respect to the phase conversion factor, ε, and the thermal conductivity, k, are very small. This indicates that ε and k cannot be estimated in this case. This also indicates that the influence of the phase conversion factor and the thermal conductivity on the transient moisture content and temperature profiles is very small in this case. This can be explained by the very small heat transfer Biot number (Bi = $hL/k = 0.08$) and consequently very small temperature gradients inside the body during the drying. For these reasons, the phase conversion factor and the thermal conductivity were treated as known quantities for the examination described below.

The relative sensitivity coefficients with respect to the dry material density, $\rho_{s,}$ 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.

Thus, it appears to be possible to estimate simultaneously the moisture diffusivity parameters, D_X and D_T, the heat capacity, c, the convection heat transfer coefficient, h, and the mass transfer coefficient, h_D, by a single thermocouple temperature response in a thin drying plate.

Determinant of the information matrix $\mathbf{J}^{\mathrm{T}}\mathbf{J}$ with normalized elements:

$$[\mathbf{J}^{\mathrm{T}}\mathbf{J}]_{m,n} = \sum_{i=1}^{i\max} \left(P_m \frac{\partial T_i}{\partial P_m} \right) \left(P_n \frac{\partial T_i}{\partial P_n} \right), \quad m, n = 1, N \tag{16}$$

has been calculated in order to define drying time. Figure 3 presents transient variations of the determinant of the information matrix if (D_X, D_T, c, h, h_D), (D_X, D_T, c, h), (D_X, D_T, h, h_D), and (D_X, D_T, h) are simultaneously considered as unknown parameters. Elements of these determinants of the information matrix were defined [21] for a large, but fixed number of transient temperature measurements (101 in this case).

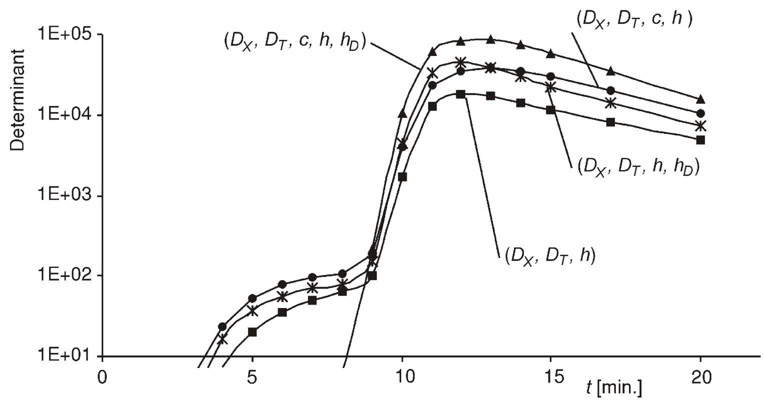

Figure 3. Determinant of the information matrix

The duration of the drying experiment (the drying time) corresponding to the maximum determinant value was used for the computation of the unknown parameters. The maximum determinant of the information matrix corresponds to the drying time when nearly equilibrium moisture content and temperature profiles have been reached, as can be seen in figs. 4 and 5.

The transient readings of the single temperature sensor located in the mid-plane of the sample were obtained by simulated experiments. The experimental 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

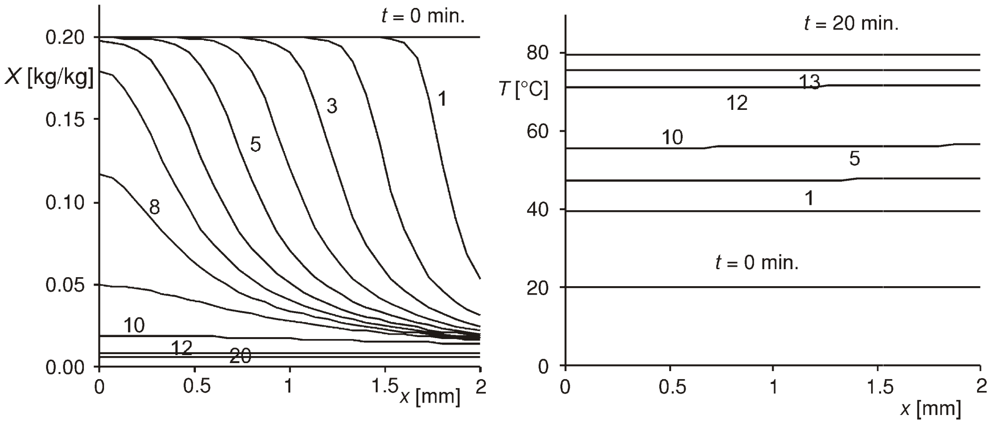

Figure 4. Transient moisture content and temperature profiles

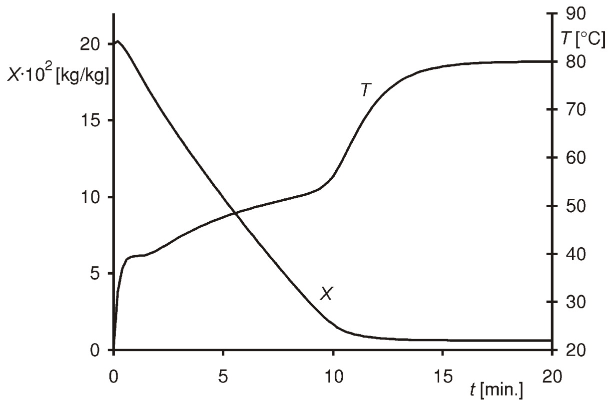

Figure 5. Volume-averaged moisture content and temperature changes during the drying

measurements, a normally distributed error with zero mean and standard deviation, σ of 0.2, 0.5, 1.0, and 1.5 ºC was added to the numerical temperature response (fig. 6).

Table 1 shows the estimated parameters for σ = 0.2, 0.5, 1.0, and 1.5 °C. For comparison, the values of exact parameters and the values estimated with errorless (σ = = 0) temperature data are shown in this table. Table 1 also shows the relative errors of the estimated parameters, ε.

From the obtained results it appears to be possible to estimate simultaneously the moisture diffusivity parameters, D_X and D_T, the heat capacity, c, the convection heat

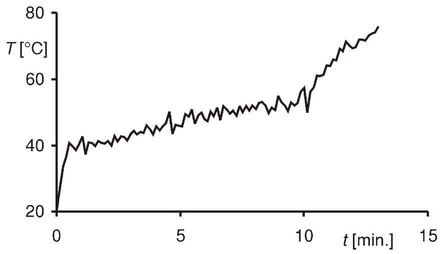

Figure 6. Simulated temperature response at $x = 0$ with a noise $\sigma = 1.5$ °C

transfer coefficient, h, and the mass transfer coefficient, h_D, by a single thermocouple temperature response. The accuracy of computing the parameters strongly depends on the noise, σ, (cases A1 to A5). Similar accuracy has been obtained if D_X, D_T, h, and h_D were simultaneously estimated (case A6). But, in the case when only the heat transfer coefficient, h, was simultaneously estimated with the moisture diffusivity parameters, D_X and D_T, the relative errors of the computed parameters were within one percent (case A7).

The very high mass transfer Biot number and the very small heat transfer Biot number can explain this. From this reason, the temperature sensitivity coefficient with respect to the convection mass transfer coefficient h_D is very small relative to the temperature sensitivity coefficient with respect to the convection heat transfer coefficient, h.

Table 1. Estimated parameters

Case		$D_X \cdot 10^{12}$ [m^2/s]	D_T [–]	c [J/kgK]	h [W/m^{2}K]	$h_D \cdot 10^2$ [m/s]
A1	Estimated	8.99	10.0	1551	83.1	9.29
$\sigma = 0$ °C	ε [%]	0.1	0.0	0.1	0.0	0.0
A2	Estimated	9.04	10.00	1550	83.2	9.12
$\sigma = 0.2$ °C	ε [%]	0.4	0.0	0.0	0.1	1.8
A3	Estimated	9.06	10.10	1551	83.3	8.88
$\sigma = 0.5$ °C	ε [%]	0.7	1.0	0.1	0.2	4.4
A4	Estimated	9.45	9.44	1597	83.5	8.62
$\sigma = 1.0$ °C	ε [%]	5.0	5.6	3.0	0.5	7.2
A5	Estimated	9.76	9.03	1627	83.8	8.31
$\sigma = 1.5$ °C	ε [%]	8.4	9.7	5.0	0.8	10.5
A6	Estimated	9.87	8.79		83.2	8.28
$\sigma = 1.5$ °C	ε [%]	9.7	12.1		0.1	10.9
A7	Estimated	8.93	9.95		83.0	
$\sigma = 1.5$ °C	ε [%]	0.8	0.5		0.1	
Exact values		9.00	10.0	1550	83.1	9.29

To overcome this problem, in this paper the mass transfer coefficient was related to the heat transfer coefficient through the analogy between the heat and mass transfer processes in the boundary layer over the drying body [22]:

$$h_D \quad 0.95\frac{D_\mathrm{a}}{k_\mathrm{a}}h \tag{17}$$

where D_a and k_a are the moisture diffusivity and thermal conductivity in the air, respectively. The obtained relation is very close to the well-known Lewis relation. By using the above relation between the heat and mass transfer coefficients, they can be estimated simultaneously, if only the heat transfer coefficient is regarded as an unknown parameter (tab. 2).

Table 2. Estimated parameters using the relation (17)

Case		$D_X \cdot 10^{12}$ [m^2/s]	D_T [–]	c [J/kgK]	h [W/m^{2}K]	$h_D \cdot 10^2$ [m/s]
B4	Estimated	8.83	10.20	1600	83.4	9.33
σ = 1.0 °C	ε [%]	1.9	2.0	3.2	0.4	0.4
B5	Estimated	8.82	10.17	1620	83.5	9.34
σ = 1.5 °C	ε [%]	2.0	1.7	4.5	0.5	0.5
B6	Estimated	8.89	10.02		83.0	9.28
σ = 1.5 °C	ε [%]	1.2	0.2		0.1	0.1
Exact values		9.00	10.0	1550	83.1	9.29

The relative errors of the computed heat capacity, c, in the cases B4 and B5 are nearly the same as in the cases A4 and A5, respectively, but the relative errors of the computed D_X, D_T, and h_D are much lower. From the obtained results in the case B6, it appears to be possible to estimate simultaneously with very high accuracy, the moisture diffusivity parameters, D_X and D_T, and the heat and mass transfer coefficients, h and h_D, by a single thermocouple temperature response even in the case with the relatively high noise of 1.5 °C.

Conclusions

A method of simultaneous estimation of the moisture diffusivity together with the other thermophysical properties of a drying body as well as the heat and mass transfer coefficients by using only temperature measurements, has been analyzed in this paper.

The Levenberg-Marquardt and the hybrid optimisation method were applied for evaluation of the unknown parameters.

The two moisture diffusivity parameters and the heat capacity of the drying body together with the heat and mass transfer coefficients were simultaneously estimated. The obtained results show good agreement between the evaluated and exact values of parameters and confirm the validity of the proposed method.

An analysis of the influence of the temperature measurements errors on the accuracy of the estimated parameters was also presented.

Nomenclature

a – water activity
c – heat capacity, [J/Kkg(db)]
C – concentration of water vapor, [kg/m^3]
D – moisture diffusivity, [m^2/s]
h – heat transfer coefficient, [W/m^{2}K]
h_D – mass transfer coefficient, [m/s]
H – latent heat of vaporization, [J/kg]
$\mathbf{I}$ – identity matrix
j_m – mass flux, [kg/m^{2}s]
j_q – heat flux, [W/m^2]
$\mathbf{J}$ – sensitivity matrix
k – thermal conductivity, [W/Km]
L – flat plate thickness, [m]
p_s – saturation pressure , [Pa]
$\mathbf{P}$ – vector of unknown parameters
t – time, [s]
T – temperature, [°C]
$\mathbf{T}$ – vector of estimated temperature, [°C]
v – velocity, [m/s]
x – distance from the mid-plane, [m]
X – moisture content (dry basis), [kg/kg(db)]
$\mathbf{Y}$ – vector of measured temperature, [°C]

Greec letters

δ – thermo-gradient coefficient, [1/K]
ε – phase conversion factor
– relative error, [%]
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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