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ESTIMATION OF THERMOPHYSICAL PROPERTIES OF MOIST MATERIALS UNDER DIFFERENT DRYING CONDITIONS

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ABSTRACT

This paper deals with a solution method for an 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 the heat and mass transfer coefficients, by using only temperature measurements. Two different physical problems, convective and contact drying, are analyzed and compared.

The present parameter estimation problem is solved by using the Levenberg-Marquardt method of minimization of the least-squares norm, by using simulated experimental data. The temperature responses during the drying are obtained from 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. An analysis of the sensitivity coefficients and the sensitivity matrix determinant is presented as well.

NOMENCLATURE

a = water activity
c = heat capacity, J/K/kg 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
ΔH = 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
κ = thermal conductivity, W/m/K
L = flat plate thickness, m
p_s = saturation pressure , Pa
$\mathbf{P}$ = vector of unknown parameters
q = heat supply rate, W/m^2
t = time, s
T = temperature, ^{0}C
$\mathbf{T}$ = vector of estimated temperature, ^{0}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, ^{0}C
δ = thermo-gradient coefficient, 1/K
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

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 describing the drying process. In the approach proposed by Luikov [1], 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 must be determined experimentally. 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 curves measurements (body mean moisture content during drying) are complex and have low accuracy.

Dantas, Orlande and Cotta [2, 3, 4] and Kanevce, Kanevce and Dulikravich [5, 6, 7, 8] recently analysed application of inverse approaches to estimation of a drying body parameters. The main idea of the applied methods is 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 drying body parameters estimation can be performed on the basis of an accurate and easy-to-perform thermocouple temperature measurements by using an inverse approach. Kanevce, Kanevce and Dulikravich [5, 6, 7, 8] analysed this idea of the drying body parameters estimation by using temperature response of a body exposed to convective drying, while Dantas, Orlande and Cotta [2, 3, 4] used contact drying experiments.

The objective of this paper is a comparison of the two kinds of experiments for estimation of the thermophysical properties of a drying body. An analysis of the influence of the drying air parameters and the drying body dimensions is presented as well. In order to perform this analysis, the sensitivity coefficients and the sensitivity matrix determinant were calculated.

A MATHEMATICAL MODEL OF DRYING

Two different physical problems, convective and contact drying, are analyzed. In the convective drying experiment (Fig. 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 (Fig. 2), one of the boundaries of the one-dimensional body is in contact with a heater that provides conductive heating. That boundary is impervious to moisture transfer. The other boundary is in contact with the drying air thus resulting in a convective boundary condition.

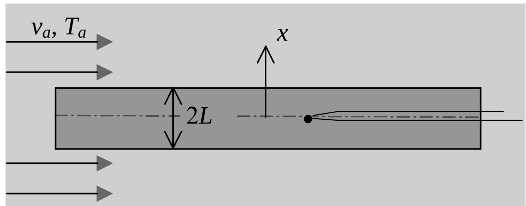


Fig. 1. Scheme of the convective drying experiment

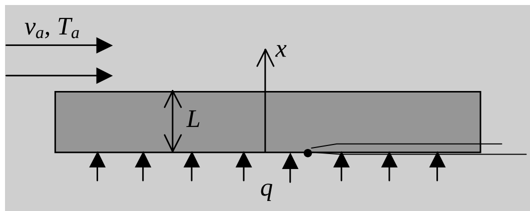


Fig. 2. Scheme of the contact drying experiment

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

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

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

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

where $T(x, t)$ and $X(x, t)$ are the unsteady temperature and moisture content fields, respectively. From the experimental and numerical examinations of the transient moisture and temperature profiles [9] it was concluded that for practical calculations, the influence of the thermodiffusion, δ, is small and can be ignored. It was also concluded that the system of two simultaneous partial differential equations could be used by treating the transport coefficients as constants, except for the moisture diffusivity, D. Consequently, the resulting system of equations for the 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

$$t=0 \quad T(x,0)=T_0\,,\;\; X(x,0)=X_0 \quad (5)$$

The boundary conditions on the specimen surfaces ($x = L$) exposed to convection are

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

where the convective heat flux, $j_q(t)$, and mass flux, $j_m(t)$, on these surface are

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

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 boundary conditions on the mid-plane of the plate ($x = 0$) are

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

In the case of the contact drying experiment the boundary conditions on the plane in contact with the heater that provides the heat supply rate q, are

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

In order to approximate the solution of Eqs. (3, 4), an explicit procedure has been used [5].

ESTIMATION OF PARAMETERS

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

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

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

A version of Levenberg-Marquardt method was applied for the solution of the presented parameter estimation problem [10]. This method is quite stable, powerful, and 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 P is achieved using the following iterative procedure

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

$$\mathbf{J}=\begin{bmatrix}\dfrac{\partial T_1}{\partial P_1} & \cdots & \dfrac{\partial T_1}{\partial P_N}\\ . & & \\ \dfrac{\partial T_{i\max}}{\partial P_1} & \cdots & \dfrac{\partial T_{i\max}}{\partial P_N}\end{bmatrix} \quad (13)$$

Near the initial guess, the problem is generally ill-conditioned so that large damping parameter is chosen thus making term $\mu\mathbf{I}$ large as compared to term $\mathbf{J}^{\mathrm{T}}\mathbf{J}$. The term $\mu\mathbf{I}$ damps instabilities due to ill-conditioned character of the problem. So, the matrix $\mathbf{J}^{\mathrm{T}}\mathbf{J}$ 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 Gauss method. In fact, this method compromises 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 stops if the norm of gradient of **E**(**P**) is sufficiently small, or if the ratio of the norm of gradient of **E**(**P**) to the **E**(**P**) is small enough, or if the changes in the vector of parameters are very small [12].

RESULTS AND DISCUSSION

For the direct problem solution, the system of equations (3) and (4) with the initial conditions, equation (5), and the boundary conditions, equations (6) and (10a,b), has been solved numerically for a model material, involving a mixture of bentonite and quartz sand with the known, experimentally determined [9] thermophysical properties: $\rho_s = 1738$ kg/m^3, c = 1550 J/K/kg db, k = 2.06 W/m/K, $\Delta H = 2.31\cdot 10^6$ J/kg and ε = 0.5.

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

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

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 $D_X = 9.0\cdot 10^{-12}$ and $D_T = 10$ are constants.

For the inverse problem investigated here, values of D_X, D_T, ρ_s, c, k, ε, h and h_D are regarded as unknown at the convective drying experiment. At the contact drying experiment there is one more unknown parameter, the heat supply rate, q. All other quantities appearing in the direct problem formulation were assumed to be known. For the estimation of these unknown parameters, the transient reading of a single temperature sensor located at the position x = 0, has been considered.

The simulated experimental data were obtained from the numerical solution of the direct problems presented above, by treating the values and expressions for the material properties as known. In order to simulate real measurements, a normally distributed error with zero mean and standard deviation, σ was added to the numerical temperature responses.

Convective drying experiment

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

$$\mathbf{P}^T = [D_x, D_T, \rho_s, c, k, \varepsilon, h, h_D] \tag{16}$$

The possibilities of simultaneous estimation of 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, were investigated in [8]. Here, we will outline the main canclusions and results.

Following the conclusions of the previous works [6, 7] the selected drying air bulk temperature, speed, and relative humidity were T_a = 80 ^{O}C, $v_{a,}$ = 10 m/s and φ = 0.12, respectively.

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

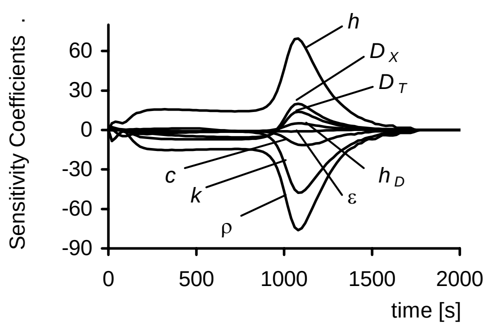


Fig.3. Relative sensitivity coefficients for the convective drying experiment

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 until the moment when the body moisture content is nearly equal to the equilibrium. Then, a rapid body temperature increase associated with a rapid evaporation rate decrease begins. After this instant in time, they are not linearly-dependent any more. This makes it possible to simultaneously estimate ρ_s and *h*, but the accuracy is much lower in the case of simultaneous estimation of ρ_s, *h*, and the other parameters. The similar conclusions are valid for the simultaneous estimation of the dry material density, ρ_s, and the heat capacity, *c*. Due to these reasons and the fact that the density of the dry plate material can be relatively easily determined by a separate experiment, the density of the dry plate material was taken as known.

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 the equilibrium. This is also a moment when a small evaporation rate and fast body temperature increase occur. Single thermocouple measurements 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.

Additional examinations are needed concerning the simultaneous estimation of the thermal conductivity and the other parameters by using a single thermocouple temperature response located in the middle of a thin drying plate.

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.

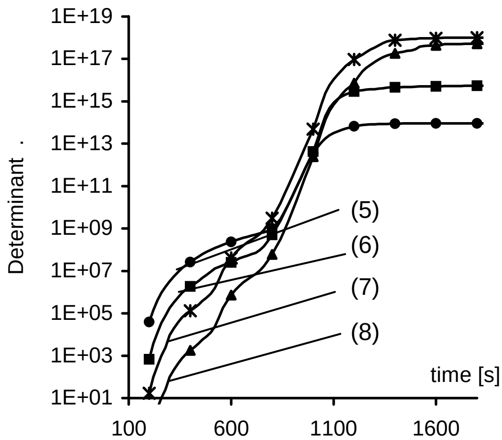


Fig.4. Determinant of the information matrix

An analysis of the determinant of the information matrix $\mathbf{J}^T\mathbf{J}$ with normalised 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, ρ_s), seven, (D_X, D_T, *c*, *h*, h_D, ρ_s, *k*), and eight, (D_X, D_T, *c*, *h*, h_D, ρ_s, *k*, ε) parameters are simultaneously considered as unknowns.

Table 1 shows the computationally obtained values of the parameters estimated with "exact" (without noise) temperature data and with simulated temperature data with added noise of σ = 0.2 and 0.5 ^{O}C. For comparison, the exact values of parameters are also shown. The obtained results show good agreement between the evaluated and exact values of parameters.

Table 1. Estimated parameters in the convective drying experiment

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

Contact drying experiment

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

$$\mathbf{P}^{\mathrm{T}} = [D_x, D_T, \rho_s, c, k, \varepsilon, h, h_D, q] \qquad (17)$$

The sensitivity coefficients analysis has been carried out for an infinite flat plate with initial moisture content of $X(x, 0) = 0.20$ kg/kg and initial temperature $T(x,0) = 20.0\ ^{\mathrm{O}}\mathrm{C}$. The possibilities of simultaneous estimation of 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 and the heat supply rate have been investigated for a variety of boundary conditions and dimensions of the drying body.

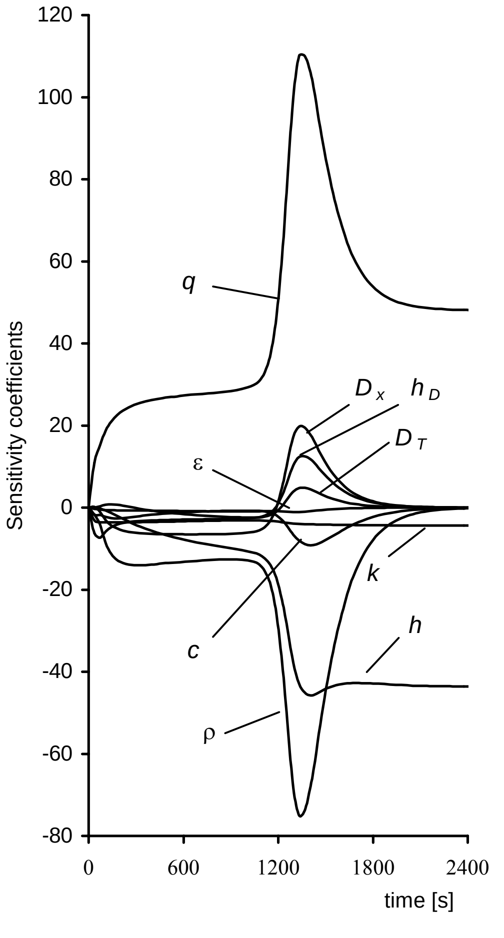


Fig.5. Relative sensitivity coefficients for the contact drying experiment

The drying air bulk temperature, T_a, was varied between 20 and 80 $^{\mathrm{O}}$C, the drying air velocity, v_a, between 3 and 10 m/s, the heat supply rate, 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 unknown parameters, was obtained with $T_a = 20\ ^{\mathrm{O}}\mathrm{C}$, $v_a = 10$ m/s, $q = 3000$ W/m^2, $L = 3$ mm. Figure 5 shows the relative sensitivity coefficients $P_j \partial T_i / \partial P_j$, i = 1, 2,…, imax, for temperature with respect to all unknown parameters, j = 1, 2,…,9. It can be seen that even in this case the relative sensitivity coefficients with respect to the heat supply rate, the dry material density, and the convection heat transfer coefficient are much higher than the relative sensitivity coefficients with respect to the phase conversion factor. This makes it impossible to simultaneously estimate all of the unknown parameters.

Due to these reasons and to the 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 transient variation of the determinant of the information matrix if nine, (D_X, D_T, c, ρ_s, k, ε, h, h_D, q), seven, (D_X, D_T, c, k, h, h_D, q), six, (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 this sensitivity determinant were defined [13] for a large, but fixed number of transient temperature measurements (501 in these cases).

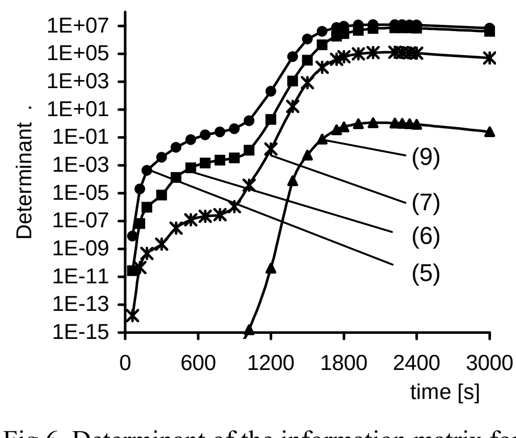
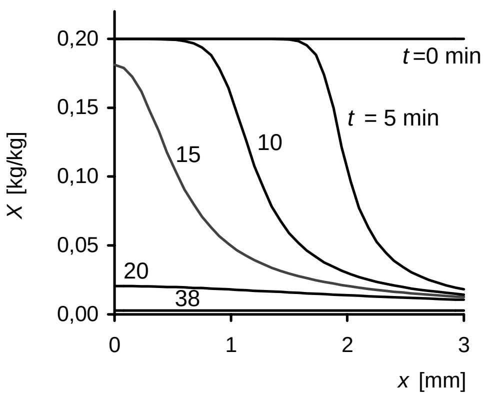


Fig.6. Determinant of the information matrix for the contact drying experiment

Table 2. Estimated parameters in the contact drying experiment

Parameters	Exact values	Initial guesses	Estimated values				Relative errors for σ = 0.5 [%]
			σ = 0	σ = 0.5	σ = 0.5	σ = 0.5	
$D_X \cdot 10^{12}$ [m²/s]	9.00	11.00	9.00	9.049	9.063	9.041	0.5
D_T [-]	10.0	12.0	10.0	9.904	9.806	9.874	1.3
c [J/K/kg]	1550	1300	1550	-	1533	1531	1.2
k [W/m/K]	2.06	2.70	2.06	-	-	2.12	3.1
h [W/m²/K]	68.7	80.0	68.70	68.697	68.64	68.59	0.2
$h_D \cdot 10^2$ [m/s]	6.94	8.00	6.94	6.90	6.89	6.82	1.7
q [W/m²]	3000	3500	3000	3000	2997	3003	0.1

The maximum determinant of the information matrix corresponds to the drying time when equilibrium moisture content and temperature profiles have been reached (Fig. 7 and 8).



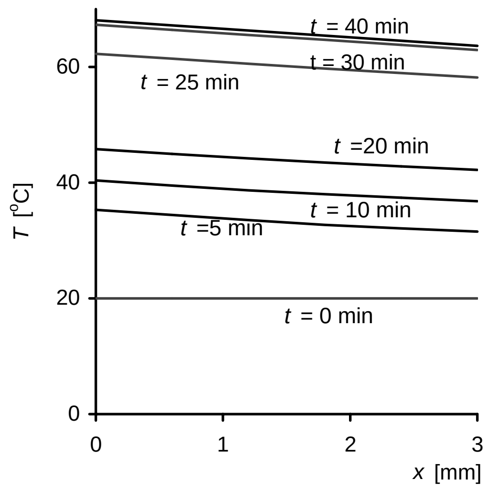


Fig.7. Transient moisture content and temperature profiles in the case of the contact drying experiment

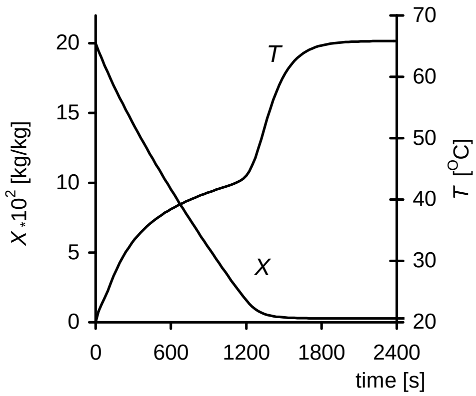


Fig.8. Volume-averaged moisture content and temperature changes during the contact drying

The unknown parameters in the contact drying experiment have been estimated using the plate of thickness L = 3 mm. The drying air bulk temperature of 20 °C, the drying air velocity of 10 m/s, and the heat supply rate of 3000 W/m² have been chosen.

Table 2 shows the computationally obtained parameters and the relative errors of the estimated parameters for σ=0.5. For comparison, the values of exact parameters and the values estimated with "exact" (without noise) temperature data are also shown. Table 2 also shows the initial guesses of the parameters for the presented estimations. Estimated values of similar accuracy have been obtained using 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 3.1%. The accuracy of computing parameters in the case when six (D_X, D_T, c, h, h_D, q) parameters were simultaneously estimated was within two percent. In the case of simultaneous estimation of the moisture diffusivity and the boundary conditions parameters, (D_X, D_T, h, h_D, q), the relative errors of the computed parameters were within one percent.

CONCLUSIONS

Aplication 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 paper.

Values of two moisture diffusivity parameters, the dry material density, the thermal conductivity, the heat capacity, the phase conversion factor, the convection heat transfer coefficient, and the mass transfer coefficient were regarded as unknown in the convective drying experiment. In the contact drying experiment an additional unknown parameter, the heat supply rate, was taken into account.

In the convective drying experiment, on the basis of a single thermocouple temperature response it is possible to estimate simultaneously five of the eight unknown parameters: the two moisture diffusivity parameters, the heat capacity, the convection heat transfer coefficient, and the mass transfer coefficient.

In the contact drying experiment it appears possible to estimate simultaneously seven of the nine unknown parameters: the two moisture diffusivity parameters, the heat capacity, the thermal conductivity, the convection heat transfer coefficient, the mass transfer coefficient, and the heat supply rate. Consequently, the aplication of the convective or contact drying experiment in the estimation of the thermophysical properties of the model drying body primarily depends on the available experimental setup.

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