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AN INVERSE METHOD FOR DRYING AT HIGH MASS TRANSFER BIOT NUMBER

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ABSTRACT

The inverse problem of using temperature measurements to estimate the moisture content and temperature-dependent moisture diffusivity together with the heat and mass transfer coefficients is analyzed in this paper. In the convective drying practice, usually the mass transfer Biot number is very high and the heat transfer Biot number is very small. This leads to a very small temperature sensitivity coefficient with respect to the mass transfer coefficient when compared to the temperature sensitivity coefficient with respect to the heat transfer coefficient. Under these conditions the relative error of the estimated mass transfer coefficient is high. To overcome this problem, in this paper the mass transfer coefficient is related to the heat transfer coefficient through the analogy between the heat and mass transfer processes in the boundary layer. The resulting parameter estimation problem is then solved by using a hybrid constrained optimization algorithm OPTRAN.

INTRODUCTION

Inverse approach to parameter estimation in last few decades has become widely used in various scientific disciplines. This paper deals with the application of the inverse approaches in drying.

Drying is a complex process of simultaneous heat and moisture transport within material and from its surface to the surroundings caused by a number of mechanisms. There are several different methods of describing the complex simultaneous heat and moisture transport processes within

drying material. In the approach initially proposed by Philip and De Vries [1] and Luikov [2] the moisture and temperature fields in the drying body are described by a system of two coupled partial differential equations. Strictly speaking, besides the temperature and water content, the gaseous pressure should be used as an independent variable. The assumption of a uniform gaseous pressure has been widely accepted for a variety of specific applications [3, 4]. The system of equations incorporates coefficients that are functions of temperature and moisture content and is non-linear. For some applications the non-linear system of two coupled partial differential equations have been used [4-6], but, for many practical calculations, the influence of the temperature and moisture content on all the transport coefficients has been neglected and the system of linear equations has been used [3, 7-9].

For many drying processes, the influence of the thermo-diffusion is small and can be ignored. In this case, the Luikov's moisture transport equation is the same as the Fick's second law equation, where concentration has been converted to moisture content on a dry basis.

The moisture diffusivity has the same meaning in both of these approaches. It accounts for various types of possible drying processes including molecular (liquid) diffusion, vapor diffusion, surface diffusion, hydrodynamic flow, Knudsen flow, and other considerations. An effective moisture diffusivity, which lumps all possible moisture transport mechanisms into a single measurable parameter, is often used to characterize the drying behavior regardless of the dominating mechanism [10]. The moisture diffusivity dependence on moisture content and temperature exerts a strong influence on the drying process calculation. This effect cannot be ignored for the majority of practical cases.

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All the coefficients except for the moisture diffusivity can be relatively easily determined by experiments [11, 12]. A number of methods for the experimental determination of the moisture diffusivity exist [13] such as: sorption kinetics methods, permeation methods, concentration-distance methods, drying methods, radiotracer methods, and methods based on the techniques of electron spin resonance and nuclear magnetic resonance.

However, there is no standard method for the experimental determination of the moisture diffusivity. The adoption of a generalized method for moisture diffusivity estimation would be of great importance, although this does not seem probable in the near future [14].

The application of the moisture diffusivity estimation methods based on the experimental drying curves in relation to the analytical solution of the differential diffusion equation seems to be the most popular experimental practice [10, 15-19]. Numerical solutions of the Fick's law differential diffusion equation with constant [20] or moisture and temperature dependant [15] diffusivity also have been used for the moisture diffusivity estimation.

The main problem in the moisture diffusivity determination by classical or inverse methods is 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 the drying) are complex and have low accuracy.

Kanevce, Kanevce and Dulikravich [21-24] and Dantas, Orlande and Cotta [25, 26] recently analyzed application of inverse approaches to estimation of drying body parameters. The main idea in this method is to take advantage of the interrelation 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 accurate and easy-to-perform thermocouple temperature measurements by using an inverse approach. We analyzed this idea of the drying body parameters' estimation by using temperature response of a body exposed to convective drying. An analysis of the influence of the drying air parameters and the drying body dimensions was conducted. In order to perform this analysis, the sensitivity coefficients and the sensitivity matrix determinant were calculated.

In the convective drying practice, usually the mass transfer Biot number is very high and the heat transfer Biot number is very small due to the low moisture diffusivity value relative to the thermal conductivity for most of the moist materials. This leads to a very small temperature sensitivity coefficient with respect to the mass transfer coefficient relative to the temperature sensitivity coefficient with respect to the heat transfer coefficient. This indicates that in these cases the mass transfer coefficient cannot be estimated simultaneously with the heat transfer coefficient with sufficient accuracy.

To overcome this problem, in this paper the mass transfer coefficient is related to the heat transfer coefficient through the analogy between the heat and mass transfer processes in the boundary layer.

The objective of this paper is an analysis of the possibility of simultaneous estimation of the thermophysical properties of a drying body and the heat and mass transfer coefficients at high mass transfer Biot number on the bases of temperature measurements by using a hybrid optimization algorithm [27] instead of a more standard Levenberg-Marquardt method [28].

NOMENCLATURE

a = water activity, -
c = heat capacity, $J K^{-1} kg^{-1} db$
C = concentration of water vapor in air, $kg\ m^{-3}$
D = moisture diffusivity, m^2/s
e = RMS error, ^0C
Gu = Gukhman number, -
h = heat transfer coefficient, $W\ m^{-2}\ K^{-1}$
h_D = mass transfer coefficient, $m\ s^{-1}$
ΔH = latent heat of vaporization, $J\ kg^{-1}$
I = identity matrix
j_m = mass flux, $kg\ m^{-2}\ s^{-1}$
j_q = heat flux, $W\ m^{-2}$
J = sensitivity matrix
κ = thermal conductivity, $W\ m^{-1}\ K^{-1}$
L = flat plate thickness, m
p_s = saturation pressure , Pa
P = vector of unknown parameters
Pr = Prandtl number, -
R = gas constant, $J\ kg^{-1}\ K^{-1}$
Re = Reynolds number, -
Sc = Schmidt number, -
t = time, s
T = temperature, ^0C
T_K = temperature, K
T = vector of estimated temperature, ^0C
V = velocity, $m\ s^{-1}$
x = distance from the mid-plane, m
X = moisture content (dry basis), $kg\ kg^{-1}\ db$
Y = vector of measured temperature, ^0C

Greek letters

δ = thermo-gradient coefficient, K^{-1}
ε = phase conversion factor, -
ε = relative error, %
σ = standard deviation, ^0C
μ = damping parameter, -
ρ = density, $kg\ m^{-3}$
φ = relative humidity, -

Subscripts

db = dry base
a = drying air
s = dry solid
wv = water vapor.

MATHEMATICAL MODEL OF DRYING

In the case of an infinite flat plate of thickness $2L$, 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

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

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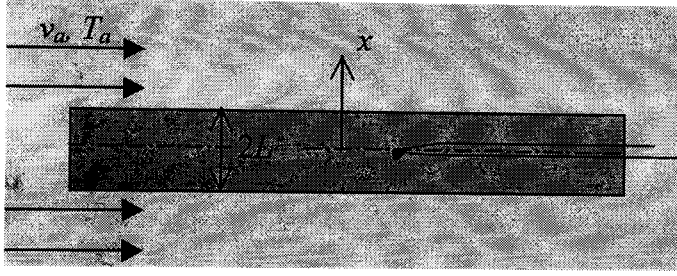

Figure 1. Scheme of the drying experiment.

Here, t, x, c, k, ΔH, ε, δ, D, ρ_s are time, distance from the mid-plane of the plate, heat capacity, 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 the dry plate material, respectively.

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

$$t = 0 \quad T(x,0) = T_0, \quad X(x,0) = X_0 \qquad (3)$$

In the convective drying experiment (Fig. 1) the surfaces of the drying body are in contact with the drying air thus resulting in a convective boundary conditions for both the temperature and the moisture content

$$-k\left(\frac{\partial T}{\partial x}\right)_{x=L} + j_q - \Delta H(1-\varepsilon)j_m = 0 \qquad (4)$$

$$D\rho_s\left(\frac{\partial X}{\partial x}\right)_{x=L} + D\delta\rho_s\left(\frac{\partial T}{\partial x}\right)_{x=L} + j_m = 0$$

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

$$j_q = h\left(T_a - T_{x=L}\right)$$

$$(5)$$

$$j_m = h_D\left(C_{x=L} - C_a\right)$$

where h is the convection heat transfer coefficient and h_D is the mass transfer coefficient, while T_a is the drying air bulk temperature.

The convection heat and mass transfer coefficients can be expressed by the Nesterenko's relations [1] for the heat and mass Nusselt numbers in drying conditions

$$Nu = 0.0270\,Pr^{0.33}\,Re^{0.9}\,Gu^{0.175} \qquad (6)$$

$$Nu_D = 0.0248\,Sc^{0.33}\,Re^{0.9}\,Gu^{0.135} \qquad (7)$$

where Pr, Sc, Re, Gu are Prandtl, Schmidt, Reynolds, and Gukhman number, respectively. The Gukhman number

$$Gu = \frac{T_{K,a} - T_{K,x=L}}{T_{K,a}} \qquad (8)$$

may be regarded as a criterion for entrainment – evaporation [29].

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

$$C_a = \frac{\varphi\, p_s(T_a)}{R_{wv}\, T_{K,a}} \qquad (9)$$

where 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 by

$$C_{x=L} = \frac{a(T_{x=L}, X_{x=L})\, p_s(T_{x=L})}{R_{wv}\, T_{K,x=L}} \qquad (10)$$

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 problem is symmetrical, and boundary conditions on the mid-plane of the plate ($x = 0$) are

$$\left(\frac{\partial T}{\partial x}\right)_{x=0} = 0, \quad \left(\frac{\partial X}{\partial x}\right)_{x=0} = 0 \qquad (11)$$

In order to approximate the solution of Eqs. (1, 2), an explicit finite-difference procedure has been used [6]. The nonlinear term has been expanded to

$$\frac{\partial}{\partial x}\left(D\frac{\partial X}{\partial x}\right) = D\frac{\partial^2 X}{\partial x^2} + \frac{\partial D}{\partial x}\frac{\partial X}{\partial x} \qquad (12)$$

The derivatives with respect to time have been represented using forward differencing at the grid point (i,j). All first- and second-order space derivatives have been approximated at time level (j) using central differencing. The moisture diffusivity, D, in the first term of Eq. (12) has been assigned its value at the grid point (i,j). Central differencing has been also applied to the boundary conditions space derivatives. The number of the space grid points was 61 in all the drying process calculation schemes.

ESTIMATION OF PARAMETERS

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

$$\mathbf{E}(\mathbf{P}) = [\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T[\mathbf{Y} - \mathbf{T}(\mathbf{P})] \qquad (13)$$

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

Application of the hybrid optimization algorithm OPTRAN and the Levenberg-Marquardt method has been analyzed for the solution of the presented parameter estimation problem.

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The Levenberg-Marquardt method belongs to a general class of damped least square methods [28, 30, 31]. The solution for vector $\mathbf{P}$ is achieved using the following iterative procedure

$$\mathbf{P}^{r+1} = \mathbf{P}^r + [(\mathbf{J}^r)^T \mathbf{J}^r + \mu^r \mathbf{I}]^{-1} (\mathbf{J}^r)^T [\mathbf{Y} - \mathbf{T}(\mathbf{P}^r)] \quad (14)$$

where r is the number of iterations, $\mathbf{I}$ is identity matrix, μ is the damping parameter, and $\mathbf{J}$ is the sensitivity matrix defined as

$$\mathbf{J} = \begin{bmatrix} \dfrac{\partial T_1}{\partial P_1} & \cdots & \dfrac{\partial T_1}{\partial P_N} \\ \cdot & & \\ \dfrac{\partial T_{i\,max}}{\partial P_1} & \cdots & \dfrac{\partial T_{i\,max}}{\partial P_N} \end{bmatrix} \quad (15)$$

The presented iterative procedure stops if the norm of gradient of $\mathbf{E}$ ($\mathbf{P}$) is sufficiently small, if the ratio of the norm of gradient of $\mathbf{E}$ ($\mathbf{P}$) to the $\mathbf{E}$ ($\mathbf{P}$) is small enough, or if the changes in the vector of parameters are very small.

This new hybrid optimization program OPTRAN [27] incorporates six of the most popular optimization algorithms: the Davidon-Fletcher-Powell gradient search [32], sequential quadratic programming (SQP) algorithm [33], Pshenichny-Danilin quasi-Newtonian algorithm [34], a modified Nelder-Mead (NM) simplex algorithm [35], a genetic algorithm (GA) [36], and a differential evolution (DE) algorithm [37]. Each algorithm provides a unique approach to optimization with varying degrees of convergence, reliability and robustness at different stages during the iterative optimization procedure. The hybrid optimizer OPTRAN includes a set of rules and switching criteria to automatically switch back and forth among 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 optimization process proceeded, the population evolved towards global minimum. The optimization 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 optimization 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 DISCUSSION

The proposed method of the moisture diffusivity estimation by temperature response of a drying body was tested for a model material that was a mixture of bentonite and quartz sand with known thermophysical properties [6]. From the experimental and numerical examinations of the transient moisture and temperature profiles [6] it was concluded that for the calculations in this study, the influence of the thermal diffusion is small and can be ignored. It was also concluded that the Luikov's system of two simultaneous partial differential equations could be used. In this case, the transport

coefficients can be treated as constants except for the moisture diffusivity.

The appropriate mean values for the model material are:

Density of the dry solid, $\rho_s = 1738$ kg m^{-3},
Heat capacity, $c = 1550$ J K^{-1} kg^{-1} db,
Thermal conductivity, $k = 2.06$ W m^{-1} K^{-1},
Latent heat of vaporization, $\Delta H = 2.31 \cdot 10^6$ J kg^{-1},
Phase conversion factor, $\varepsilon = 0.5$, and
Thermo-gradient coefficient, $\delta = 0$.

The following expression can describe the experimentally obtained relationship for the moisture diffusivity.

$$D = 9.0 \cdot 10^{-12} X^{-2} \left(\frac{T_K}{303} \right)^{10} \quad (16)$$

The experimentally obtained desorption isotherm of the model material is presented by the empirical equation

$$a = 1 - \exp(-1.5 \cdot 10^6 T_K^{-0.91} X^{(-0.005 T_K + 3.91)}) \quad (17)$$

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

For the direct (analysis) problem solution, the system of equations Eq. (1) and Eq. (2) with the initial conditions Eq. (3) and the boundary conditions Eq. (4) and Eq. (11) was solved numerically with the experimentally determined thermo physical properties.

For the inverse (ill-posed) problem investigated in this paper, values of the moisture diffusivity, D, and, heat and mass transfer coefficients, h and h_D, are regarded as unknown. All other quantities appearing in the direct problem formulation were assumed to be known. The moisture diffusivity of the model material has been represented by the following function of temperature and moisture content

$$D = D_X X^{-2} \left(\frac{T_K}{303} \right)^{D_T} \quad (18)$$

where D_X and D_T are constants.

Thus, the vector of unknown parameters is

$$\mathbf{P}^T = [D_X, D_T, h, h_D] \quad (19)$$

For the estimation of these unknown parameters, the transient readings of a single temperature sensor located in the mid-plane of the sample were considered (Fig. 1.). The simulated 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 measurements, a normally distributed error with zero mean and standard deviation, σ of 1.5 °C was added to the numerical temperature response (Fig. 2.).

The sensitivity coefficients analysis was carried out for a plate of thickness $2L = 4$ mm, with initial moisture content of $X(x, 0) = 0.20$ kg/kg and initial temperature $T(x, 0) = 20$°C. Following the conclusions of the previous works [3, 4, 5] the drying air bulk temperature of $T_a = 80$ °C, and drying air speed of $V_a, = 10$ m/s, have been chosen. The relative humidity of the drying air was $\varphi = 0.12$.

Figure 3 shows the relative sensitivity coefficients $P_m \partial T_i / \partial P_m$, i = 1, 2,..., 100, for temperature with respect to all unknown parameters, D_X, D_T, h, h_D (m = 1, 2, 3, 4).

It can be seen that the temperature sensitivity coefficient with respect to the convection mass transfer coefficient h_D is very small relatively to the temperature sensitivity coefficient with respect to the convection heat transfer coefficient h.
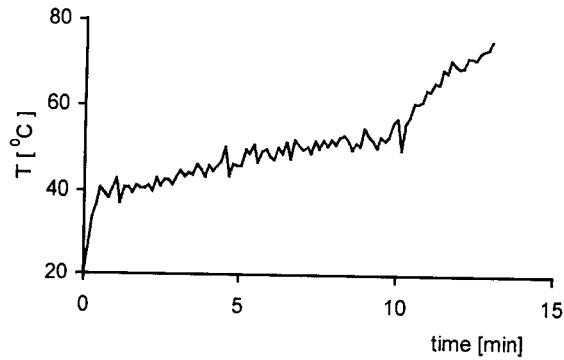

Figure 2. Simulated temperature response at x=0.

The very high mass transfer Biot number and the very small heat transfer Biot number can explain this. The heat transfer Biot number is 0.08. The mass transfer Biot number ranged from 200 to $1 \cdot 10^6$ and changed during the drying with local moisture content and temperature change.
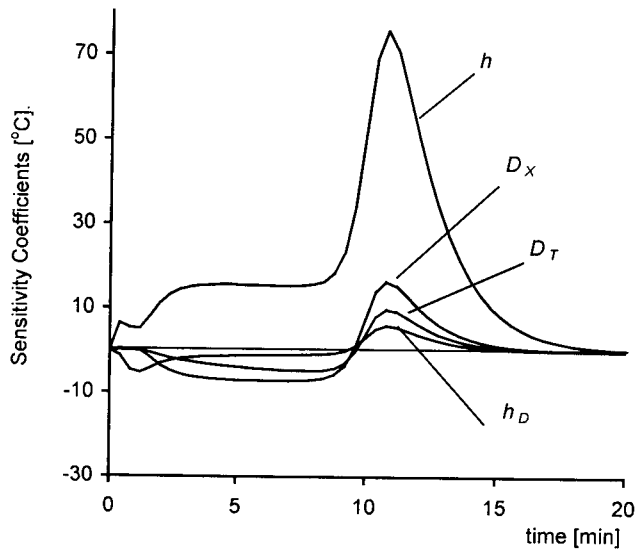

Figure 3. Relative sensitivity coefficients for the convective drying experiment.

Figure 4 presents transient variation of the determinant of the information matrix if four, (D_X, D_T, h, h_D) and three (D_X, D_T, h) parameters are simultaneously considered as unknown. Elements of this sensitivity determinant were defined [31] for a large, but fixed number of transient temperature measurements (100 in these cases). The duration of the simulated drying

experiment (the drying time) corresponding to the maximum determinant value was used for the computation of the unknown parameters.
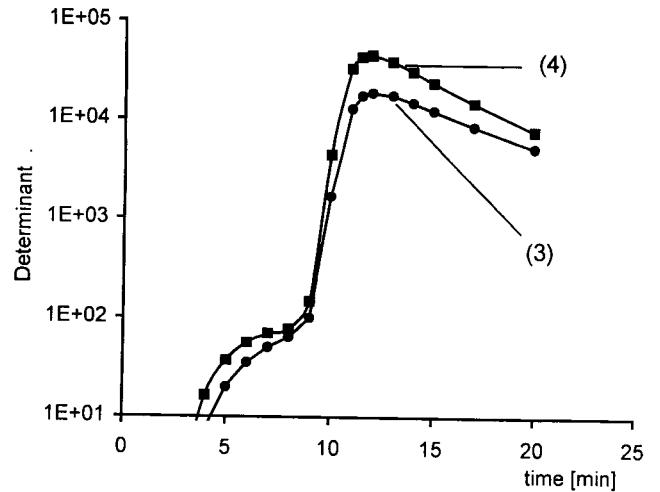

Figure 4. Determinant of the information matrix.

Table 1 shows the computationally obtained results. For comparison, the exact values of parameters are shown in the bottom row. The relative errors of the estimated parameters, ε, as well as the RMS errors, e, are also shown in the table. The RMS error is defined as

$$e = \sqrt{\frac{E(P_{est})}{i\,\max}} \qquad (20)$$

where P_{est} is the vector of estimated parameters.

Table 1. Estimated parameters ($\sigma = 1.5\ ^\circ C$)

Case		$D_X 10^{12}$ [m²/s]	D_T [-]	h [W/m² K]	$h_D \cdot 10^2$ [m/s]	e [°C]
P3	Initial	0.5	5.0	50.0		
	Estimated	8.93	9.95	83.03		1.49
	$|\varepsilon|$ [%]	0.83	0.54	0.09		
P4a	Initial	0.5	5.0	50.0	5.0	
	Est. OPTRAN	9.87	8.79	83.17	8.28	1.48
	$|\varepsilon|$ [%]	9.61	12.08	0.08	10.87	
	Estimated LM	3.37	1.01	49.9	6.16	5.42
	$|\varepsilon|$ [%]	62.6	89.9	39.9	33.7	
P4b	Initial	9.87	8.79	83.17	8.28	
	Estimated	8.89	10.02	83.02	9.28	1.49
	$|\varepsilon|$ [%]	1.27	0.24	0.09	0.09	
	Exact values	9.00	10.0	83.1	9.29	

From the obtained results in the case P3, it appears to be possible to estimate simultaneously the moisture diffusivity parameters, D_X and D_T, and the convection heat transfer

coefficient, h, by a single thermocouple temperature response with the relatively high noise of 1.5 $^{\circ}$C, by using OPTRAN algorithm as well as the Levenberg-Marquardt method.

However, in the case of simultaneous estimation of the moisture diffusivity parameters, D_X and D_T, and the convection heat and mass transfer coefficients, h and h_D (case P4a) local minimum has been obtained with the Levenberg-Marquardt (LM) method.

On the other hand, when using the hybrid optimization algorithm OPTRAN the solutions do not depend on the initial guesses and the global minimum has been obtained.

Even when using a superior optimization algorithm like OPTRAN, the accuracy of computing parameters is small. The very small values of the relative sensitivity coefficient with respect to the mass transfer coefficient (Fig. 3.) can explain this. To overcome this problem, in this paper the mass transfer coefficient was related to the heat transfer coefficient through Eqs. (6) and (7), obtained from the analogy between the heat and mass transfer processes in the boundary layer over the drying body. From Eqs. (6) and (7), with accuracy within one percent, following relationship can be obtained

$$h_D = 0.95 \frac{D_a}{k_a} h \qquad (21)$$

where D_a and k_a are 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 with the moisture diffusivity parameters with high accuracy (case P4b in Table 1).

CONCLUSIONS

An analysis of the possibility of simultaneous estimation of the thermophysical properties of a drying body and the heat and mass transfer coefficients at high mass transfer Biot number by using only temperature measurements was presented. By using an interrelation between the heat and mass transfer coefficients, they were simultaneously estimated with the two moisture diffusivity parameters with high accuracy. Application of the hybrid optimization algorithm OPTRAN has been analyzed for the solution of the presented parameter estimation problem.

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