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**MOISTURE DIFFUSIVITY ESTIMATION BY TEMPERATURE RESPONSE OF A
DRYING BODY**

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ABSTRACT

The paper presents a method for the moisture diffusivity estimation from experimentally measured temperature response of a drying body by using inverse approach. The mathematical model of drying and the numerical procedure for solution of direct drying problem are given. The Levenberg-Marquardt method is used for estimation of the moisture content and temperature dependent moisture diffusivity. Experiments using numerically simulated temperature data are presented to verify the applicability of the method. Good agreement between the exact and estimated parameter values were obtained.

KEYWORDS

Parameter estimation, drying, moisture diffusivity, inverse approach

INTRODUCTION

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 drying process, but there is no single theory for wet material drying prediction, which encompasses all transfer mechanisms. In the approach proposed by Luikov [5] based on the concepts of irreversible thermodynamics the moisture and temperature fields in the dried body are described by a system of two coupled partial differential equations. The system of equations incorporates coefficients which are functions of temperature and moisture content. These coefficients must be determined experimentally. For practical calculations, the influence of the temperature and moisture content on all the transport coefficients except for the moisture diffusivity is small and can be neglected. The moisture diffusivity dependence on moisture and temperature exerts a strong influence on the drying process calculation. This effect can not be ignored for the most of practical cases. 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 work 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 surroundings. The objective is the development of a method of the moisture diffusivity estimation on the basis of a temperature response by using inverse approach. Local moisture content measurements are practically unfeasible especially for small drying objects. Standard drying curves (body mean moisture content during the drying) are complex and of low accuracy. In this paper, a substitute method is proposed that is based on easy and accurate temperature measurements. The temperature response during convective drying is obtained by numerical experiments. As a representative drying body, a mixture of bentonite and quartz sand with known thermophysical properties has been chosen.

MATHEMATICAL MODEL OF DRYING

In the case of an infinite flat plate of thickness $2L$, if the shrinkage of the material during drying can be neglected ($\rho_s = \text{const}$), the resulting system of equations for the temperature, $T(x, t)$, and moisture content, $X(x, t)$, can be expressed as

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

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

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

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

The boundary conditions on the free plate surface ($x = L$) are:

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

In the case of convective drying of the sample, the convective heat flux, $j_q(t)$, and mass flux, $j_m(t)$, on the surface of evaporation are:

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

where h is the heat convection and h_D the mass transfer coefficient, T_a is the drying air bulk temperature, and C_a is the concentration of water vapor in the drying air. The water vapor concentration of the air in equilibrium with the free surface of the body is calculated by

$$C_{x=L} = \varphi(T_{x=L}, X_{x=L}) \cdot p_s(T_{x=L}) / 461.9 / (T_{x=L} + 273) \quad (6)$$

where p_s is the saturation pressure and φ is the relative humidity. The relative humidity of the air in equilibrium with the sample at the surface temperature and moisture content is calculated from the experimental water sorption isotherms.

The problem is symmetrical, and boundary conditions on the axis of the plate are:

$$\left(\frac{\partial T}{\partial x} \right)_{x=0} = 0, \quad \left(\frac{\partial X}{\partial x} \right)_{x=0} = 0 \quad (7)$$

THE DRYING BODY PROPERTIES

The presented idea of the moisture diffusivity estimation by temperature response of a drying body has been tested for a model material, a mixture of bentonite and quartz [4]. From the experimental and numerical examinations of the transient moisture and temperature profiles [3] it was concluded that for practical calculations, the influence of the thermal diffusion is small and can be ignored. It was also concluded that the Luikov's system of simultaneous partial differential equations could be used by treating of the transport coefficients as constants except for the moisture diffusivity. The appropriate mean values for the model material are: the density of dry solid, $\rho_s = 1738 \text{ kg/m}^3$, heat capacity, $c = 1550 \text{ J/(kgK)}$, thermal conductivity, $k = 2.06 \text{ W/(mK)}$, latent heat of vaporization, $\Delta H = 2.31 \cdot 10^6 \text{ J/kg}$, ratio of water evaporation rate to the reduction rate of the moisture content, $\epsilon = 0.5$, thermo-gradient coefficient, $\delta = 0.0$. The following expression can describe the experimentally obtained relationship for the moisture diffusivity [4].

$$D = 9.0 \cdot 10^{-12} \cdot X^{-2} \cdot \left(\frac{T + 273}{303} \right)^{10} \quad (8)$$

The dependence of desorption isotherms of the model material on temperature and moisture content is [2]:

$$\varphi = 1. - \exp(-1.5 \cdot 10^6 \cdot (T + 273)^{-0.91} \cdot X^{(-0.005 \cdot (T+273)+3.91)}) \quad (9)$$

where φ is the relative humidity of the air in equilibrium with the sample at temperature T and moisture content X .

NUMERICAL DRYING EXPERIMENTS

The drying experiments have been carried out numerically. The system of equations (1) and (2) with the initial (3) and the boundary conditions (4) and (7) has been solved with the

experimentally determined thermophysical properties. In order to approximate the solution of the equations (1) to (7), an explicit numerical integration procedure was used. The nonlinear term has been expanded to

$$\frac{\partial}{\partial x} \left(D \frac{\partial X}{\partial x} \right) = D \frac{\partial^2 X}{\partial x^2} + \frac{\partial D}{\partial x} \frac{\partial X}{\partial x} \quad (10)$$

The derivatives with respect to time have been represented by forward difference form at the grid-point (i,j). All first and second derivatives in space have been approximated at time level (j) by central difference forms. The moisture diffusivity, D, in the first term of (10) has been assigned its value at the grid point (i,j). The applied procedure leads to the difference equations

$$X_{i,j+1} = (R_D - R_{\Delta D}) X_{i-1,j} + (1 - 2R_D) X_{i,j} + (R_D + R_{\Delta D}) X_{i+1,j} \quad (11)$$

$$T_{i,j+1} = R_\alpha T_{i-1,j} + (1 - 2R_\alpha) T_{i,j} + R_\alpha T_{i+1,j} + \frac{\varepsilon \Delta H}{c} (X_{i,j+1} - X_{i,j}) \quad (12)$$

where

$$R_D = \frac{\Delta t}{(\Delta x)^2} D_{i,j}; \quad R_{\Delta D} = \frac{\Delta t}{(\Delta x)^2} \frac{D_{i+1,j} - D_{i-1,j}}{4} \quad (13)$$

and

$$R_\alpha = \frac{\Delta t}{(\Delta x)^2} \alpha. \quad (14)$$

Thermal diffusivity has been calculated as $\alpha = k/(c\rho_s)$.

In order to approximate the boundary conditions, central difference form has been applied to the grid points (1,j) and (M,j) that lie on the boundaries $x = 0$ and $x = L$, respectively.

A sufficient condition for the numerical stability of this simple explicit method is that the values of the ratios R_D and R_α are less or equal to 0.5. The computations were performed with the time increment, Δt , corresponding to the value of 0.4 for R_D and R_α . While R_α is a constant, R_D varies with the moisture diffusivity. At most of the grid-points (i,j), R_α was below 0.01.

The numerical drying experiments have been carried out for the plate of thickness $2L = 3.0$ mm, with initial moisture content of $X(x, 0) = 0.2$ kg/kg and initial temperature $T(x,0) = 20.0$ °C. The drying air bulk temperature was $T_a = 80.0$ °C and the relative humidity was $\varepsilon = 0.12$. The convection heat transfer coefficient was $h = 45.1$ W/(m²K) and the mass transfer coefficient was $h_D = 4.87 \cdot 10^{-2}$ m/s. Satisfactory accuracy was achieved with $M = 41$ grid points.

Figure 3 shows the volume-averaged moisture \bar{X} and temperature \bar{T} changes during drying as well as the drying rate $|d\bar{X}/dt|$ or mass flux, $j_m(t) = -\rho_s L d\bar{X}/dt$.

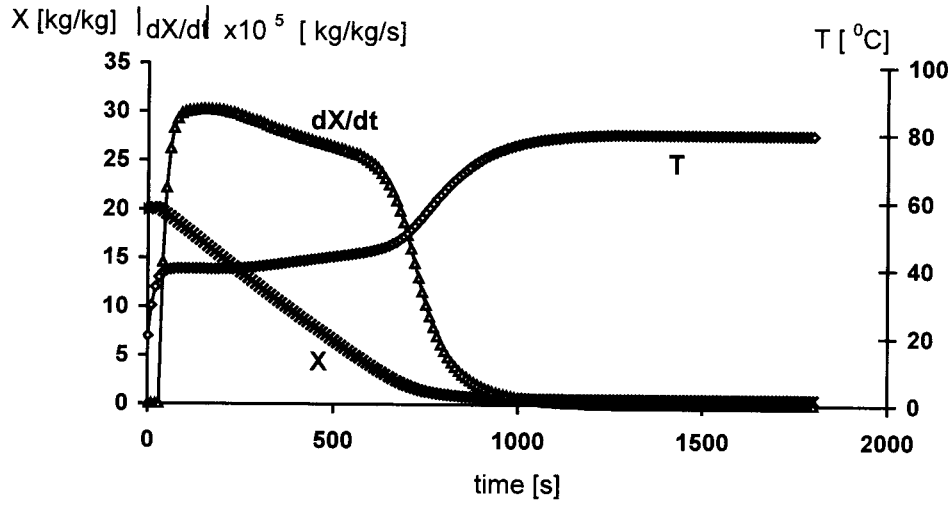


Fig. 3. Predicted moisture, temperature, and drying rate curves

MOISTURE DIFFUSIVITY ESTIMATION

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

$$E(P) = [Y - T(P)]^T [Y - T(P)] \quad (15)$$

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

A version of Levenberg-Marquardt method was applied for the solution of the presented parameter estimation problem [6]. This method is quite stable, powerful, and straightforward and has been applied to a variety of inverse problems [7]. It belongs to a general class of damped least square methods [1]. The solution for P is achieved using the following iterative procedure

$$P^{r+1} = P^r + [(J^r)^T J^r + \mu^r I]^{-1} (J^r)^T [Y - T(P^r)] \quad (16)$$

where I is identity matrix, μ is damping parameter, and J represents the sensitivity matrix defined as:

$$J = \begin{bmatrix} \frac{\partial T_1}{\partial P_1} & \frac{\partial T_1}{\partial P_2} & \cdots & \frac{\partial T_1}{\partial P_N} \\ \frac{\partial T_2}{\partial P_1} & \frac{\partial T_2}{\partial P_2} & \cdots & \frac{\partial T_2}{\partial P_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial T_i}{\partial P_1} & \frac{\partial T_i}{\partial P_2} & \cdots & \frac{\partial T_i}{\partial P_N} \end{bmatrix} \quad (17)$$

The term μI damps instabilities due to the ill-conditioned character of the problem. Near the initial guess, the problem is generally ill-conditioned and damping parameter is chosen large making term μI large as compared to term $J^T J$. Therefore, the matrix $J^T J$ is not required to be non-singular at the beginning of iterations when the procedure tends towards a steepest descent method. As the iteration process approaches the converged solution, the damping parameter decreases, and the Levenberg-Marquardt method tends towards Gauss method [1,7]. In fact, this method compromises between the steepest descent and Gauss method 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 [8].

RESULTS AND DISCUSSION

For the various drying materials, including the model material considered here, the moisture diffusivity could be represented by the following function of temperature and moisture content

$$D = \frac{D_1}{D_2 + X^2} \cdot \left(\frac{T + 273}{303} \right)^{10} \quad (18)$$

where D_1 and D_2 are constants. For the inverse problem investigated here, values of D_1 and D_2 are regarded as unknown and all other quantities involved in direct problem formulation were assumed to be known. Thus, $P^T = [D_1, D_2]$.

Numerical experiments have been conducted to verify the proposed method. Since the sample is very thin (3.0 mm), a single thermocouple has been located in the middle of the infinite flat plate. Two analyses of the simulated data have been considered. In the first analysis, parameters have been estimated using "exact" temperature data at the sensor location obtained by the solution of direct problem for the exact values of the parameters. Adding an error term to exact temperature response then simulated the data for the second analysis. The errors were additive and normally distributed with zero mean and a standard deviation $\sigma = 0.5$ °C generated by RANDN routine of the MATLAB program for normally distributed random numbers. The results obtained by applying the present method to the estimation of the unknown parameters for the case with exact data and the data with noise are shown in the Table 1.

Table 1. Performance of the method without and with the simulated measurement noise

	σ	D_1	D_2	RMS error	Iterations
Exact values	-	9.0×10^{-12}	0.	-	-
Values obtained with "exact" T data	0	9.0019×10^{-12}	$3.7796 \cdot 10^{-7}$	$4.3955 \cdot 10^{-4}$	21
Values obtained with added noise	0.5	9.0602×10^{-12}	$1.3277 \cdot 10^{-5}$	$4.6684 \cdot 10^{-1}$	14

It can be seen that a good agreement is achieved in both cases. The root mean squared difference between experimental and obtained values tends to zero in the first case and tends to standard deviation of measured temperature data in the second case. Figure 4 shows the residual. Normally distributed errors can be seen.

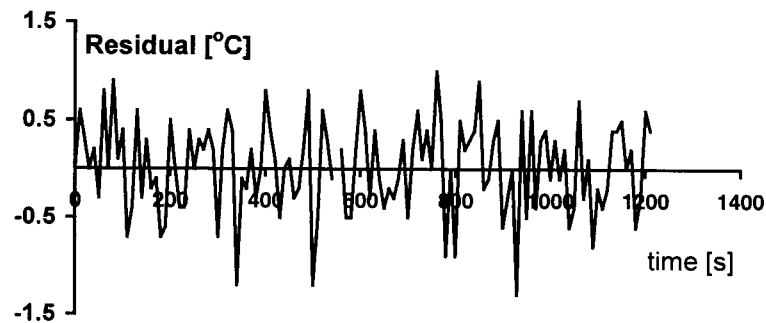


Fig. 4. The residual

The initial guess ($D_{1init} = 5.0 \cdot 10^{-11}$ and $D_{2init} = 0.1$) for both cases was the same and it was very far from the exact values of parameters in order to test the stability of the proposed method. Consequently, the number of iterations is high. Figure 5 shows the RMS changes and Figure 6 illustrates the approaching of parameters to the final values during iterative process for the case with the added noise.

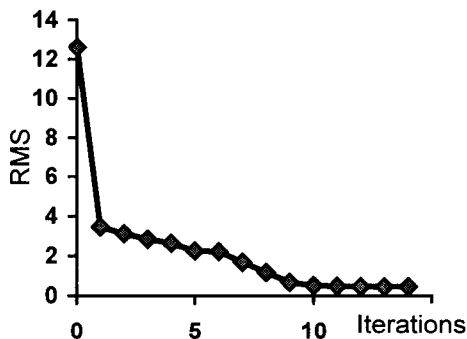


Fig. 5. RMS – Error

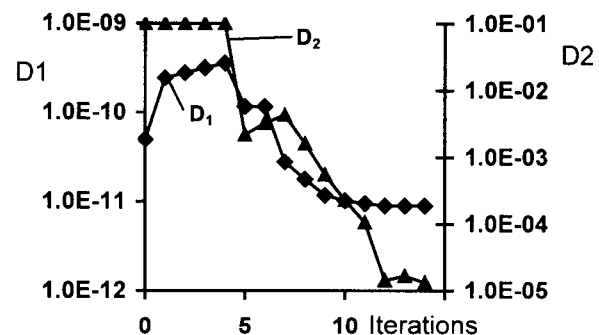


Fig. 6. Moisture diffusivity coefficient

Since the exact value of D_2 for model material equals zero and the performed analysis shows that the second parameter value is zero compared to the X^2 values in this case, the analysis with one parameter has been conducted also. The relation for moisture diffusivity (13) was used with $D_2 = 0.0$, and the parameter D_1 was evaluated by the same method. The similar results were obtained.

In order to investigate the influence of drying time, determinant of the sensitivity matrix $J^T J$ (Eq.17) with normalized elements

$$[J^T J]_{m,n} = \sum_{i=1}^I \left(P_m \frac{\partial T_i}{\partial P_m} \right) \left(P_n \frac{\partial T_i}{\partial P_n} \right), \quad m, n = 1, N \quad (19)$$

has been calculated. Figure 7 shows $|J^T J|$ for one parameter analysis for the entire drying time until the equilibrium temperature and moisture content of the body were reached. Figure 8 illustrates changes of the relative sensitivity coefficient during drying process.

$$J_{i,l} = P_l \frac{\partial T_i}{\partial P_l}, \quad i=1,2,\dots,I; \quad l=1,2,\dots,N \quad (20)$$

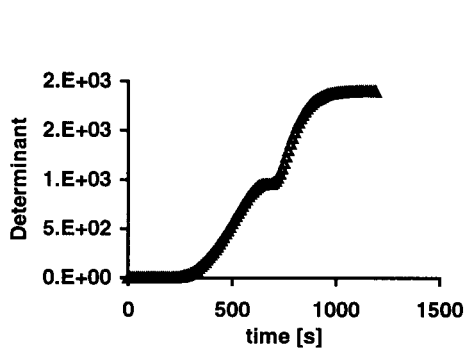


Fig. 7. Sensitivity determinant

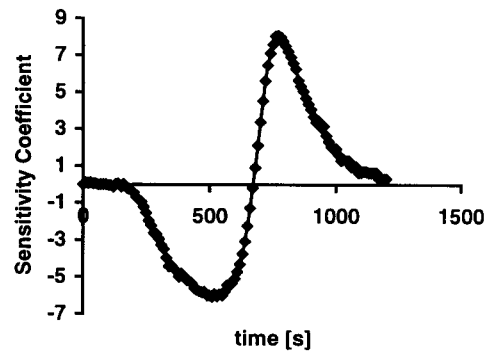


Fig. 8. Sensitivity coefficient

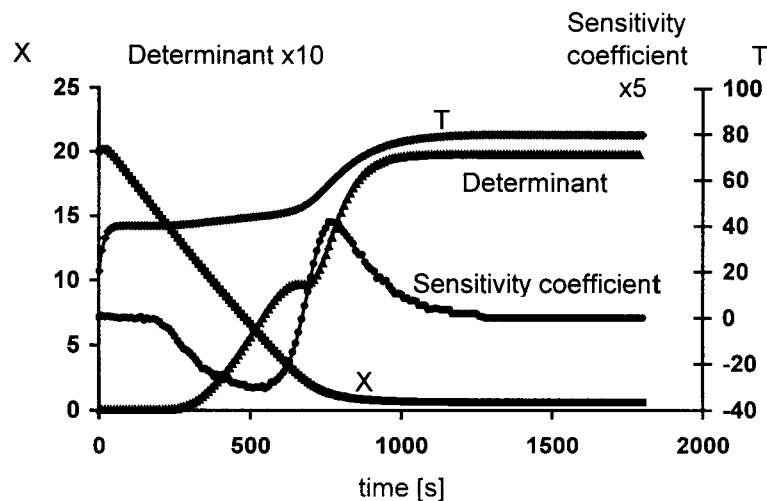


Fig. 9. Comparison of moisture, determinant, sensitivity coefficient, and temperature

Two plateaus can be seen on the presented curve. The first plateau corresponds to the moment (Fig. 9) when the body moisture content is nearly equal to the equilibrium. After this instant in time, rapid body temperature increase occurs associated with a rapid evaporation rate decrease. The second plateau corresponds to the moment when nearly equilibrium temperature has been reached. In all analyses presented here, drying time corresponding to the end of the first plateau (720 s) has been taken. For the drying times shorter than that, the problem is ill-posed and local minimum can be obtained depending on the initial guesses.

CONCLUSIONS

A method is presented for estimation of moisture diffusivity on the basis of temperature transient response of a drying body by using an inverse approach. The numerical procedure for solution of direct drying problem with appropriate convergence conditions was outlined. Numerical results for transient moisture content and temperature profiles as well as predicted moisture, temperature and drying rate curves are shown. The iterative Levenberg-Marquardt method is applied for evaluation of unknown constants in moisture diffusivity model of its dependence on moisture and temperature. The estimation method is demonstrated using data obtained from a simulation of the experimental design. The results of the numerical experiments, in the case with errorless measurements as well as with measurements containing random errors, show good agreement between evaluated and exact parameter values and confirm the validity of the proposed method. Conducted sensitivity analysis confirms that proper duration of drying experiment has been chosen.

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