DETERMINATION OF CROSS-COEFFICIENTS FOR COUPLED HEAT AND MASS TRANSPORT IN POROUS MEDIA

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Abstract

Determining the moisture dependent cross transport coefficients based on the solution of the inverse problem of the parameter estimation involving coupled heat and mass transfer in porous media, is presented. The parameter estimation problem is solved with Levenberg-Marquardt's method of minimization of the least-squares norm by using a set of temperature measurements at two sensor location inside the body. Moisture content measurement is not considered. The solution of the corresponding direct problem is obtained using control-volume approach with central-difference scheme.

Keywords: heat and moisture transfer, inverse problem, cross transport coefficients

1 Introduction

Heat and mass transfer in capillary porous media has practical applications in several different areas including, among others, drying and the study of moisture migration in soil and building materials. In building energy analysis, calculated heat conduction through walls usually neglects the storage and transport of moisture in the porous structure of the walls. However, walls are normally submitted to both thermal and moisture gradients, so that an accurate heat transfer determination requires a simultaneous calculation of both, sensible and latent effects. For the mathematical modelling of such phenomena, Luikov [1] has proposed his widely know formulation, based on system of coupled partial differential equations, which takes into account the cross effects: the temperature gradient is associated with moisture migration and the moisture gradient causes heat transfer.

The main difficulty in dealing with mathematical models based on the fundamental conservation principles is the need for the transport properties contained in the governing equations. This is especially true for the experimentally hard to determine internal mass transfer coefficients.

This paper deals with the method for determining moisture-dependent cross transfer coefficients for heat and moisture transfer in porous media, which is based on the solution of the inverse problem referred as parameter estimation. The solution of this inverse problem requires a finite set of temperature measurements taken inside the body and one assumes that the investigate moisture-temperature dependent coefficients belong to set polynomials. The effectiveness of inverse problem's solution is substantially dependent on the numerical realisation of the direct problem's solution. Here the control-volume method with central-difference scheme is used. Parameter estimation problem is fairly difficult, since the described equations are non-linear with respect to the unknown quantities. Therefore experiment is arranged where the specimen is designed in the simplest shape and the heat and moisture transport is chosen in a simple way, in order to make determining of the unknown coefficients as easy as possible. Articles dealing with the solution of inverse heat transfer problems are quite common in the literature nowadays. However, it is interesting to note that any fewer articles are available on the solution of inverse problems of coupled heat and mass transfer [2].

2 Formulation of the problem

The physical problem involves a one-dimensional capillary porous sample, initially at uniform temperature and uniform moisture content. One of the boundaries, which one is impervious to moisture, is in direct contact with heater. The other boundary is in contact with the dry surrounding air, thus resulting in a convection boundary condition for both the temperature and the moisture content.

The governing partial differential equations, for the modelling of such physical problem, were derived from conservation of mass and energy flow in a 1-D element volume of porous material by Luikov [1]. These are written as

$$\rho c_m(T,u)\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(\lambda(T,u)\frac{\partial T}{\partial x}\right)-l(T)\frac{\partial}{\partial x}\left(a_u(T,u)\frac{\partial u}{\partial x}\right) \tag{1}$$

$$\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}\left(D_u(T,u)\frac{\partial u}{\partial x}+D_T(T,u)\frac{\partial T}{\partial x}\right) \tag{2}$$

where T is temperature, u is volume basic moisture content, ρ is density solid matrix, c_m is specific heat of sample, λ is thermal conductivity of sample, ρ_m is the water density, l is latent heat of vaporization, D_u is moisture transport coefficient associated to moisture content gradient, D_T and a_u are transport cross coefficients.

Boundary conditions are expressed as follows

$$\left(\lambda(T,u)\frac{\partial T}{\partial x}\right)_{x=0}=-q(t) \qquad \text{for } t>0 \tag{3}$$

$$\left(D_u(T,u)\frac{\partial u}{\partial x}+D_T(T,u)\frac{\partial T}{\partial x}\right)_{x=0}=0 \qquad \text{for } t>0 \tag{4}$$

$$\left(\lambda(T,u)\frac{\partial T}{\partial x}\right)_{x=L}+\left(l(T)a_u(T,u)\frac{\partial u}{\partial x}\right)_{x=L} \qquad \text{for } t>0 \tag{5}$$
$$=h(T_\infty-T_{x=L})+l(T)h_m(u_\infty-u_{x=L})$$

$$\left(D_u(T,u)\frac{\partial u}{\partial x}+D_T(T,u)\frac{\partial T}{\partial x}\right)_{x=L}=\frac{h_m}{\rho_m}(u_\infty-u_{x=L}) \qquad \text{for } t>0 \tag{6}$$

where $h(T_\infty-T_{x=L})$ represents the heat exchanged with the ambient air and $h_m(u_\infty-u_{x=L})$ is the phase change energy term, h is surface conductance, h_m is mass convection coefficient.

Initial conditions are

$$T(x,0)=T_0 \qquad \text{at} \qquad x\in<0,L> \tag{7}$$

$u(x,0) = u_0 \quad \text{at} \quad x \in <0, L>$ (8)

Considering the temperature range of interest in building applications, temperature dependence of lime mortal cross transport coefficients is, here, neglected when compared to their moisture content dependence. The objective is to determine coefficients $D_T(u)$ and $a_u(u)$ as well as to calculate the temperature and moisture fields within the specimen under consideration.

3 Solution of the direct problem

The mathematical model (2) -(8) is discretized by using the control-volume method and the interpolation is realised by the central-difference scheme. The space element is defined by nodes x_{i-1}, x_i, x_{i+1} and $\Delta x_i = x_{i+1} - x_i$; similarly we discretize the time variable introducing time interval $\Delta t_k = t_{k+1} - t_k$.

For internal points, the governing equations are written as

$$\left(\rho_0 c_{k,i} \frac{\Delta x_i}{\Delta t_k} + \frac{\lambda_{k,i-1}}{\Delta x_{i-1}} + \frac{\lambda_{k,i+1}}{\Delta x_{i+1}}\right) T_{k,i} = \frac{\lambda_{k,i}}{\Delta x_{i-1}} T_{k.i-1} + \frac{\lambda_{k,i+1}}{\Delta x_{\mathrm{i+1}}} T_{k,i+1} + \rho_{\mathrm{o}} c_{k-,i} \frac{\Delta x_i}{\Delta t_{k-1}} T_{k-1,i} + \\ 1_{\mathrm{k\text{-}1,i\text{-}1}} \rho_l \left(\frac{D_{u,k-1,i-1}\left(u_{k-1,i-1} - u_{k-1,i}\right)}{\Delta x_{i-1}} - \frac{D_{u,k-1,i+1}\left(u_{k-1,i} - u_{k-1,i+1}\right)}{\Delta x_{i+1}}\right) \tag{9}$$

$$\left(\frac{\Delta x_i}{\Delta t_k} + \frac{D_{u,k,i-1}}{\Delta x_{i-1}} + \frac{D_{u,i+1}}{\Delta x_{i+1}}\right) u_{k,i} = \frac{D_{u,k.i-1}}{\Delta x_{i-1}} u_{k,i-1} + \frac{D_{u,k,i+1}}{\Delta x_{i+1}} + \frac{\Delta x}{\Delta t_{k-1}} u_{k-1,i} + \\ \left(\frac{D_{T,k-1,i-1}}{\Delta x_{i-1}}\left(T_{k-1,i-1} - T_{k-1,i}\right) - \frac{D_{T,k-1,i+1}}{\Delta x_{i+1}}\left(T_{k-1,i} - T_{k-1,i+1}\right)\right) \tag{10}$$

where $k = 0,1,2,...K$ refers to time step ($k = 0$ refers to the initial condition) and $i = 1,2,3,..., I+1$ refers to spatial grid points ($i = 1$ and $i = I+1$ refers to the boundaries). In the same way, boundary conditions are put in discrete form to obtain the following expressions for the half volume node at the boundaries ($x = 0$ and $x = L$)

$$\left(\rho_0 c_{k,i-1} \frac{\Delta x}{2\Delta t} + \frac{\lambda_{k,i-1}}{\Delta x} + \frac{L\rho_l D_{Tvk,i-1}}{\Delta x} + h\right) T_{k,0} = \left(\frac{\lambda_{k,i-1}}{\Delta x} + \frac{L\rho_l D_{Tv,i-1}}{\Delta x}\right) T_{k,1} + \\ \rho_{\mathrm{o}} c \frac{\Delta x}{2\Delta t} T_{k-1,0} + L\rho_l D_{uv,k,i-1}\left(\frac{u_{k-1,1} - u_{k-1,0}}{\Delta x}\right) + hT_\infty + Lh_m\left(\rho_{v,\infty} - \rho_{v,0}\right) \tag{11}$$

$$\left(\frac{\Delta x}{2\Delta t} + \frac{D_{u,k,i-1}}{\Delta x}\right) u_{k,0} = \frac{D_{u,k,i-1}}{\Delta x} u_{k,1} + \frac{\Delta x}{2\Delta t} u_{k-1,0} + D_{T,k,i-1}\left(\frac{T_{k-1,1} - T_{k-1.0}}{\Delta x}\right) \\ + \frac{h}{\rho_l}\left(\rho_{v,\infty} - \rho_{v,0}\right) \tag{12}$$

Equations (9) - (12) have the form

$$\mathrm{A}_{k,i} \cdot \psi_{k,i} = \mathrm{A}_{k,i-1} \cdot \psi_{k,i-1} + \mathrm{A}_{k,i+1} \cdot \Psi_{k,i+1} + \mathrm{A}_{k-1,i} \cdot \psi_{k,i+1} + D$$

where $D = \mathrm{A}_{k-1,i} \cdot \psi_{k-1,i} + B$ and ψ is a dependent variable (T or u).

The source term D contains non-linear functions of the dependent variables. As the solution method is iterative, the values calculated for T and u from the previous iteration are used for calculating the source terms in the above equations. Mass and energy conservation equations are as coupling terms always evaluated at a previous iteration.

4 Inversion procedure

For inverse problem of interest here, cross transport coefficients $D_T(u)$ and $a_u(u)$ are regarded as unknown quantities. For the determining of such quantities, we assuming that the functions $D_T(u)$ and $a_u(u)$ are taken as the polynomials

$$D_T(u) = D_0 + D_1 u + D_2 u^2 \tag{13}$$

$$a_u(u) = a_0 + a_1 u + a_2 u^2$$

and we consider available the transient temperature measurements Y_{km} taken at the locations x_m, $m = 1,2$; $\mathrm{x_m} \in (0, L)$. The subscript k refers to the time at which the measurements are taken. The temperature measurements contain random errors, but all the other quantities appearing in the formulation of the direct problem are supposed to by known exactly. The solution of the present parameter estimation problem is based on minimizing the least-squares norm. Such a norm can be written as

$$S(\mathbf{P}) = [\mathbf{Y} - T(\mathbf{P})]^{\mathrm{T}} [\mathbf{Y} - T(\mathbf{P})] \tag{14}$$

where $\mathbf{P} = [D_0, D_1, D_2, a_0, a_1, a_2]$ denotes the vector of unknown parameters. The superscript T above denotes transpose and $[\mathbf{Y} - T(\mathbf{P})]^{\mathrm{T}}$ is given by

$$[\mathbf{Y} - T(\mathbf{P})]^{\mathrm{T}} \equiv [(\vec{Y}_1 - \vec{T}_1), (\vec{Y}_2 - \vec{T}_2), \ldots, (\vec{Y}_K - \vec{T}_K)]$$

where $(\vec{Y}_k - \vec{T}_k)$ is a row vector containing the differences between the measured and estimated temperatures at the measurement positions x_m, $m = 1,2$, at time t_k, that is,

$$(\vec{Y}_k - \vec{T}_k) = [\vec{Y}_{k1} - \vec{T}_{k1}, \vec{Y}_{k2} - \vec{T}_{k2}]$$

The estimated temperatures T_{km} are obtained from the solution of the direct problem, at the measurement location x_m and time t_k, by using estimates for the unknown parameters $\mathbf{P}$. Here minimization of the least-squares norm $S(\mathbf{P})$ is solved with the Levenberg-Marquardt method [3]. The iterative procedure is given by

$$\mathbf{P}^{j+1} = \mathbf{P}^j + [(\mathbf{J}^j)^{\mathrm{T}} \mathbf{J}^j + \mu^j \Omega^j]^{-1} (\mathbf{J}^j)^{\mathrm{T}} [\mathbf{Y} - T(\mathbf{P}^j)]$$

where $\mathbf{J}$ is sensitivity matrix μ^j is a positive scalar named damping parameter, Ω^j is a diagonal matrix and the superscript j denotes the iteration number. The sensitivity matrix is defined as $\mathbf{J}(\mathbf{P}) \equiv \left[\frac{\partial T^{\mathrm{T}}(\mathbf{P})}{\partial \mathbf{P}} \right]^{\mathrm{T}}$. The subroutine OBCLSJ of the IMSL [2] was used in the present work.

The procedure is repeated until difference $\mathbf{Y} - T(\mathbf{P})$ is small enough and satisfied the criterion for terminating the minimizing process $\left\| \mathbf{P}^{j+1} - \mathbf{K}^{j} \right\| < \varepsilon$.

5 Results

The present parameter estimation problem is classified as non-linear, because the sensitivity coefficients are function of the unknown parameters. As results, the analysis of the sensitivity coefficient and of the determinant of the matrix $\mathbf{J}^{T}\mathbf{J}$ respectively is not global, that is, it is depend on the value chosen in advantage for unknown parameters. The design of optimum experiments is of capital importance in parameter estimations - this problem is beyond the scope of this contribution, but by following the same approach of reference [4], we consider the applied heat flux $q(t)$ to be in the form of a step function in time, that is, $q(t) = q_0$ for $0 < t < t_h$ and $q(t) = 0$ if $t > t_h$ (15)

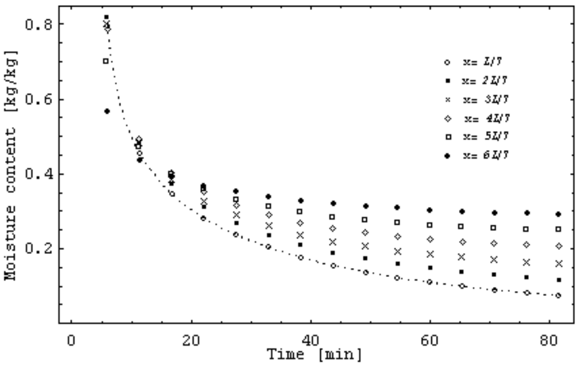
Because the heat flux given by (15) is a piecewise constant function, the solution technique for direct problem needs to be sequentially for the heating period $0 < t < t_h$ and then for the post-heating period.

Let us consider in this paper the test-case involving the following values of material properties for lime mortar: $\rho_0 = 2050.0\,(\mathrm{kg/m^3})$, $c_m = 950 + 0.041\mathrm{T} + 38\mathrm{u}$ (J/kgK), $\lambda = 0.58 + 0.003\mathrm{T} + 0.4\mathrm{u}$ (W/Km), $h = 0.32$ (W/km^2), $h_m = 4.7 \cdot 10^3$ (kg/m$^2 s$). $D_u = 9.3 \cdot 10^{-7} + 3 \cdot 10^{-10}\mathrm{T} + 6 \cdot 10^{-7} u\,(\mathrm{m^2/s})$. We present in Table 1 results obtained for the estimated parameters for standard deviation $\sigma = 0.01\,\mathrm{T_{max}}$. Normalised standard deviations are computed by dividing the original standard deviations by the maximum measured temperature.

Table1.Estimated parameters

Test	Experimental conditions	Parameter	Start guess	Estimated parameter	Normalised stand. deviation
1	$q_0 = 40\ \mathrm{W \cdot m^{-2}}$	a_0	1	1.2112×10^{-8}	0.0023
	$\mathrm{t_h} = 40$ min	a_1	7	5.9917×10^{-8}	0.0041
	$\mathrm{t_f} = 60$ min	a_2	4	3.1123×10^{-8}	0.0076
		D_0	4	4.362×10^{-5}	0.0057
		D_1	8	7.3725×10^{-5}	0.0037
		D_2	2	1.3271×10^{-4}	0.0045
2	$q_0 = 10\ \mathrm{W \cdot m^{-2}}$	a_0	1.2	1.2283×10^{-8}	0.0073
	$\mathrm{t_h} = 40$ min	a_1	6	5.9712×10^{-8}	0.0051
	$\mathrm{t_f} = 60$ min	a_2	3	3.1106×10^{-8}	0.0078
		D_0	4.3	4.3549×10^{-5}	0.0087
		D_1	7.1	7.3412×10^{-5}	0.0071
		D_2	1.2	1.3153×10^{-4}	0.0083

Figure 1 and 2 present the temperature and moisture content variations at several points inside the body, respectively, for $t_h = 40\,\text{min}$, $t_f = 60\,\text{min}$, $q_0 = 40\,\text{W. m}^{-2}$. As result of evaporation and moisture transfer to the surrounding air, the moisture content is smaller near the open boundary for up to $t = 3\,\text{min}$. For larger times, the moisture content near the heater boundary becomes smaller than that near the open boundary, as a result of the moisture flow from the regions at higher temperatures.



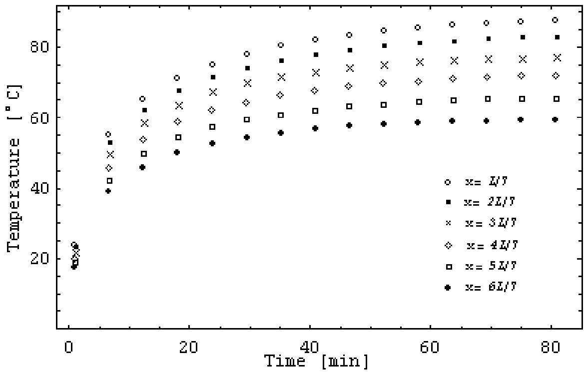


Figure 1 and 2 Temperature and moisture content variation inside the body for q = 40 W.m^{-2} and 30 iteration with $\sigma = 0.01$

Conclusion

In this paper we present the solution for a non-linear inverse problem of parameter estimation in the 1-D porous media, by using Luikov's model for coupled heat and mass transfer processes. This method can determine moisture dependent cross-transfer coefficients: mass transfer coefficient associated to temperature gradient and vapor phase transport coefficient associated to moisture gradient.

Numerical results demonstrate excellent estimations on the moisture distribution; the fact that experimentally determining moisture distribution is rather difficult account for why the proposed method is highly promising for designing a moisture sensor for some solids.

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