Numerical Solutions of Luikov and Philip and De Vries Equations of Heat and Mass Transfer in Porous Media

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Abstract: This paper presents a numerical solution of combined heat and moisture transfer in porous media of thickness L and width W using two models. The first formulation of this coupled heat and mass transfer phenomena is based on the simplified model of Philip and De Vries where it is assumed that the heat transfer due to the mass transfer is negligible and that the time variation of the condensed water is also negligible. The second is based on the luikov’s approach; contrariwise the heat transfer equation has been modified by the introduction of a new term known as the phase change rate. The system of equations is numerically solved when the sides of the slab are subjected to ambient and initial conditions in terms of temperature and moisture content using Incremental unknown scheme.

Keywords: Coupled heat and mass Transfer, Incremental unknowns, Finite element method, numerical method, and Porous media.

1. Introduction

Moisture is one of the most important factors limiting building’s service life. Moisture damage has been identified as one of the main reasons for building envelope deterioration. More recently recognized are the potential serious health hazards of mould and other organisms which flourish in buildings and constructions with excessive moisture [1]. Therefore, it is necessary to do research on the heat and moisture transfer in the buildings for getting a better thermal comfort. For decades, many researchers have devoted to the work of modeling of heat and moisture transfer in building envelope [2]. As early as 1960s, Luikov [3] has firstly proposed a mathematical model for simultaneous heat and mass (moisture) transfer in building porous materials. The conservation equations include the mass, the momentum and the energy conservation equations. The constitutive equations are described by Darcy’s law, Fick’s law and Fourier’s law. However, the solutions are either numerical or complicated involving complex eigenvalues. Cary and Taylor [4] use irreversible thermodynamics to describe the interactions of the forces and fluxes involved. A mechanistic approach based on physical models of the phenomenological processes that occur in the soil was established by Philips and De [5]. Whitaker [6] averaged the transport equation on a representative elementary volume (REV) at the continuum level and obtained the governing equations in a higher level. This modeling method overcomes the modeling difficulty that porous media are heterogeneous. But the transport coefficients of the model can not be getting easily without the complex experiments. These models have been adopted widely by many researchers [7], [8], [9] and [10]. According to the models of Philip, De Vries, Luikov and Whitaker, Liu [11] developed the multiphysics-phase change-diffuse model recently based on the Navier-Stokes equation. This model has seven field variables. Besides, there are more models established by the researchers’ [12], [13], [14], [15], [16] and [17]. The purpose of this paper is to clarify the influence of the phase change rate on the heat and moisture behaviour in the building envelope under the natural condition.

2. Equation of the Coupled Heat and Mass Transfer

Simultaneous heat and moisture transfer in a porous material involves complex physical phenomena. The strength of this complexity depends on how the mutual effect of heat on mass transfer and vice-versa is dealt with. In reality the relative humidity RH of the surroundings affects greatly the thermal characteristics of the porous medium where at high relative humidity some of the pores may contain water at liquid phase. Early investigations of moisture migration considered the diffusion of vapor through air within the pores as done by Henry [18] and since then many models were presented. They can be categorized owing to their level of complexity. Example of these models can be found in Philip and De Vries, De Vries, Luikov, Whitaker, Benet [19]. We restrict ourselves to the simplified model of De Vries, in which both vapor and liquid fluxes are considered and expressed in terms of the volumetric moisture concentration.

2.1 Simplified model of Philip and DeVries

Simplified model of Philip and DeVries assumes that the heat transfer due to the mass transfer is negligible, and that the time variation of the local condensed water vapor is also negligible. In these conditions the heat and moisture transfer system can be written as follow:

\[ \frac{\partial w}{\partial t} = d w (D_w \nabla \cdot w + D_v \nabla \cdot T) - \frac{\partial K}{\partial z} \] (1)

\[ \frac{\partial T}{\partial t} = d v (\alpha L \nabla w \cdot \nabla w + (A + \rho L D_v) \nabla \cdot T) \] (2)

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2.2 Luikov’s model

The model proposed by LUIKOV is based on the same assumptions as the simplified model PHILIP-DE VRIES. It leads to a mass transfer equation similar to that obtained in the previous system. By against the heat transfer equation has been modified by the introduction of a new term known as the phase change rate and noted by . The coupled equations can be written as follows:

\[
\frac{\partial w}{\partial t} = d_{w} \left( D_{w} \nabla w + \frac{\rho_{l}}{\rho_{v}} D_{T} \nabla T \right) - \frac{\rho_{l} \delta K}{\rho_{v}} \frac{\partial T}{\partial z} \tag{3}
\]

\[
\frac{\partial T}{\partial t} = \kappa \left( \nabla^{2} T \right) + \varepsilon L \frac{\partial w}{\partial t} \tag{4}
\]

Equations (3) and (4) have another complication: the value of changes from 0 to 1 depending on the significance of liquid transfer relative to the vapor diffusion within the material and, in turn, depending on the nature of the material. We expect it to increase with temperature. The effect of the phase change coefficient on the moisture and temperature regimes can be explored using the model given by (3) and (4).

3. 1-D test problem

3.1 Linearization of the system

The present study deals with a transient 1-D horizontal heat and moisture transfer in a homogeneous porous slab of thickness with constant transport coefficients. Its two ends are subjected to initial and boundaries conditions. Under these assumptions, the system of equations describing the transient moisture and heat diffusion can then be written in the following general form when neglecting the moisture transport by gravity:

\[
\frac{\partial w}{\partial t} = A_{ww} \frac{\partial^{2} w}{\partial x^{2}} + A_{wT} \frac{\partial^{2} T}{\partial x^{2}} \tag{5}
\]

\[
\frac{\partial T}{\partial t} = A_{T} \frac{\partial^{2} T}{\partial x^{2}} \tag{6}
\]

3.2 Analytical solution of the 1-D problem

Analytical solutions of heat and mass transfer problems in all models are restricted to 1D situation with constant coefficients. Example of these solutions is given in Dinulescu and Eckert [20], Liu and SHUNG [21]. In the present study we solve the linearized system with constant coefficient of the matrix when subjected to the following initial and boundary conditions

\[
w(x, t = 0) = w_{0}(x) \quad T(x, t = 0) = T_{0}(x)
\]

\[
w(x = 0, t) = w_{0}(t) \quad T(x = 0, t) = T_{0}(t)
\]

\[
w(x = L, t) = w_{l}(t) \quad T(x = L, t) = T_{l}(t)
\]

The analytical solution of the system (2) in conjunction with initial and boundary conditions was obtained by using Green Functions. Details of the solution methodology are presented in Lefebvre and Izquierdo [22] and in Saadani et al. [23]. The vectorial form of the exact solution is given by

\[
\begin{bmatrix} w(x, t) \\ T(x, t) \end{bmatrix} = \left( I - \frac{x}{L} \right) \begin{bmatrix} w_{0}(t) \\ T_{0}(t) \end{bmatrix} + \frac{x}{L} \begin{bmatrix} w_{L}(t) \\ T_{L}(t) \end{bmatrix}
\]

Where denote the eigen values of the matrix which are the diffusivities of heat and moisture.

The analytical solution is an infinite series. The influence of the order of the series on the value of the temperature is given in figure 1 where we plot the temperature time variation at the location according to for three different order . We can see that beyond an order of 11 the exact solution remains the same. Nevertheless, the series used in the exact solution in the following sections is truncated at .

![Figure 1: Analytical solution at $x = 0.125L$ according to $n$.](image)

3.3 Numerical Procedure

Numerical solutions of the mono-dimensional linear heat and moisture transfer equations were obtained by using a time
marching procedure until the steady state is reached. The incremental unknowns (IU) were introduced by Temam [24]. In these new numerical schemes the large scale component $U$ for the unknown and its small scale component $Z$ are treated differently.

Consider a discretized approximate solution on $N$ equally spaced grids to be $U = \left( u(h) \right)_{h=1}^{N}$ where $h = \frac{1}{N}$. We split $U$ into two components $Y$ and $Z$ by the means of a matrix of passage noted $S$, which gives:

$$ U = S \begin{bmatrix} Y \\ Z \end{bmatrix}, \quad \text{and} \quad \begin{bmatrix} Y \\ Z \end{bmatrix} = S^{-1}U \quad (8) $$

Based on the above consideration the relationship between variables at two successive time steps is given by

$$ 'SS Y^m + \Delta t' SAS Z^m = 'SS Y^{m-1} + \Delta t' SS Z^{m-1} + \Delta t' SS F_{t}^m $$

Many new schemes can be designed by using the IU principle. Its Crank-Nicolson like scheme is written in the following form:

$$ 'SS + \Delta t' SAS Y^m = ('SS Y^{m-1} + \Delta t' SS F_{t}^m) $$

### 3.4 Result and Discussion

The boundary conditions, the pre-simulation time period (warm-up), the size of the physical domain, the simulation time step, the grid refinement, the convergence errors and the required computer run time are important simulation parameters, which have to be chosen very carefully in order to accurately predict temperature and moisture content profiles in mortar slab under different sort of weather data.

In this subsection we present the results of the linear 1D problem. The boundary conditions and the initial conditions, as well as the geometry remain the same. The situation under study is one-dimensional heat and mass transfer in a homogeneous porous mortar of thickness $L$ similar to the tests problems used by Lefebvre and Izequierdo [1998], with the initial and boundary conditions for both temperature and moisture content:

$$ w(x, t=0) = 0.07 \text{ kg/kg} ; \quad T(x, t=0) = 20 \text{°C} $$
$$ w(x=0, t) = 0.031 \text{ kg/kg} ; \quad T(x=0, t) = 5 \text{°C} $$
$$ w(x=L, t) = 0.025 \text{ kg/kg} ; \quad T(x=L, t) = 23 \text{°C} $$

The temperature and the moisture content were monitored at the positions $x=0.125L$ (near the cold end). The sensitivity of the computed result was checked by running two different space girding $n=200$ and $n=300$ in conjunction with two different time steps $\Delta t = 0.1$ and $1$ s. The results obtained with these time and space grid sizes did not show any differences neither in convergences nor in accuracy for both temperature and moisture content except that with $\Delta t = 1$s convergence toward the steady state is reached in fewer computation steps. We can safely conclude that the results presented in this paper are grid free solutions. The accuracy of the numerical method used to solve this problem is compared to the exact solution.

The temperature decay profiles near the cold end obtained with the different models are plotted in figure 2, figure 3 and figure 4 along with the analytical linear solution for comparison purposes. The moisture results at these same locations are presented in figure 5 and figure 6.

A perfect matching between the computational results of the incremental unknown scheme and the analytical solution is obtained. The influence of taking into account the phase change rate is not that significant for the temperature evolution. However, as presented in figure 6 results of the moisture content decay show clearly that the evolution is strongly affected by the presence of the phase change rate.

![Figure 2: Evolution of temperature at $x = 0.125L$ of the mortar slab (Philip and DeVries’s model).](image)

![Figure 3: Evolution of temperature at $x = 0.125L$ of the mortar slab (Luikov’s model).](image)

![Figure 4: Evolution of temperature at $x = 0.125L$ of the mortar slab (Philip and DeVries and Luikov’s model).](image)
Numerical experiment was conducted in order to assess the impact of the phase change rate on time variation of temperature and moisture content in a homogenous porous material. For the water transport two phenomena take place. First, the increasing product temperature leads to an increase of partial vapor pressure of water, and therefore the partial vapor pressure for water in the region close to surface is higher than in the center. Due to the pressure differences, the water vapor moves both to the centre and to the surface.

4. Conclusion

The stationary 1D heat and moisture transfer test problems show that solution of the water content in the porous material is greatly affected when phase change rate is taken into account while the transient temperature solution remains mainly identical for both models. These remarks should be taken into account when predicting the water content and temperature evolution during thermal processes of porous material. For the water transport two phenomena take place. First, the increasing product temperature leads to an increase of partial vapor pressure of water, and therefore the partial vapor pressure for water in the region close to surface is higher than in the center. Due to the pressure differences, the water vapor moves both to the centre and to the surface.

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