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An adaptive simulation of nonlinear heat and moisture transfer as a boundary value problem

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ABSTRACT

This work presents an alternative view on the numerical simulation of diffusion processes applied to the heat and moisture transfer through porous building materials. Traditionally, by using the finite-difference approach, the discretization follows the Method Of Lines (MOL), when the problem is first discretized in space to obtain a large system of coupled Ordinary Differential Equations (ODEs). Thus, this paper proposes to change this viewpoint. First, we discretize in time to obtain a small system of coupled ODEs, which means instead of having a CAUCHY (Initial Value) Problem (IVP), we have a Boundary Value Problem (BVP). Fortunately, BVPs can be solved efficiently today using adaptive collocation methods of high order. To demonstrate the benefits of this new approach, three case studies are presented, in which one of them is compared with experimental data. The first one considers nonlinear heat and moisture transfer through one material layer while the second one considers two material layers. Results show how the nonlinearities and the interface between materials are easily treated, by reasonably using a fourth-order adaptive method. Finally, the last case study compares numerical results with experimental measurements, showing a good agreement.

1. Introduction

The hygrothermal transfer through porous structures is a matter of concern in many areas such as building physics, geophysics, environmental engineering and energy systems whose the transient evolution of heat and moisture migration plays an important role. Particularly, in the area of building physics, the heat and moisture transfer process through the porous envelope, roofing systems and the ground can strongly affect the energy efficiency, the thermal comfort of the occupants and the durability of the components [1–3]. Therefore, reliable assessment of hygrothermal transfer in building materials is a major issue, requiring efficient numerical tools for heat and moisture transfer in building materials [4].

As building material properties are temperature- and moisture-dependent and the boundary conditions are driven by weather variables, the models included in those tools are based on numerical approaches using discrete representations of the continuous equations. To compute the solution, standard discretization and incremental techniques are applied, such as the EULER implicit scheme in Refs. [5,6] to solve large systems of equations. Furthermore, when dealing with nonlinearities, hygrothermal properties of porous materials have to be updated as a function of the temperature and moisture content fields at each iteration [7]. The difficulties to compute the solution increase, particularly when using implicit schemes that require sub-iterations to treat those issues. In the literature [8–10], the important numerical costs of simulation tools are also mentioned and it is a matter of concern due to the substantial scale of buildings, where heat and moisture transfer phenomena have to be simulated.

In addition, in the models proposed in literature, the problem previously described is generally solved by traditional approaches such as the finite-difference method [11], the finite-volume method [5,12,13] and the finite-element method [14–16], which are well established in the fields of thermal sciences and building physics. In these classical approaches, the higher accuracy obtained for the space discretization of the numerical schemes is to order $\mathcal{O}(\Delta x^2)$. For a space standard discretization $\Delta x = 10^{-2}$, it implies that the error ε on the solution of the equations cannot be lower than $\mathcal{O}(10^{-4})$. Within the issue of comparing the model numerical predictions with experimental observations

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as carried out for instance in Refs. [17–19], it is of major importance to control the accuracy of the solution.

For sure, the accuracy of the computed solution can be increased by reducing the space and time discretization parameters. However, as mentioned before, the standard approaches proposed in literature has a high degree of freedom. Therefore, increasing the number of spatial and temporal grid points will inevitably increase the computational time of the numerical model. With high-order numerical schemes, it is possible to have the same precision of low-order numerical schemes but with a lower computational cost, as shown in Ref. [20]. For this reason, these traditional methods have to be improved or even replaced by innovative and efficient ways of numerical simulation [21], particularly with the issue of comparing the model predictions with experimental observations.

Therefore, this article aims at contributing to the numerical development of hygrothermal transfer, by proposing a new approach to simulate the one-dimensional heat and moisture diffusive transfer trough single and multilayered building porous materials. The Method of Horizontal Lines is here proposed to solve the nonlinear heat and moisture transfer to increase significantly the accuracy in space with a low computational time of the numerical model. Usually, when using finite-differences, the discretization follows the Method of Lines (MOL). It means that the problem is first discretized in space to obtain a large system of coupled ODEs. Here, a different point of view is proposed based on discretizing first in the time domain to obtain a Boundary Value Problem (BVP). Such problems can be easily solved using adaptive collocation methods of high order. This approach is investigated in this paper to compute with high accuracy combined heat and mass transfer problems in porous materials.

The manuscript is organized as follows. Section 2 details the physical model of heat and moisture transfer while fundamentals of the proposed method are shown in Section 3. Numerical results are discussed in Section 4 and simulation are compared with experimental data in Section 5. Finally, in Section 6, the main conclusions are outlined with future perspectives.

2. Physical model

The physical problem considers one-dimensional heat and moisture transfer through a porous material defined by the spatial domain $\Omega_x = [0,\ L]$ and time domain $\Omega_t = [0,\ \tau]$. The following convention is adopted: $x = 0$ corresponds to the surface in contact with the inside room and, $x = L$, corresponds to the outside surface. The moisture transfer occurs due to capillary migration and vapour diffusion. The heat transfer is governed by diffusion and latent mechanisms. The physical problem can be formulated as [22,23]:

$$\frac{\partial \rho_w}{\partial t} = \frac{\partial}{\partial x}\left(k_l \frac{\partial P_c}{\partial x} + \delta_v \frac{\partial P_v}{\partial x} \right), \tag{1a}$$

$$(\rho_0 c_0 + \rho_w c_w)\frac{\partial T}{\partial t} + c_w T \frac{\partial \rho_w}{\partial t} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x} + L_v \delta_v \frac{\partial P_v}{\partial x} \right), \tag{1b}$$

where ρ_w is the volumetric moisture content of the material, δ_v and k_l, the vapour and liquid permeabilities, P_v, the vapour pressure, T, the temperature, R_v, the water vapour gas constant, P_c, the capillary pressure, c_0, the material heat capacity, ρ_0, the material density, c_w, the water heat capacity, λ, the thermal conductivity, and, L_v, the latent heat of evaporation. Equation (1a) can be written using the vapour pressure P_v as the driving potential. For this, we consider the physical relation, known as the KELVIN equation, between P_v and P_c, and the CLAUSIUS–CLAPEYRON equation:

$$P_c = \rho_l R_v T \ln\left(\frac{P_v}{P_s(T)}\right),$$

$$\frac{\partial P_c}{\partial P_v} = \frac{\rho_l R_v T}{P_v}.$$

where P_v comes from the relation $\phi = P_v/P_s(T)$, in which ϕ is the relative humidity. Thus, by neglecting the variation of the capillary pressure and the mass content with temperature [16], the partial derivative of P_c can be written as:

$$\frac{\partial P_c}{\partial x} = \frac{\partial P_c}{\partial P_v}\frac{\partial P_v}{\partial x} + \frac{\partial P_c}{\partial T}\frac{\partial T}{\partial x} \simeq \frac{\rho_l R_v T}{P_v}\frac{\partial P_v}{\partial x}.$$

In addition, we have:

$$\frac{\partial \rho_w}{\partial t} = \frac{\partial \rho_w}{\partial \phi}\frac{\partial \phi}{\partial P_v}\frac{\partial P_v}{\partial t} + \frac{\partial \rho_w}{\partial T}\frac{\partial T}{\partial t} \simeq \frac{\partial \rho_w}{\partial \phi}\frac{\partial \phi}{\partial P_v}\frac{\partial P_v}{\partial t}.$$

Considering the relation $\rho_w = w(\phi)$, obtained from the sorption isotherm, and from the relation between the vapour pressure P_v and the relative humidity ϕ, we get:

$$\frac{\partial \rho_w}{\partial t} = \frac{w'(\phi)}{P_s(T)}\frac{\partial P_v}{\partial t}.$$

We denote by

$k_M \overset{\text{def}}{:=} k_l \frac{\rho_l R_v T}{P_v} + \delta_v$:the total moisture transfer coefficient under vapour pressure gradient

$k_{TM} \overset{\text{def}}{:=} L_v \delta_v$:the total moisture transfer coefficient under vapour pressure gradient

$k_T \overset{\text{def}}{:=} \lambda$:the heat transfer coefficient under temperature gradient

$c_M \overset{\text{def}}{:=} \frac{w'(\phi)}{P_s(T)}$:the moisture storage coefficient

$c_T \overset{\text{def}}{:=} \rho_0 c_0 + w(\phi) c_w$:the energy storage coefficient

$c_{TM} \overset{\text{def}}{:=} c_w T \frac{w'(\phi)}{P_s(T)}$:the coupling storage coefficient.

Considering the previous notation, Equation (1) can be rewritten as:

$$c_M(T,\ P_v)\frac{\partial P_v}{\partial t} = \frac{\partial}{\partial x}\left(k_M(T,\ P_v)\frac{\partial P_v}{\partial x} \right), \tag{2a}$$

$$c_T(T,\ P_v)\frac{\partial T}{\partial t} + c_{TM}(T,\ P_v)\frac{\partial P_v}{\partial t} = \frac{\partial}{\partial x}\left(k_T(T,\ P_v)\frac{\partial T}{\partial x} + k_{TM}(T,\ P_v)\frac{\partial P_v}{\partial x} \right). \tag{2b}$$

Finally, the problem of interest is a coupled system of two nonlinear parabolic partial differential equations, with vapour pressure P_v and temperature T gradients as driving potentials. Their boundary conditions are expressed as:

$$\mathbf{n}\cdot\left(k_M(T,\ P_v)\frac{\partial P_v}{\partial x} \right) = h_M(P_v - P_{v,\infty}(t)) - g_\infty(t),$$

$$\mathbf{n}\cdot\left(k_T(T,\ P_v)\frac{\partial T}{\partial x} + k_{TM}(T,\ P_v)\frac{\partial P_v}{\partial x} \right) = h_T(T - T_\infty(t)) - q_\infty(t) + L_v h_M(P_v - P_{v,\infty}(t)),$$

where $P_{v,\infty}$ and T_∞ stand for the vapour pressure and temperature of the air, h_M and h_T are the convective transfer coefficients and $\mathbf{n}$ is the normal that assumes $+1$ or -1 at the left or right boundary sides. If the bounding surface is in contact with the *outside* air, g_∞ is the liquid flow from wind driven rain and q_∞ is the sensible heat from the rain:

$$q_\infty = g_\infty \cdot H_l,$$

where, H_l is the water enthalpy. If the bounding surface is in contact with the *inside* building air then $g_\infty = 0$ and the variable q_∞ is the enclosure and long-wave radiative heat exchanged among the room surfaces:

$$q_\infty = \sum_{j=1}^{m} s\,\xi\,\sigma[(T_j(x=0))^4 - (T(x=0))^4],$$

where s is the view factor between two surfaces, σ is the STEFAN–BOLTZMANN constant, ξ is the emissivity of the wall surface, j represents the m bounding walls.