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Modeling Simultaneous Heat and Mass Transfer in Porous Media

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***Abstract* — We assess the performances of incremental unknown method when used in solving a time dependent 2D coupled linear and nonlinear heat and mass transfer in a homogenous porous slab of thickness L and width W. The formulation of this coupled heat and mass transfer phenomena is based on the simplified model of 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 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 and the results are compared to those obtained using finite difference schemes and finite element method. Validation tests are performed in 2D situation the system is solved in linear and nonlinear cases using the Incremental Unknowns, classical finite differences and finite element method and results obtained from different schemes are compared among them. Time marching solution is achieved in all cases using ADI method. The numerical results show clearly the perfect agreement between the numerical scheme and finite element method also the transient evolution is greatly affected when non linear effects are taken into account.**

***Keywords* – Coupled Heat And Mass Transfer, Incremental Unknowns, Finite Element Method, Numerical Method, Porous Media.**

I. Introduction

Investigation of the coupled heat and mass transfer in porous materials is of interest to many engineering and environmental fields. Examples of such applications range from thermal insulation in buildings to moisture migration during drying in manufacturing process. During the last few years, important experimental and analytical studies as well as computational modeling were conducted in an effort to understand the mechanism of the coupled diffusive phenomena Petkovic [1], Pel [2]. The present study is a numerical contribution to these efforts. Our primary focus is on the applicability and the performances of a new class of numerical methods termed as the Incremental Unknowns methods when implemented in transient, 2-D coupled heat and mass transfer problems. Results obtained with finite element method are compared to those obtained using their incremental unknowns and classical numerical schemes.

II. 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 vis-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 [3] 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 [4], De Vries [5], Luikov [6], Whitaker [7], Benet [8]. We restrict ourselves to the simplified model of De Vries [5], in which both vapor and liquid fluxes are considered and expressed in terms of the volumetric moisture concentration.

In addition to the assumptions made in the generalized model, the simplified model of De Vries 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. Although both Luikov and De Vries models give a satisfactory approach in explaining the physical phenomena occurring inside the porous material, when applied to a multilayered material, the water content value at the interface of each layer presents a discontinuity. To overcome this problem Duforestel [9] used the vapor pressure as a potential and shows that his model is equivalent to De Vries model. In these conditions the heat and moisture transfer system can be written as follow:

$$\frac{\partial w}{\partial t} = div\left(D_w gradw + D_T gradT\right) - \frac{\partial K}{\partial t} \qquad (1)$$

$$\left(\rho_m C\right)\frac{\partial T}{\partial t} = div\left(\rho_L LD_{wv} gradw + \left(\lambda + \rho_L LD_{Tv}\right) gradT\right)$$

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The heat and the mass diffusion coefficients appearing in the above equations depend on the vapor pressure and are similar in their analytical expression to the one used by Duforestel [9]. Values of the isothermal sorption as well as the permeability of water needed for numerical implementation were derived from the experimental work of Miquel [10].

III. 2-D Test Problem

The 2D test problem considered in this section deals with a square homogeneous material with a length L of each side. The material properties are similar to the mortar considered to the test problem used by Saadani [11]. The test was conducted by considering constant diffusion coefficients. In the linear case the diffusion coefficients are constant and the system 1 can be written in the following form:

$$\frac{\partial w}{\partial t} = A_{ww}\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}\right)+A_{wT}\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right) \qquad (2)$$
$$\frac{\partial T}{\partial t} = A_{Tw}\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}\right)+A_{TT}\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)$$

IV. Computational Modeling

Numerical solutions of the two-dimensional linear heat and moisture transfer equations were obtained by using a time marching procedure until the steady state is reached. In addition to the classical finite differences schemes (classical Crank-Nicolson) see for example Patankar [12], Anderson et al. [13], we implemented a novel scheme that is the Incremental Unknowns.

The incremental unknowns were introduced by R. Temam [14], as a mean to approach approximate inertial manifold in the case of finite differences discretization. This concept leads to the introduction of large classes of new numerical schemes for which the large scale component Y for the unknown and its small scale component Z are treated differently, leading to an improved conditioning for elliptic problem and to an improved stability condition for evolution problems.

Consider a discretized approximate solution on N equally spaced grids to be $U = (U(ih))_{i=1,\dots N}$ 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:

$$U = S\begin{pmatrix} Y \\ Z \end{pmatrix}$$

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

$$\left({}^tSS + \Delta t\,{}^tSAS\right)\begin{pmatrix} Y^m \\ Z^m \end{pmatrix} = \left({}^tSS\right)\begin{pmatrix} Y^{m-1} \\ Z^{m-1} \end{pmatrix} + \Delta t\,{}^tSS\begin{pmatrix} F_Y^m \\ F_Z^m \end{pmatrix} \qquad (3)$$

Where the matrix S is of order $(2N-1)\times 2N$, the matrix ${}^tSS$ is of order $(2N-1)$ and the matrix ${}^tSAS$ of order $(2N-1)$, and are respectively written in the following forms:

$$S = \begin{pmatrix} I_{N-1} & 0 \\ G & I_N \end{pmatrix} \quad {}^tSS = \begin{pmatrix} B & {}^tG \\ G & I_N \end{pmatrix} \quad {}^tSAS = \begin{pmatrix} \frac{A^*}{2} & 0 \\ 0 & \frac{2}{h_1^2} I_N \end{pmatrix}$$

G is a matrix of order $N\times(N-1)$, I_N is the matrix of identity of order $N\times N$, the matrix B of order $N-1$ and A^* is a matrix of order $N-1$ with $h_1 = \frac{1}{2N}$:

$$B = \begin{pmatrix} \frac{3}{2} & \frac{1}{4} & 0 \\ \frac{1}{4} & \ddots & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{3}{2} \end{pmatrix} \quad G = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & \ddots & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad A^* = \frac{1}{2h_1^2}\begin{pmatrix} 2 & -1 & 0 \\ -1 & \ddots & -1 \\ 0 & -1 & 2 \end{pmatrix}$$

We can write the expression of (2) as:

$$\begin{cases} \left(B+\Delta t A_{ww}\frac{A^*}{4}\right)Y^m + \left({}^tG+\frac{\Delta t}{h_1^2}A_{wT}\right)Z^m = \\ \left(B-\Delta t A_{ww}\frac{A^*}{4}\right)Y^{m-1} + \left({}^tG-\frac{\Delta t}{h_1^2}A_{wT}\right)Z^{m-1} \\ \left(G+\Delta t A_{Tw}\frac{A^*}{4}\right)Y^m + \left(1+\frac{\Delta t}{h_1^2}A_{TT}\right)Z^m = \\ \left(G-\Delta t A_{Tw}\frac{A^*}{4}\right)Y^{m-1} + \left(1-\frac{\Delta t}{h_1^2}A_{TT}\right)Z^{m-1} \end{cases} \qquad (4)$$

V. Results of the 2D Test Problem

Runs of the 2D linear and non linear test problems were obtained with fifty and hundred space grid nodes and with time steps of 0.1 and 1s. Results from different time steps and different space grids did not show any differences for the case tested except that the runs of 1s and 100 nodes required less iterations to reach the steady state solution especially for the evolution of the moisture content which exhibited with a higher grid node number a very slow convergence rate due to the strongly nonlinear character of the mass transfer diffusion coefficients. We present in this section results of the 2D linear along with the nonlinear obtained with 1s and 100 grid nodes. The system of equations was solved when the square slab is subjected to the boundary conditions

$$w(0,y,t) = 0.031 \qquad w(1,y,t) = 0.025$$
$$w(x,0,t) = 0.031 \qquad w(x,1,t) = 0.025$$
$$T(0,y,t) = 5°C \qquad T(1,y,t) = 23°C$$
$$T(x,0,t) = 5°C \qquad w(x,1,t) = 23°C$$

and with initial conditions

$$w(x,y,0) = 0.07 \qquad T(x,y,0) = 20°C$$

Values of temperature and moisture content decay were monitored at two different positions (x, y) = (0.125L, 0.125L) and at (x, y) = (0.875L, 0.875L) termed respectively as the cold corner and the warm corner. In figure 1 we present the temperature decay obtained with the classical finite difference scheme and the Incremental Unknowns schemes both for the linear and the non linear system. We can note that alike the result of the 1D case

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Saadani [11] the temperature evolution is almost not affected by taking into account the nonlinearity. The same remarks apply also for the temperature decay at the warm corner figure 2. However, as presented in figure 3 and 4 results of the water content decay show clearly that the evolution is strongly affected by the nonlinearity. Non linear results present a slower convergence of the water content toward the steady state solution. This is a similar to the slow convergence noticed in the 1D non-linear case mentioned above and also a confirmation of the result obtained by Lefebvre and Izequirdo [15] when they compared their 1D linear moisture decay to the result of 1D nonlinear case of Kallel et al. [16]. The diffusion coefficients depend strongly on the water content rather than on temperature as it was mentioned by Perrin and Javels [17]. These plots show also that in the 2-D non linear situation the results of the IU when compared to these obtained with the standard finite difference schemes show a difference in the accuracy.

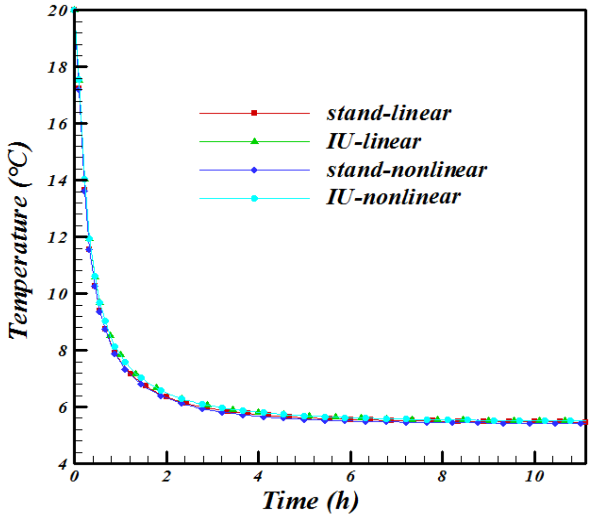

Fig.1. Evolution of temperature at the location *(0.125L, 0.125L)*

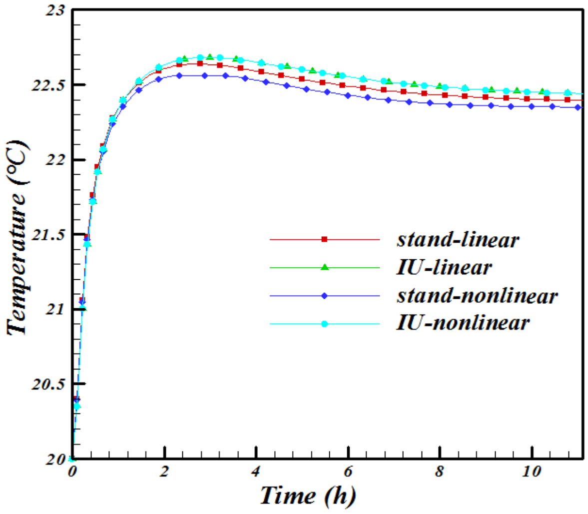

Fig.2. Evolution of temperature at the location *(0.875L, 0.875L)*

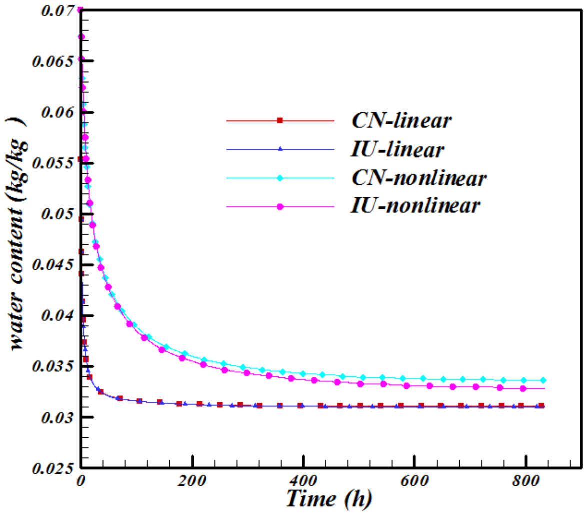

Fig.3. Evolution of the water content at the location *(0.125L, 0.125L)*

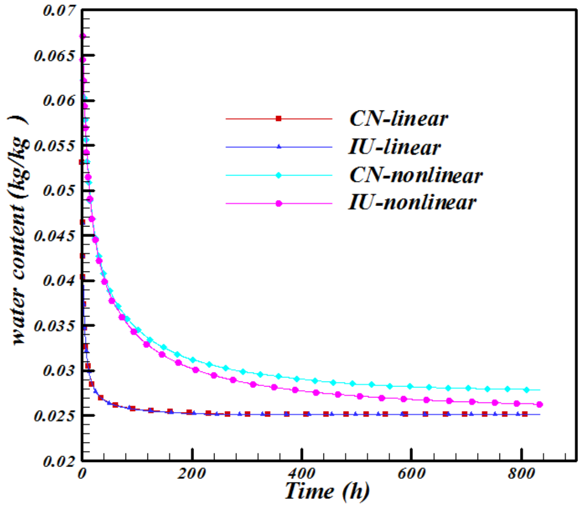

Fig.4. Evolution of the water content at the location *(0.875L, 0.875L)*

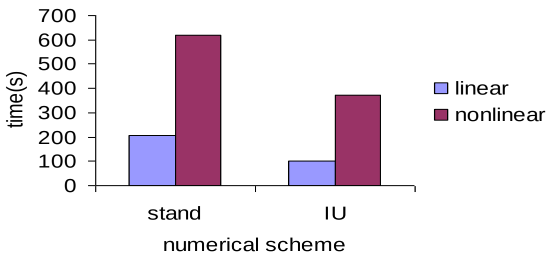

Fig.5. CPU time of temperature

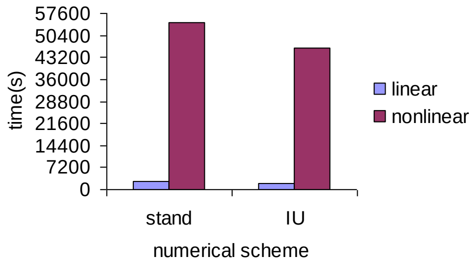

Fig.6. CPU time of water content

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The difference in accuracy of the nonlinear results obtained with the two numerical methods (i. e : Finite Differences Scheme and the Incremental Unknowns) is achieved at the expense the CPU time required for the solution to reach the steady state as indicated in figure 5 and 6. The classical finite differences scheme required a 40% CPU time for temperature computing and extras 2 hours of CPU time for computing the moisture content.

VI. Comparison with other Simulation

The last numerical simulation is a comparison with the numerical predictions calculated with finite element method. We use the same initial and boundary conditions. When compared to the decay of water content obtained in the present study for similar locations respectively plotted in figure 7 for temperature and figure 8 and 9 for water content they exhibit the same transient behaviour during the most significant.

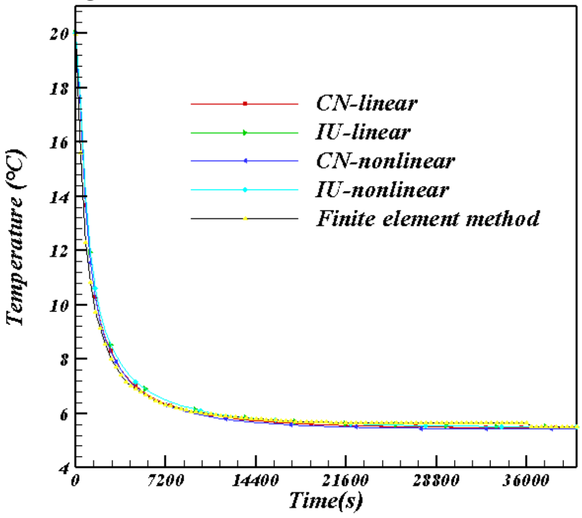

Fig.7. Evolution of temperature at the location *(0.125L, 0.125L)*

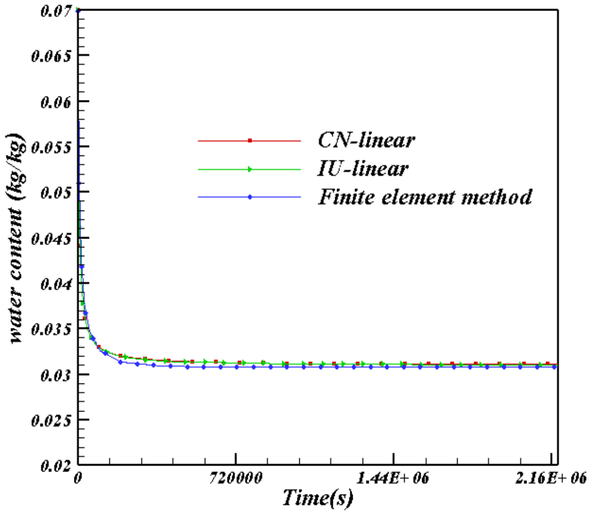

Fig.8. Evolution of the water content at the location *(0.125L, 0.125L)*

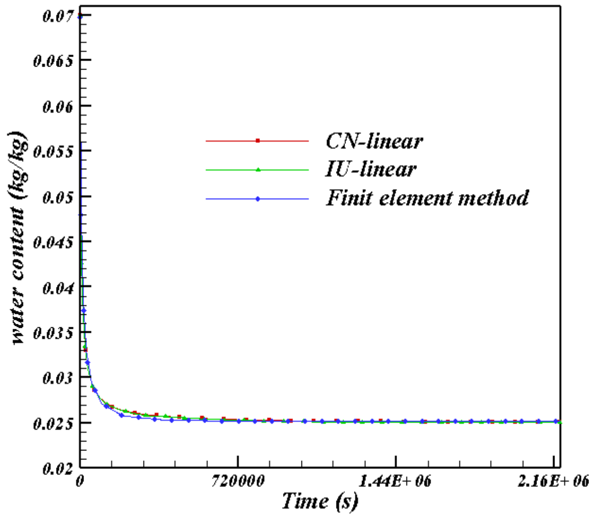

Fig.9. Evolution of the water content at the location *(0.875L, 0.875L)*

VII. Conclusion

Numerical experiment was conducted in order to assess the impact of the nonlinearity on time variation of temperature and moisture content in a homogenous porous material also compared the results obtained with finite element method to those obtained using their incremental unknowns and classical numerical schemes. The transient 2D heat and moisture transfer problem as formulated by De Vries is solved with different numerical schemes. The 2D nonlinear test problems show that transient solution of the water content in the porous material is greatly affected when non constant diffusion coefficients are taken into account while the transient temperature solution remains mainly identical to the evolution of the linear case. These remarks should be taken into account when predicting the water content and temperature evolution during thermal processes of porous material. The linear 2D test problem shows that results obtained with finite element method perform very well in term of accuracy when compared to the numerical schemes solution of heat and moisture transfer in a mortar slab.

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