Numerical modeling of coupled heat and water steam flow in spatially variable permeability of saturated porous media

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Abstract

The aim of this paper is to present an efficient numerical strategy for the simulation of convection-diffusion phase change problems in saturated porous media with spatially variable permeability. An efficient and accurate finite volume method is used to discretize in space leading to a semi discrete differential algebraic system DAE. Suitable numerical techniques are implemented to solve the stiff system resulting from the strong coupling between the equations of the model. The proposed method is applied on evaporation in heterogeneous saturated porous media. 1D and 2D simulations are presented, where we suppose that the soil is constituted by blocks of different permeability.

Keywords: Heat transfer, Phase change, Variable permeability, Drying process.

1. Introduction

Heat flow accompanied by a phase change with variable permeability, occurs in many important practical problems. In particular the heat diffusion in the ground saturated by water has pressed upon the attention to develop new methods for more precise representative simulations. The large number of published papers on heat transfer and fluid flow through porous media demonstrates clearly that this area of fluid mechanics has been studied extensively during the last three decades [4], [5].

Actually, the aim of this work is to present the applied mathematics used to study prehistoric fires. It is related to the drying process problem studied, among others by [7] and [8]. The idea is to apply a numerical model to calculate the heat conduction in porous soils subjected to intense heat from above. This particular geometry requires that the heat prevents the usual behavior of water in the ground, because the vapor ascends to the heated surfaces. Subsequently, the mathematical model delineating our problem is described by coupled systems of moving boundary problem with phase change and the convection phenomenon under a downward facing heated surface.

Due to the absorption or release of latent heat and the presence of complex interfacial structures that characterize the problem of evaporation, the exact solution of conservation equations is impossible. Here, we choose a model consisting of a single region that utilizes a system of conservation equations that can be equally applied to both phases [1], [2]. The latent heat evolution is accounted for in the energy equation by the enthalpy formulation [1], while no explicit conditions on the interface are required and the numerical solution can be carried out on a fixed grid. However, the numerical treatment of phase change problems requires special attention to handle the latent heat evolution associated with the phase change and the high nonlinearity presented in the system of equations due to the fact that all the soil properties are temperature dependent.

The purpose of this paper is to use an efficient and accurate numerical method to deal with binary water-vapor phase change problem in a heterogeneous saturated porous medium; this numerical has been presented elsewhere [2]. A control volume numerical method combined with a modified Newton method is be used, and there is a coupling between the energy equation and the water steam flow model, like in [6].

In this paper the authors would like to show the effects of the heterogeneity on the position of the interface of phase change at 100℃.

2. Mathematical formulation

Consider a horizontal surface embedded in a water saturated porous medium of variable permeability as shown in Fig. 1. The temperature of the surface facing downward is T_c, which is greater than the temperature T_∞ of the medium.

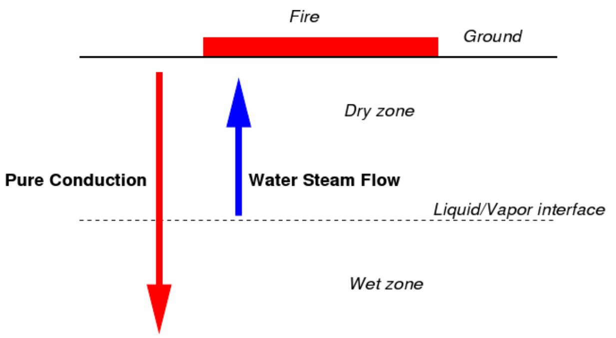

Fig. 1 Physical description of the medium.

When a heated region in the soil reaches T_v (temperature of evaporation which is approximately 100°C), the water existing in the soil turns into vapor flowing in the ground. As the bottom of the domain is closed, the only possibility for the water steam to escape the porous medium is to flow upward to the ground, leading a counter-current heat flow, as shown in Fig. 1.

2.1. Model equations

In order to model the heat transfer in the soil, we use the energy equation. We assume that the two phases (porous matrix and fluid phase) are in local equilibrium, so that the energy conservation equation is expressed as

$$(\rho c)_e \frac{\partial T}{\partial t} + (\rho c)_f V_f.\nabla T = div(k_e \nabla T) \quad (1)$$

where T represents the temperature, ρ is the density, c is the apparent capacity, k is the conductivity, V_f is the filtration velocity of the fluid; the subscripts e and f indicate respectively the equivalent parameters of the medium and the properties of the fluid.

The effective calorific capacity being additive, the effective value $(\rho c)_e$ is then defined by

$$(\rho c)_e = \phi \rho_f c_f + (1-\phi)\rho_s c_s \quad (2)$$

Where the subscript s indicates the properties of the porous matrix, ρ_s, c_s are constants, otherwise, ρ_f, c_f are temperature dependent. The porosity ϕ is used as the water content in the soil (we suppose that the medium is saturated by water).

On the other hand, in order to model the fluid motion through the porous medium, we use the Darcy flow model formulation

$$V_f = -\frac{K}{\mu_f}\nabla P_f \quad (3)$$

where V_f is the filtration velocity of the fluid, K is the permeability (variable in space and constant in time), μ_f is the viscosity of the fluid phase (water or vapor) and P_f is the fluid pressure. Hence, the continuity equation is given by

$$\phi \frac{\partial \rho_f}{\partial t} + div(\rho_f V_f) = 0 \quad (4)$$

The resulting equation obtained by coupling Eq. 2 and Eq. 3, which models the water steam flowing in the heterogeneous media, is thus given by

$$\begin{aligned} div(\nabla P_f) = {} & \frac{\phi \mu_f}{K \rho_f}\frac{\partial \rho_f}{\partial t} + \frac{1}{\mu_f}\nabla \mu_f.\nabla P_f \\ & - \frac{1}{\rho_f}\nabla \rho_f.\nabla P_f - \frac{1}{K}\nabla K.\nabla P_f \end{aligned} \quad (5)$$

The system of equations is completed by adequate initial and boundary conditions.

2.2. Apparent heat capacity formulation (AHC)

To avoid the tracking of the interface, the AHC method is used because it allows for a continuous treatment of a system involving phase transfer. In this method [1], the latent heat is calculated by integrating the heat capacity over the temperature, and the domain is considered to be treated as one region. A direct evaluation, in fact, can be expressed to lead to satisfactory numerical integrations only if the thermo-physical properties versus temperature curves do not present sharp peaks in the range of interest. If, instead, a "true" evaporation process is considered, difficulties are likely to arise.

In fact, when the temperature approaches the phase change temperature, the equivalent heat capacity tends to the shape of the Dirac σ function and, therefore cannot be satisfactory represented across the peak, by any smooth function. Such extreme problems can be successfully tackled by the technique already presented in [2], where a more appropriate averaging process is employed.

To alleviate the singularity presented in the formulation of thermo-physical properties defined by [1] (see Fig. 2 continuous lines), the Dirac delta function can be approximated by the normal distribution

$$d\sigma / dT = (\varepsilon \pi^{-1/2}) \exp\left[-\varepsilon^2 (T - T_v)^2\right] \quad (6)$$

in which ε is chosen to be $\varepsilon = 1/2^{1/2}\Delta T$, where ΔT is one-half of the assumed phase change interval and T_v is the phase change temperature. Consequently, the integral of $d\sigma / dT$ yields the error functions approximations for the initial phase fraction. With conventional finite volume method, the initial phase fraction derived from $d\sigma / dT$ integration should be used to avoid the numerical instabilities arising from the jump in the values of the volumetric fraction of initial phase from zero to one. In our approach, the smoothed coefficients (see Fig. 2 dashed lines) could be written as

$$c_f = c_l + (c_v - c_l)\sigma(T) + L\frac{d\sigma}{dT} \quad (7)$$

and

$$k_f = k_l + (k_v - k_l)\sigma(T) \quad (8)$$

where L is the latent heat of phase change and the subscripts l and v indicate respectively the properties of the liquid phase (water) and the properties of the vapor.

Similar techniques are used in the model for the best determination of the other physical properties of the medium (density and viscosity).

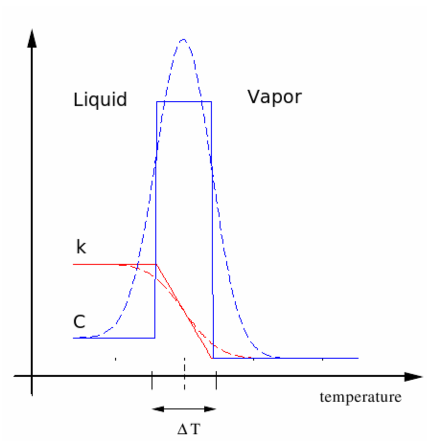

Fig. 2 Equivalent thermo-physical properties in the AHC method.

The mathematical description of these coefficients allows a global treatment of the system. However, the matrices of the thermo-physical properties are now strongly time dependent (the set of equations modeling the problem is highly non-linear), through the variation of coefficients with temperature, and a completely new solution has to be obtained at each stage. The evaluation of temperature dependent quantities requires special care, particularly if a rather coarse mesh is employed and spatial variation of the quantities is abrupt.

3. Numerical strategy

The problem to be solved may be written in vectorial form with adequate initial and boundary conditions

$$\begin{cases} \dfrac{\partial T}{\partial t} = f(t,x,T) \\ \gamma \dfrac{\partial T}{\partial t} + \theta \dfrac{\partial P}{\partial t} = g(t,x,T,P) \end{cases} \tag{9}$$

where γ and θ depend on $\sigma(T)$ and $d\sigma/dT$.

The first equation of the system (Eq. 9) is an ordinary differential one, on the other hand, the second equation is a differential algebraic equation of index one, because θ may be zero.

Among the large variety of existing approaches used to solve such systems, the following methodology has been chosen:

- The use of the method of lines where space and time discretizations are considered separately
- Spatial discretization: finite volume method
- An appropriate DAE solver is used

After the spatial discretization by the finite volume method in 2D, we obtain the semi-discrete system of DAE, which writes

$$\begin{cases} T' = A(T)T \\ \gamma T' + \theta P' = B(T,P)P \end{cases} \tag{10}$$

Let $Y = [T,P]^T$. By classical transformations, the system can be written with the general form

$$\begin{cases} F(t,Y,Y') = 0 \\ Y(t_0) = Y_0 \\ Y'(t_0) = Y'_0 \end{cases} \tag{11}$$

In order to solve (Eq. 11), the integration method used in our model is the variable order, variable coefficient BDF (Backward Differentiation Formula), in fixed leading-coefficient form. Actually, the BDF method is well adapted to our problem which becomes more and more stiff as ΔT decreases. The numerical calculation is performed with the use of the MUESLI FORTRAN library [3] which is based on the DASSL DAE solver of SLATEC. The model has been implemented in 1D and 2D geometric configurations.

4. Some validation examples

4.1. Heat conduction in a saturated homogeneous soil

Several experiments have been done at the archaeological soil of Pincevent to study the minimal duration of prehistoric fire. In this example we provide a comparison between numerical simulation and results coming from a real experiment. A real fire is lighted at the surface of a clay soil and the temperature is measured at different depths in the soil using sensors inserted at different positions under the fire.

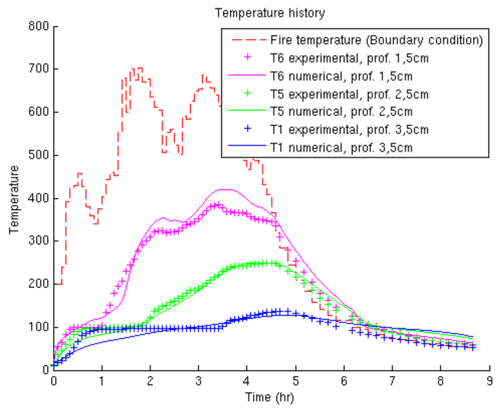

Fig. 3 Comparison between numerical results and experimental data (realized on the archaeological hearths at Pincevent site; a real fire has been used).

We suppose that the permeability of the medium is uniform, so we have:

$$\frac{1}{K} \nabla K . \nabla P_f = 0 \tag{16}$$

Figure 3 shows the comparison at different depths. The temperature of the real fire was measured at the center of the fire and used as a boundary condition for the simulation (we supposed that the temperature of the fire is uniform). The predicted temperatures from the numerical simulation in Fig. 3 almost match the experimental values of temperatures with a very small difference especially at the plateaus location (the plateaus at the phase change temperature observed in (Fig. 3) are due to the phase change phenomenon).

Possible explanations for these deviations include the fact that domain size is too small to accurately represent the zero-flux boundaries. Moreover, we are uncertain about the values of the thermal properties for the soil. But the main idea of this paper is to test whether the plateau of Fig. 3 (in the T1 sensor) is related to variable permeability of the soil.

4.2. Heat conduction in a saturated soil with spatially variable permeability

In this section, we examine how the phenomenon of spatial variable permeability affects the flow and heat transfer from a uniform temperature heated surface. In particular, we assume that the medium consists of different blocks of constant permeability which can take many patterns. In the following, red blocks are of permeability 10^{-12} m^2 and the blue ones are of 10^{-14} m^2. We suppose that the considered soil is a water saturated clay soil initially at 20°C, the temperature of the supposed fire at the surface of the soil is 400°C. The heating process is 12 hours long. Domain extents is 0.025 m long and 0.10 m deep. Numerical grid is 12 by 48.

Let's consider first the 1D problem. Figure 4 shows the phase-change interface (at 100°C) position when the soil is considered as horizontal layers of constant permeability. An important point, already emphasized in [2] is that the coupling between the water steam flow and the heating process delays the displacement of the interface (green curve compared to the blue one). Another interesting point is that a sudden increase in permeability also delays the interface movement.

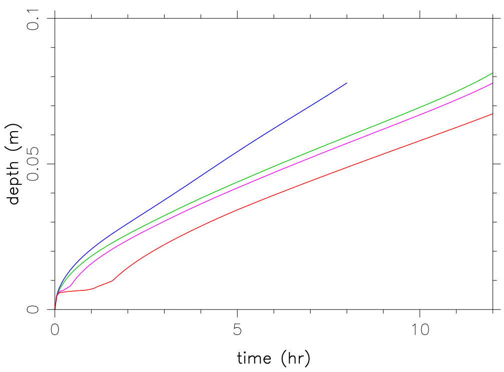

Fig. 4 Phase-change interface position for different cases: (blue) heating without coupling, (green) homogeneous permeability, (magenta) weak difference in permeability and (red) strong difference.

Figure 5 presents the time evolution of temperature at each 15 first node, like sensors. In this case, the ratio in the permeability is 10. We can notice that for some sensors, there is a long plateau, like in the experiments of Fig 3.

If we consider now vertical blocks (permeability ratio of 10), the simulation must be done in 2D. As before, the heat transfer is delayed in the less permeable block, as shown in Fig. 6

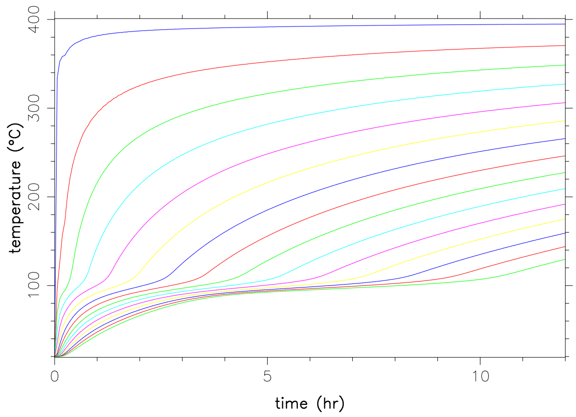

Fig. 5 Temperature evolution at each node of the mesh (along the vertical direction).

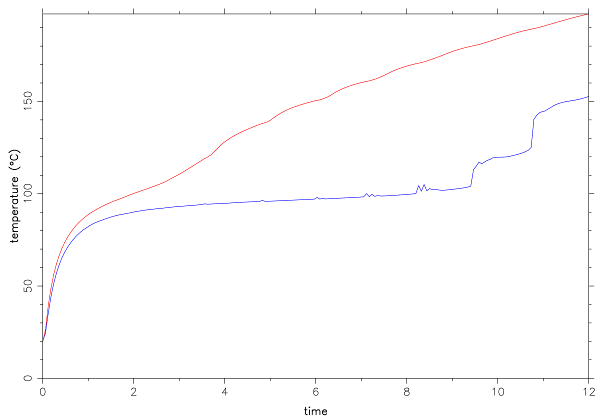

Fig. 6 Temperature evolution for two fixed sensors, when the soil is constituted by two vertical blocks: each curve has the same color as the corresponding block.

Lastly, we consider the heating of a soil made by squared blocks, as shown in Fig. 7. Whole temperature field is shown in Fig 8 in pseudo colors, whereas two fixed sensors reveal temperature evolution in Fig. 7.

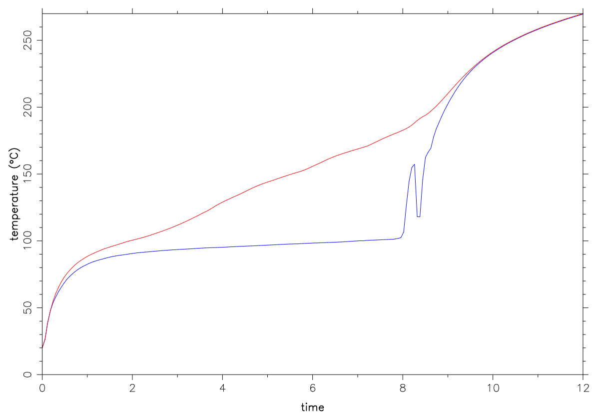

Fig. 7 Temperature evolution for two fixed sensors, when the soil is constituted by repeated square blocks.

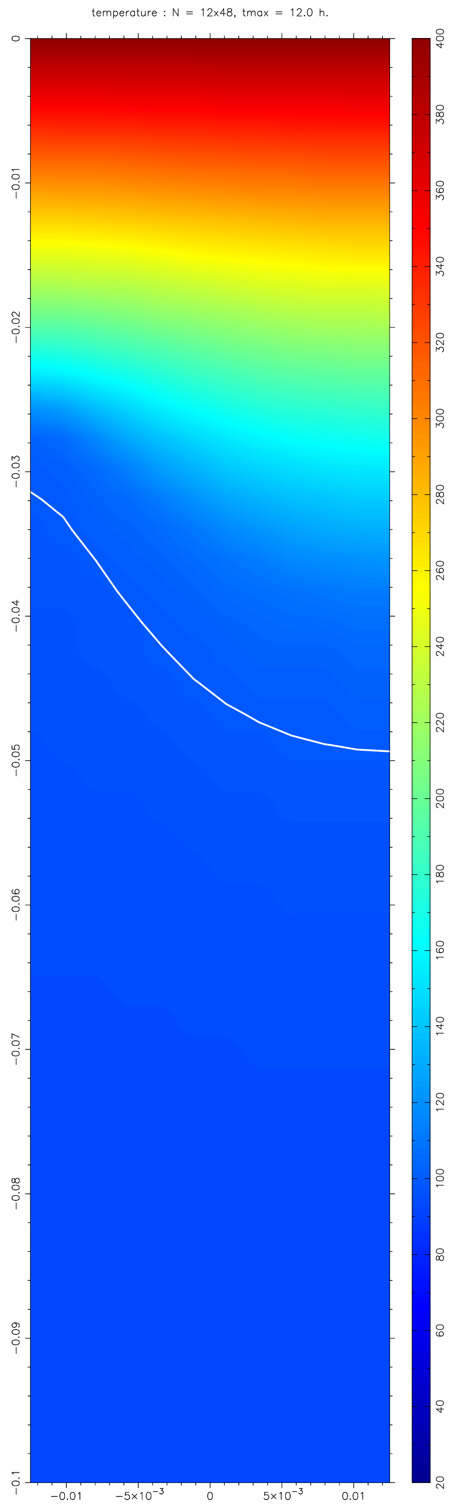

Fig. 8 Temperature field. Phase-change interface is shown by the white line.

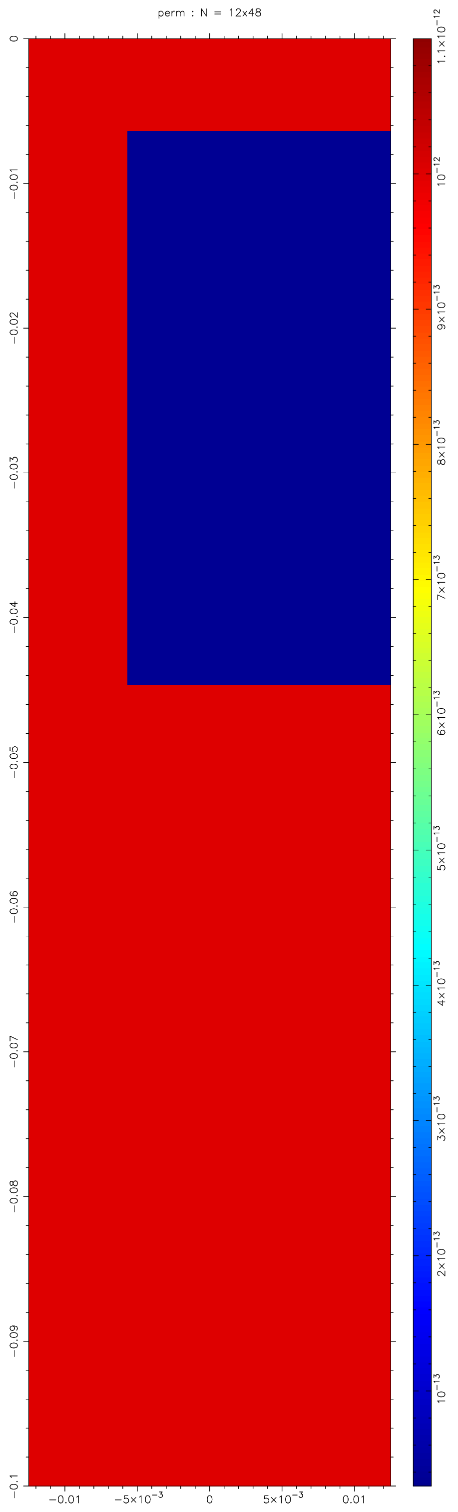

Fig. 9 Pattern for the simulation. Due to symmetry, only the half of the square blocks is considered. Dirichlet condition is applied on the top, whereas Neumann condition is applied to others.

5. Conclusions

In this work, different heterogeneous cases have been studied. While the 1D and 2D cases are very simple, numerical simulations shows interesting features; one of them is the plateau in the temperature evolution for specific sensors. As this is our first results, work is in progress to improve the scheme in the codes, in order to suppress the numerical instabilities, shown in fig. 6 and 7. Last, we hope to obtain other results for finest grids.

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