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Simulation of Heat Transfer With Phase Change in 3D Saturated Porous Media

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Abstract. *We investigate in this paper the forced heat conduction in a real 3D saturated porous media. To avoid the follow of the "dry/wet" phase change front we used the apparent heat capacity method (AHC). A new method is proposed to avoid the singularity presented in the physical parameter modelized by (AHC). In term of numerics the discretization is based on the mixed hybrid finite element method. The validation stage of our code is provided by comparing numerical results with experimental and analytical existing ones.*

1 Introduction

The aim of this paper is to present the applied mathematics to the study of Prehistoric fire explaining the rules of human behavior related to the use of fire. We deal with a problem of heat diffusion in a 3D water saturated heterogeneous porous media subjected to intense heat from above, which presents the inherent difficulties associated with the non-linearity of the interface conditions and the unknown location of the moving boundary (front of dry/wet phase change). Due to the powerlessness of classical methods like the finite element or finite difference methods in manipulating these systems where usually the primary variable and its derivative need to be approximated, the mixed and mixed-hybrid finite element methods are developed to handle such problems. The main favorable property of these methods is that both the primary unknown and its gradient are approximated simultaneously with the same order of convergence. Besides, they fulfill the physics of the problem, i.e. conserve mass locally and preserve the continuity of fluxes.

The parabolic governing equation for the unknown temperature T is given by

$$\begin{array}{lll} (\rho C)_e(T)\dfrac{\partial T(x,t)}{\partial t} + \nabla.(-k_e(T)\nabla T(x,t)) = f(x,t) & \text{in} & \Omega \times (0, t_{end}], \\ T(x,0) = T^0(x) & \text{in} & \Omega, \\ T(x,t) = T^D(x,t) & \text{on} & \Gamma^D \times (0, t_{end}], \\ T(x,t).\nu = q^N(x,t) & \text{on} & \Gamma^N \times (0, t_{end}]. \end{array} \quad (1)$$

where Ω is a bounded domain in $\mathbb{R}^3$ with boundary $\partial\Omega = \Gamma^D \cup \Gamma^N$; $(\rho C)_e = \phi(\rho C)_f + (1-\phi)(\rho C)_s$ represents the apparent capacity of the medium (ρ is the density, C is the apparent heat capacity, ϕ is the porosity, the subscripts e, f and s indicate respectively the equivalent parameters of the medium, the properties of the fluid and the porous matrix properties); k_e is the conductivity, it is assumed to be a diagonal tensor with components in $L^\infty(\Omega)$ (k_e is calculated using the harmonic mean between k_f and k_s); ν indicates the outward unit normal vector along $\partial\Omega$; $f \in L^2(\Omega)$ represents the source function; T^D and q^N are respectively the Dirichlet and Neumann boundary conditions. The form of equation (1) shows that only conductional heat transfer is considered and the convection in the phase change sub-domain is neglected. It should be emphasized that the thermophysical properties of the fluid are temperature dependent.

To solve this problem we modified `TRACES` [3] (Transport of RadioACtive Elements in Subsurface) which is a computer program for the simulation of flow reactive transport in saturated porous media. To take into account the evaporation phenomenon (phase change problem) in the porous medium, the apparent heat capacity approach (AHC) [1], presented below, has been implemented in this code.

2 Apparent heat capacity method (AHC)

To avoid the follow of the interface, the apparent heat capacity method will be used because the AHC formulation 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 expected to lead to satisfactory numerical integrations only if the thermophysical 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 δ function and, therefore, cannot be satisfactorily represented across the peak, by any smooth function. Such extreme problems can be successfully tackled by the technique proposed here, where a more appropriate averaging process is employed.

To alleviate the singularity presented in the formulation of thermophysical properties defined by [1] (see Figure 1, continuous lines), the Dirac delta function can be approximated by the normal distribution function $d\sigma/dT = (\epsilon\pi^{-1/2})exp[-\epsilon^2(T-T_v)^2]$, in which ϵ is chosen to be $\epsilon = 1/\sqrt{2}\Delta T$, 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 element method, the initial phase fraction derived from $d\sigma/dT$ by 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 Figure 1, dashed lines) could be written as:

$$C_f = C_l + (C_v - C_l)\sigma + L\frac{d\sigma}{dT} \text{ and } k_f = k_l + (k_v - k_l)\sigma \tag{2}$$

Similar techniques are used in the program for the best determination of the other physical properties of the medium.

The mathematical description of these physical coefficients allows a global treatment of the system. The proposed approach has been implemented using the mixed-hybrid finite element method with different type of elements (tetrahedron, parallelepiped and prism). However, the matrices of thermophysical properties are now strongly time dependent (the set of equations (1) 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.

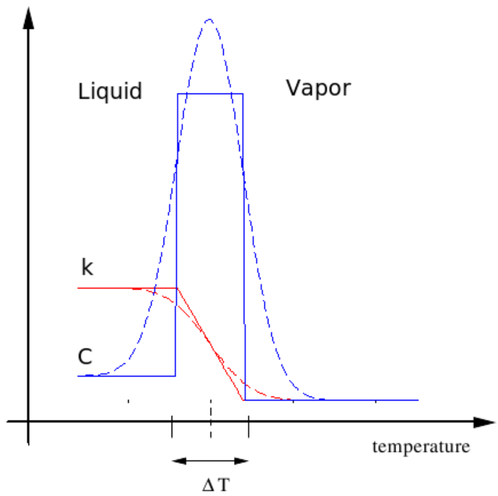

Figure 1: Estimation of thermophysical properties in phase change problems.

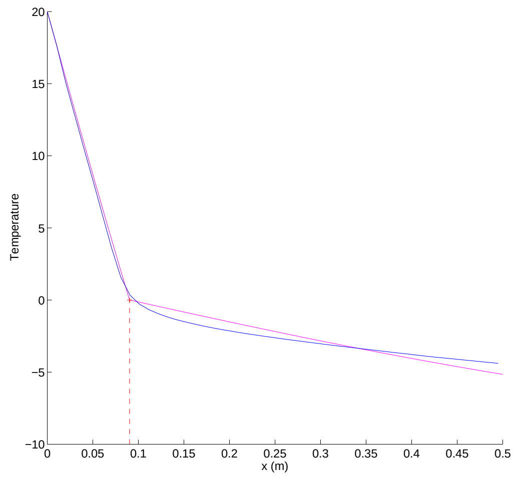

Figure 2: Temperature profile at $t = 50\ h$. $\Delta T = 1°C$. Analytical (red) and numerical (blue) solutions.

3 Some validation examples

In this paper, two validation examples which are of a comparative nature are presented. The first one deals with a simple configuration of the Stefan problem for which analytical solutions exist. The second one is a comparison with a real experiment of heat conduction in a saturated porous media.

Example 1. Melting of a corner region Melting of an ice in an internal corner with the surfaces of the wedge maintained at equal temperatures higher than the melting temperature was considered in order to allow a comparison of the results obtained from the present method with exact analytical solutions in 2D case [2]. Medium is initially at $-10°C$ and the two conductive wedges are suddenly kept at $20°C$. Figure (2) illustrates the comparison between numerical solution and analytical one representing the fusion profile at one of the non-conductive boundaries. Figure (3) shows a comparison for the temperature history at $(x, y) = (5\ cm, 5\ cm)$.

Example 2. Heat conduction in 3D saturated porous media Several experiments have been done at the archaeological sites of Etiolles and Pincevent to study the prehistoric fire. In this

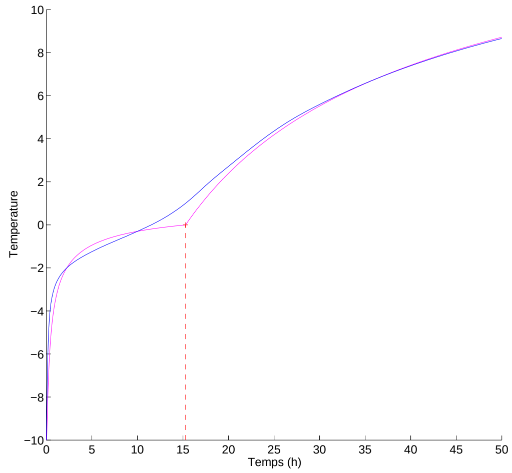

Figure 3: Temperature history at $(x, y) = (5\ cm, 5\ cm)$. Analytical (red) and numerical (blue) solutions.

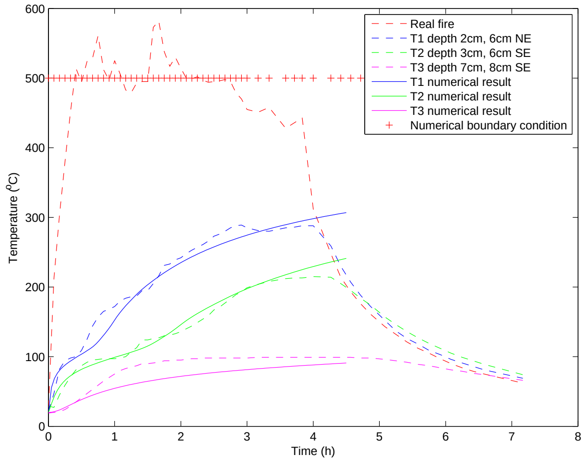

Figure 4: Comparison between numerical results and experimental ones.

example we provide a comparison between numerical simulation and results coming from a real experiment. The experiment has been done at the soil of Etiolles. 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. Figure (4) shows the comparison at different depths. The temperature of the real fire was measured at the center of the fire. However, for the simulation we supposed that the temperature of the fire is uniform and we used $500°C$ as a boundary condition at the surface. A non uniform progressive mesh has been used.

4 Conclusion

The presented approach in this paper used to solve non-linear heat conduction problems in a saturated porous media with phase change presented is very efficient. The proposed algorithm is very relevant and the examples presented show the accuracy obtained even when dealing with a real complicated case as shown in example 2. The developed code can deal with 2D and real 3D cases.

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