

NON-ISOTHERMAL EFFECTS ON MULTI-PHASE FLOW IN POROUS MEDIUM

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Key words: Non-isothermal multi-phase flow, partially saturated porous media, object-oriented finite element method

Summary. In this paper a ppT -formulation for non-isothermal multi-phase flow is given including diffusion and latent heat effects. Temperature and pressure dependencies of governing parameters are considered, in particular surface tension variation on phase interfaces along with temperature changes. A weak formulation of the governing equations is obtained by applying Galerkin's method of weighted residuals. The numerical model is implemented in the framework of the open source scientific software OpenGeoSys based on object-oriented programming (OOP) principles allowing model applications in various geotechnical areas. The classic benchmark for two-phase flow by McWhorter and Sunada¹ is used as a reference case on which non-isothermal effects and non-linear material behavior are studied.

1 INTRODUCTION

Numerical simulation of fluid flow and heat transport processes in the multi-phase flow model is conducted in various fields of practical applications. In many occasions, multi-phase/ multi-component processes are strongly affected by non-isothermal processes. In particular, when temperature is high enough in the domain of fluid flow, several non-linear physical phenomena need to take into account in the simulation. Such phenomena are vaporization, diffusion and capillary effects. Capillary effect due to interface curvature inside pores is induced by surface tension that alters the equilibrium between liquid water and water vapor. But this tension force is very sensitive to temperature and need to incorporate its variation with temperature. Normally liquid phase flow is very slow intact with a low permeable host medium. However even in such environments water vapor flow can develop due to a high thermal gradient present, therefore it is important to consider non-isothermal effects in those geological environments. It has several practical

applications such as groundwater remediation, geothermal energy or waste isolation. For instance, nuclear waste repositories in the deep to the earth are influenced by several interfering physical processes.

A general formulation for fluid flow and heat transport through a partially saturated porous medium is needed in order to show the clear picture of phase transitions by vaporization. In this sequence Baggio et al.² and Sanavia et al.³ has presented various types of governing partial differential equation for non-isothermal effects on multi-phase flow with their physical meaning. They emphasized on necessity of the heat source for vaporization and mention that through Kelvin equation it is possible to define a simple relation for water saturation, which is depending on capillary pressure and temperature. Numerical and experimental analysis of the hydro-thermal behavior of concrete with dehydration process at high temperatures is presented by Gawin et al.⁴ and Pont and Ehlacher⁵. A simple test problem was solved by Krejci⁶ in order to show the difference between linear and non-linear solution at high temperature. Basu et al.⁷ examined multi-phase flow of gaseous methane and liquid water during the drainage of methane from a coal seam in mining operations which has some considerable significance for mine safety with regard to explosion. Olivella and Gens⁸ presented vaporization of liquid water in unsaturated soil subjected to temperature gradients with capillary effect. They also made a distinction between the geothermal reservoir and the non-isothermal unsaturated soil approaches. Benet and Jouanna⁹ derived a phenomenological relation for phase change of liquid water in the porous medium when water vapor pressure is different from saturated water vapor pressure. Theoretical and experimental analysis has been conducted by Ruiz and Benet¹⁰ on phase change of a volatile liquid in unsaturated soil. They provided an expression for rate of phase change of liquid water present in the pores of solid skeleton.

Modeling of fluid flow and heat transport through undeformable (rigid) porous media has been presented in this study. Here pore of solid skeleton is filled with compressible fluid phase (dry air and water vapor). We have considered mass balance equation for each fluid phase and an energy balance equation. It is more convenient to separate water vapor and dry air masses in order to formulate mass balance equation for each phase. Sum of liquid water and water vapor masses represents liquid phase mass balance equation and dry air mass for gas phase mass balance equation. With this we developed a ppT formulation to describe the full system. Here, state of the porous medium is described by capillary pressure p^c , gas pressure p^g and temperature T .

2 NUMERICAL EXAMPLE

In the recent numerical study simulation has been performed about displacement process in the horizontal column. We assume that horizontal column is a partially saturated porous medium, initially the pores of the solid skeleton are filled with binary mixture of dry air and water vapor at temperature equal to 353.15 K. We solve the problem in one-dimensional domain with 260 linear finite elements up to the time duration 7.0×10^3 s. The non-linear iteration is restricted with maximum of 25 iterations.

Under isothermal condition McWhorter and Sunada¹ have presented a quasi-analytical solution for displacement of oil by water in a one-dimensional horizontal column. In order to verify the present numerical method we selected this problem as a benchmark test. In the benchmark, displaced and displacing fluids have common density and viscosity, i.e. density equal to $1.0 \times 10^3 \text{ kg m}^{-3}$ and viscosity equal to $1.0 \times 10^{-3} \text{ Pa s}$. Material parameters of the porous medium are presented in Table 1. We conducted a simulation on identical setup as in the McWhorter's problem and found that present water saturation is matching well with those of quasi-analytical solution. In Fig. 1 we show the comparison of water saturation profile for $7.0 \times 10^3 \text{ s}$ and we found that present water saturation is in close agreement.

Table 1: Material parameters of solid phase used in the computations.

Meaning	Symbol	Value/ Ref.	Unit
Density	ρ^s	2.0×10^3	kg m^{-3}
Heat capacity	c_p^s	1.091×10^3	$\text{J kg}^{-1} \text{K}^{-1}$
Thermal conductivity	κ^s	0.42	$\text{W m}^{-1} \text{K}^{-1}$
Entry pressure	p_{d0}	5.0×10^3	Pa
Absolute permeability	\mathbf{k}	1.0×10^{-10}	m^2
Total porosity	ϕ	0.3	-
Water saturation	S^l	Eq. (1)	-
Relative permeability	\mathbf{k}_{rel}	Brooks Corey	-

Water saturation is defined as extensive quantity per unit volume of pore space. In the present study, water saturation S^l is depending on capillary pressure p^c and temperature T . Brooks and Corey¹¹ present the relationship between water saturation and capillary pressure. Baggio et al.² mentioned that water saturation depends on temperature, and can be estimated through Kelvin equation. From this information it is possible to solve a simple differential equation in order to get the desired relation for water saturation.

$$S^l = \left(\frac{p_d T_0}{p^c T} \right)^m \quad (1)$$

Here, T_0 is the temperature at which water saturation S^l equals to one and m is the parameter related to the pore size distribution (small values represent single grain size material and large one for highly non-uniform material) and hydraulic parameter p_d referred as entry pressure.

Entry pressure is the measure of capillary pressure regarding to the start of the displacement. Surface tension σ on the phase interface induces a movement of fluids until a local equilibrium is reached. This equilibrium depends on several physical quantities and

temperature is one of them. Hence, it is possible to define a relation for entry pressure varies with temperature. Since capillary pressure can be scaled with surface tension, so

$$p_d = p_{d0} \left(\frac{\sigma(T)}{\sigma(T_0)} \right), \quad (2)$$

where, p_{d0} is assumed 5.0×10^3 Pa at temperature T_0 . Following correlation for surface tension has been used in the present study

$$\sigma(T) = 0.3258 \left(1.0 - \frac{T}{647.3 \text{ K}} \right)^{1.256} - 0.148 \left(1.0 - \frac{T}{647.3 \text{ K}} \right)^{2.256}. \quad (3)$$

Hence, entry pressure is a decreasing function of the temperature.

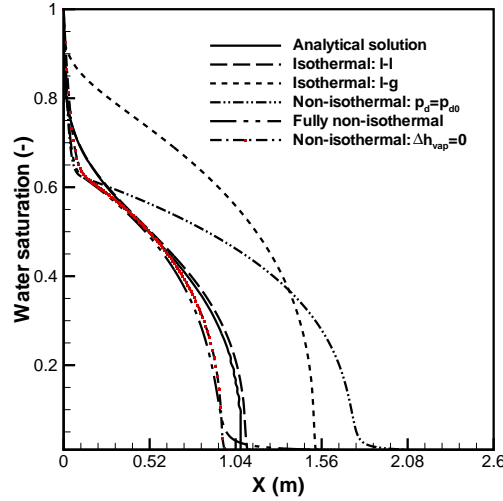


Figure 1: Water saturation S^l in the column from different conditions along with quasi-analytical solution at time 7.0×10^3 s.

In Fig. 1 we have presented the water saturation profile in the column from different cases/ conditions along with quasi-analytical solution at time 7.0×10^3 s. From the water saturation profile it is possible to make some prediction about displacement, i.e. how easily liquid water can move and how far it can reach in the column. Water saturation curve corresponding to the case when displaced and displacing fluids have common density and viscosity is included for reference, and it is close to quasi-analytical solution.

In many experimental studies it has found that a better displacement can be achieved with use of higher entry pressure. We have shown effect of temperature dependent entry pressure on pressure and temperature fields in Fig. 2. There we included curves corresponding to the condition of zero enthalpy of vaporization, i.e. $\Delta h_{vap} = 0$ and constant

entry pressure, i.e. $p_d = p_{d0}$ along with fully nonisothermal case at time 7.0×10^3 s. Fig. 2c show a significant difference in temperature profile corresponding to fully non-isothermal and zero enthalpy of vaporization condition. Hence, it is important to consider heat transport through latent heat of vaporization in the present study.

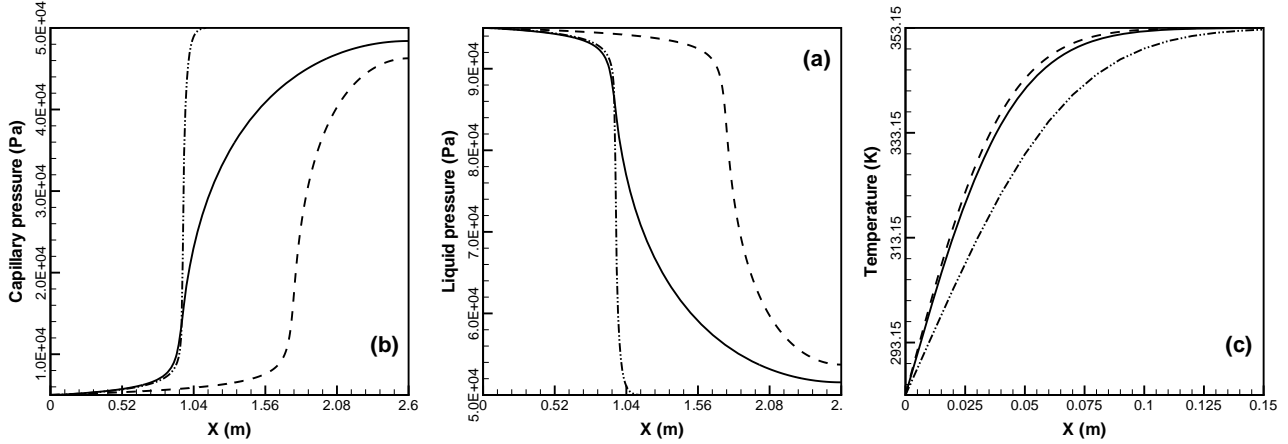


Figure 2: (a) Capillary pressure p^c ; (b) liquid pressure p^l ; (c) temperature T emerging from fully non-isothermal case (—); $p_d = p_{d0}$ (---); $\Delta h_{vap} = 0$ (-·-·-) at time 7.0×10^3 s.

We have presented liquid water and gas phase densities in Figs. 3 for time 1.0×10^3 , 4.0×10^3 and 7.0×10^3 s. Liquid water density is calculated by $\rho_w^l = \rho_w^l(T_0) (1 - \beta_T (T - T_0))$, here we used a temperature dependent thermal expansion coefficient $\beta_T (= -\frac{1}{\rho_w^l(T_0)} \frac{\partial \rho_w^l}{\partial T})$. Density of liquid water is measured by temperature and thermal expansion coefficient (which itself increasing with temperature). On increment in temperature, liquid water density is lowered by both quantities, i.e. temperature and thermal expansion coefficient. Distribution of the gas density depends on gas pressure and temperature. And what we have shown in Fig. 3b represents that at the left end gas density is maximum. A sharp decrement has been observed while moving toward right end. Vapor mole-fraction x_w^g is used for the approximation of dynamic viscosity, heat capacity and thermal conductivity for the gas phase.

Dynamic viscosity of the pure water depends on the temperature whereas binary mixture of gas also dose on its composition in addition to the temperature. Unlike the viscosity of pure water dry air viscosity is increasing with increase of temperature. However increase in temperature results in development of water vapor. So at high temperature gas phase is assumed a binary mixture of water vapor and dry air. The addition of water vapor in the gas phase, forces gas viscosity to behave as a decreasing function of temperature. Pruess¹² and Hirschfelder et al.¹³ computed viscosity of binary mixture of water vapor and dry air; whereas water vapor viscosity is according to IFC¹⁴.

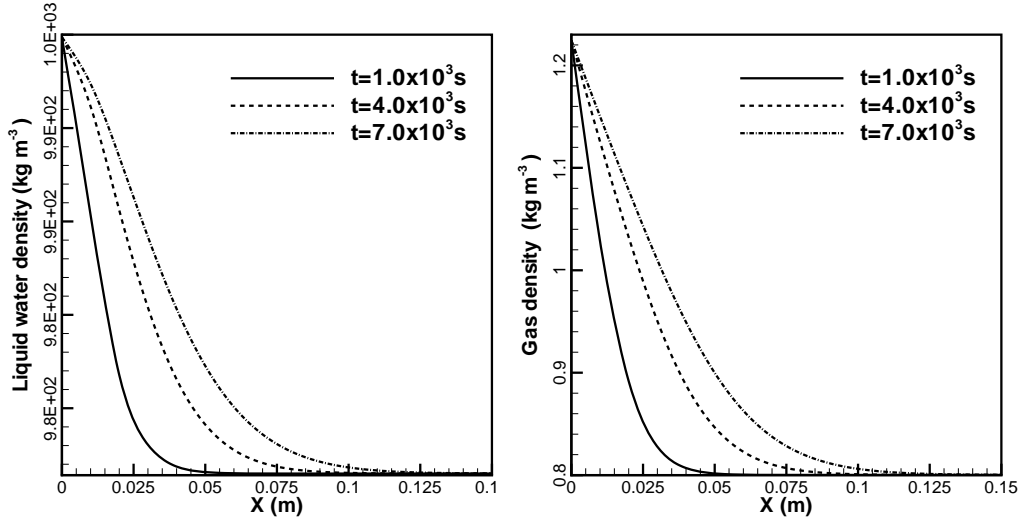


Figure 3: Density distribution of the liquid water and gas.

Gas viscosity μ^g shows the trend which is exactly the same as described by Pruess¹², i.e. it starts increasing with increase of temperature until gas phase has only dry air. As soon as enough water vapor has been added into the gas phase it starts decreasing and asymptotically reaches to the viscosity value of water vapor and dry air mixture at 353.15 K, i. e. 1.7402×10^{-5} Pa s. And liquid water viscosity μ^l shows that at left end where temperature is 283.15 K liquid water viscosity has the maximum value then it start decreasing with increase of temperature up to a certain distance beyond it becomes uniform.

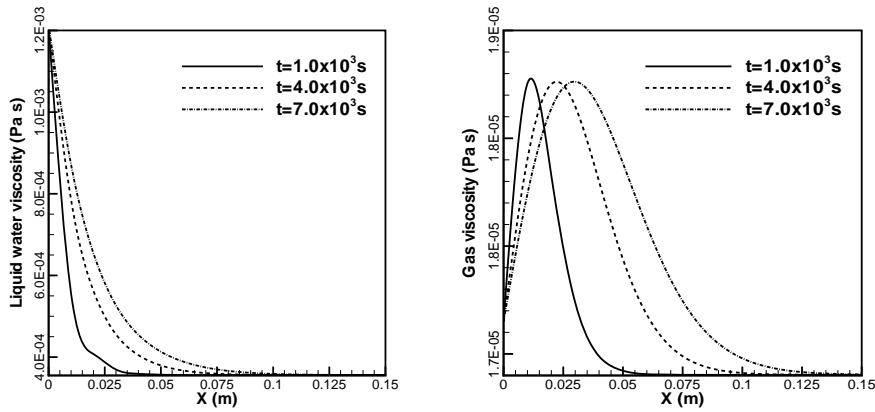


Figure 4: Resulting profile of viscosity for time 1.0×10^3 , 4.0×10^3 and 7.0×10^3 s.

3 CONCLUSIONS

In this paper a numerical non-isothermal multi-phase model has been developed for the analysis of geotechnical problems. The following progress has been achieved in the presented work.

- A ppT formulation of the governing equations for non-isothermal multi-phase flow through a partially saturated porous medium has been developed, i.e. the chosen primary variables are gas and capillary pressures as well as equilibrium temperature. In comparison to commonly used pST formulations the ppT concept has advantages in particular for the accuracy of the finite element method with no upwind technique. Temperature effects have been included by means of the general Clausius-Clapeyron equation of state for phase change. Densities of water vapor and dry air have been calculated by ideal gas law. The variability of the complete material properties of porous medium and fluids such as capillarity, relative permeability, mobility, density, viscosity, heat capacity and thermal conductivity has been investigated in detail.
- We used a combined monolithic / staggered coupling scheme with automatic control of time stepping, i.e. monolithic for the multi-phase flow and staggered for the heat transport.
- We proved the importance of latent heat effects on vaporization by showing the significant difference in temperature profiles when comparing with $\Delta h_{vap} = 0$ (see Fig. 2c).
- In a previous work Olivella and Gens⁸ estimated the entry pressure required to initiate the desaturation process in an unsaturated porous medium. We further developed this scaling technique to investigate temperature dependent entry pressure for fluid displacement. The entry pressure can be used to estimate temperature effects on sorption equilibrium due to curvature of concave meniscus separating liquid water and water vapor. We used this sorption equilibrium to study how the water saturation changes with temperature. A new relation is presented which is accounting to both temperature and capillary effects.
- The numerical scheme has been implemented in the framework of object-oriented FEM and, therefore, allows an easy extension of the numerical non-isothermal multi-phase model for multi-dimensional problems.

4 Acknowledgements

The authors acknowledge the funding by the German Federal Ministry of Education and Research (BMBF) within the framework of the CO₂-MoPa and the CLEAN joint projects as parts of the Special Programme GEOTECHNOLOGIEN.

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