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MULTIPHYSICS MODELING OF CRACKS IN MULTIPHASE POROUS MATERIALS – PRELIMINARY VALIDATION

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Abstract. This paper presents a coupled multiphysics model for the simulation of crack initiation and propagation in multiphase porous materials, integrating a Thermo-Hydro-Mechanical (THM) model with a crack phase-field (PF) approach for brittle fracture. The fully coupled THM governing equations are formulated within the Hybrid Mixture Theory, describing the THM behavior of saturated and non-isothermal porous media. The proposed model aims to simulate the fracture evolution under diverse mechanical, hydraulic, thermal and environmental loadings. Validation cases including tensile test and thermo-mechanical thermal shock demonstrate the model's accuracy through comparisons with established finite element codes or analytical solutions.

1 INTRODUCTION

The numerical simulation of coupled phenomena in multiphase porous materials is essential for predicting and understanding the behavior under multiple interacting physical processes up to the material and structural failure. This study develops an efficient coupled approach to analyze the multiphysics interactions in multiphase porous media, taking into account fluids flow, heat transfer and mechanical deformation up to the crack initiation and propagation. The governing equations are derived at the macroscopic scale within the Hybrid Mixture Theory. The phase-field approach is integrated to represent brittle fracture, providing a robust numerical framework for crack evolution. This work enhances previous models by incorporating gas pressure and temperature effects, extending validations to complex multiphysics scenarios. The proposed model has broad relevance to engineering fields such as geomechanics, materials science, and porous media analysis.

2 GOVERNING EQUATIONS

This section summarizes the coupled THM and fracture model to characterize crack initiation and propagation in multiphase porous materials. The THM fields are fully coupled, incorporating interactions between thermal, hydraulic and mechanical phenomena at the macroscopic level, while the fracture process is modeled through a crack phase-field approach. The macroscopic balance equations reported below are derived from [1] for liquid saturated deformable porous media.

2.1 Balance equations of the THM problem

The transient thermo-hydro-mechanical behavior for the water saturated porous media under study is described using macroscopic balance equations formulated according to Hybrid Mixture Theory [1]. Quasi-static loading conditions are assumed in these equations and developed in the geometrically linear framework according to [2].

The equilibrium equations in terms of effective Cauchy's stress are expressed as:

$$\nabla \cdot (\boldsymbol{\sigma}' - p^w \mathbf{1}) + \rho \mathbf{g} = \mathbf{0} \tag{1}$$

in which $\sigma'(\boldsymbol{x}, t)$ denotes the effective stress tensor, $\rho(\boldsymbol{x}, t)$ represents the mixture density defined as $\rho = [1 - n]\rho^s + n\rho^w$, $n(\boldsymbol{x}, t)$ the porosity, g the gravity acceleration vector and 1 is the second order identity tensor.

The mass conservation equation for the liquid water is,

$$\rho^w \nabla \cdot \left(\frac{\partial \mathbf{u}}{\partial t} \right) - \nabla \cdot \left(\rho^w \frac{\mathbf{k}}{\mu^w} \left[\nabla p^w - \rho^w \mathbf{g} \right] \right) - \rho^w \beta_{sw} \frac{\partial T}{\partial t} = 0 \tag{2}$$

where $\mathbf{k}(\boldsymbol{x}, t)$ is the intrinsic permeability tensor and $\mu^w(\boldsymbol{x}, t)$ the dynamic water viscosity. $\beta_{sw}(\boldsymbol{x}, t) = [1 - n]\beta_s + n\beta_w$ is the cubic thermal expansion coefficient of the medium, β_s and β_w being the solid and water cubic thermal expansion coefficient, respectively. In equation (2), the water flux has been described using the Darcy law.

The energy balance equation accounts for convective and conductive heat transfer within the porous medium has the following form:

$$(\rho C_p)_{eff} \frac{\partial T}{\partial t} - \left(\rho^w C_p^w \frac{\mathbf{k}}{\mu^w} \left[\nabla p^w - \rho^w g \right] \right) \cdot \nabla T - \nabla \cdot (\chi_{\text{eff}} \nabla T) = 0 \tag{3}$$

where $(\rho C_p)_{\text{eff}} = (1-n)\rho^s C_p^s + n\rho^w C_p^w$ is the effective thermal capacity of porous medium, C_p^s and C_p^w the specific heat of solid and water, respectively, and χ_{eff} the effective thermal conductivity of the porous medium. This balance equation neglects the terms related to the mechanical work induced by density variations due to temperature changes of the phases and induced by volume fraction changes.

2.2 Phase-field evolution equation

Brittle fracture propagation is modeled in this paper adopting the crack phase-field variable d. This variable represents the damage state of the material up to crack initiation and propagation, evolving in time according to an equation derived from the principle of energy minimization and the variational derivative of the fracture energy functional [3, 4, 5]:

$$\frac{G_c}{l}(d - l^2\Delta d) - 2(1-d)\boldsymbol{H} = 0 \tag{4}$$

Here, G_c is the critical energy release rate (fracture toughness), l is the internal length scale parameter controlling the diffusive crack width, and $\boldsymbol{H}$ is the history variable protecting crack irreversibility by storing the maximum tensile energy density attained.

To numerically solve the coupled system of equations governing displacements, water pressure, temperature and phase-field variables, a nested staggered iterative scheme is employed. This approach solves the THM equations (1) - (3) monolithically and, sequentially, the phase-field evolution equation (4), promoting both computational stability and convergence efficiency.

3 MODEL VALIDATION

In this section, the robustness and accuracy of the proposed coupled THM phase-field fracture model is validated against benchmark problems across different couplings. To this end, validation tests encompass mechanical, hydro-mechanical and thermo-mechanical problems are solved and compared with established numerical codes, analytical benchmarks and experimental observations available in the literature. In the following, only two cases are described.

3.1 Mechanical validation with phase-field

The mechanical validation focuses on assessing the implemented phase-field fracture framework within the Comes-Geo software [1, 2] by benchmarking its results against those obtained via the GRIPHFiTH finite element code [6], widely recognized for its accuracy in phase-field simulations.

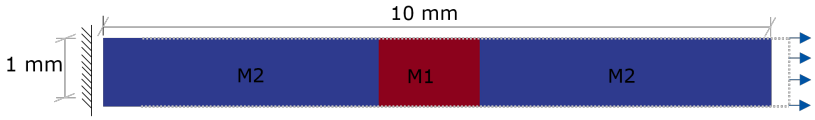

Figure 1: Geometry tension test bar

Table 1: Parameters of the tensial bar with a weaker material in the middle

Material	M1	M2
Tensile strength (GPa)	21	210
Fracture Toughness-Gc (kN/mm)	0.0027	
Internal Length (mm)	0.4	
Number of Elements	625	

The validation test consists of a uniaxial tensile mechanical experiment conducted on a bar composed of two materials with differing mechanical strengths. The specimen geometry features a weaker intermediate zone material M1) sandwiched between stronger outer zones (material M2), which introduces a stress concentration for the crack initiation within the weaker region. The right boundary of the specimen undergoes displacement-controlled loading with total displacement increment of 0.05 mm in 100 incremental loading steps, applied as a Dirichlet boundary condition, simulating a tensile test. This setup is illustrated in Fig. 1. The introduction of the weak zone section effectively mimics heterogeneous material behavior frequently

encountered in engineering applications, thereby serving as an insightful benchmark for fracture propagation modeling.

The material parameters defining tensile strength and fracture toughness (Gc) for each material are summarized in Table 1. Notably, material M1 exhibits significantly lower tensile strength, creating a preferential crack path centrally within the specimen.

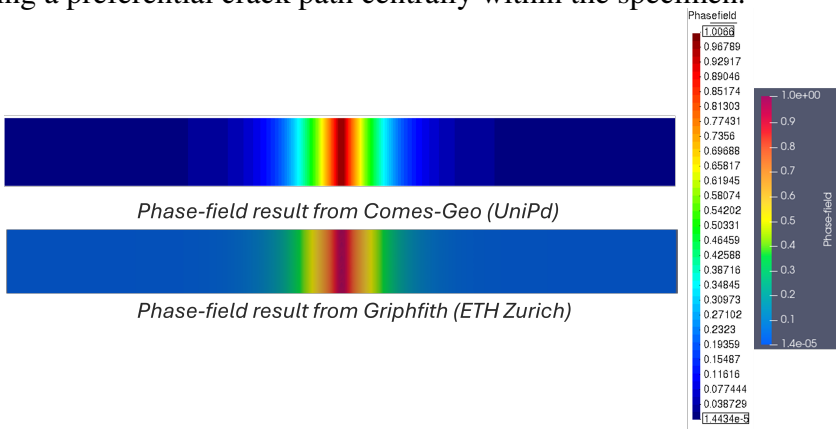

Figure 2: Comparison of phase-field solutions obtained from GRIPHFiTH and ComesGeo codes

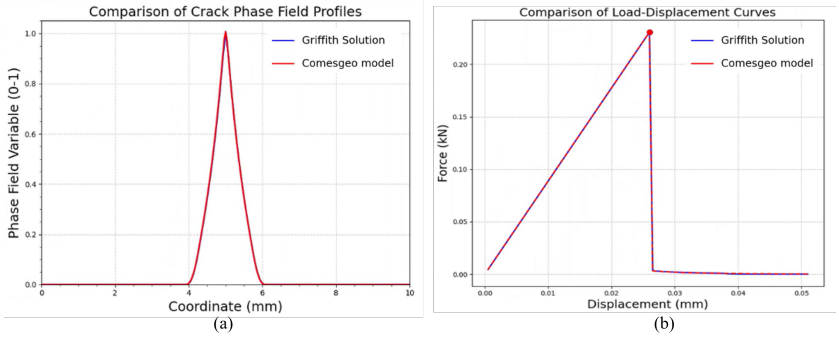

Figure 3: Comparison of phase-field solution profiles (x-direction) and force–displacement response obtained from GRIPHFiTH and Comes-Geo codes

The phase-field solution generated by both ComesGeo and GRIPHFiTH codes at the point of final tensile failure exhibits excellent visual agreement, as depicted in Fig. 2. Quantitative comparison further reinforces this agreement, with phase-field profiles along the horizontal axis at the final loading step and force-displacement curves evolving over time showing negligible discrepancies (Figures 3a and 3b, respectively). These results confirm the ability of the implemented numerical framework to accurately resolve crack patterns and mechanical response during progressive tensile loading.

3.2 Thermo-Mechanical validation with phase-field

The final stage of validation involves assessing the thermo-mechanical component of the proposed model by comparing it against the one-dimensional analytical solution through a benchmark case [7, 8]. To align with the benchmark setup, the governing equations (1)-(3) were simplified from a multiphase porous medium description to that of a dense solid ceramic plate

by assigning $n = 0$ and $\alpha = 0$. The system is initialized at a uniform temperature of T_0 = 300 °C and subsequently quenched to a surface temperature of T^* = 20 °C. A time increment of $d_t = 1 \times 10^{-4}$ s is employed, with the simulation carried out until 2000×10^{-4} s. The geometry and boundary conditions are illustrated in Fig. 4. The analytical solution for the temperature distribution, T_{ana}, is given by [7, 8],

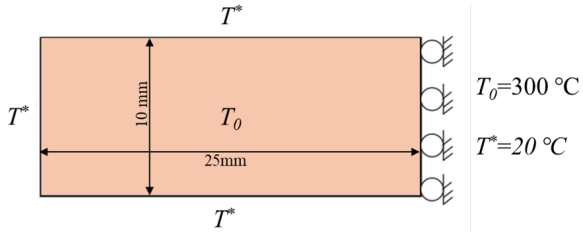

Figure 4: geometry and boundary condition

E	370 GPa
v	0.3
χ_{eff}	31 W/(mk)
ρ^s	3980 kg/m^3
C_p	880 $J/(kgK)$
β_s	7.5×10^{-6} K^{-1}

Table 2: Material properties

$$T_{ana}(x,t) = T^* + 4\,(T_0 - T^*) \times \sum_{i=1,3,5,\ldots} \left(\frac{\sin(i\pi x/L)}{i\pi} \exp\left(-\frac{i^2\pi^2 D}{L^2} \cdot t \right) \right) \tag{5}$$

where L is the specimen height, and the thermal diffusivity is defined as $D = \frac{\chi_{eff}}{\rho_s C_p}$.

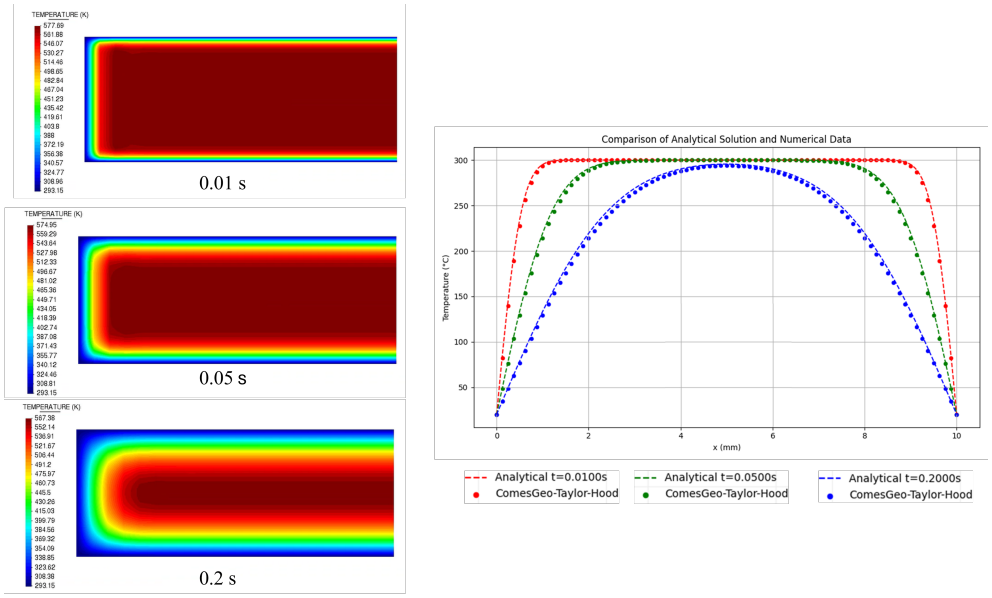

Figure 5: Quenching simulation: numerical temperature contours at $t = 10, 50$, and $200\,\mathrm{ms}$ (left), and comparison of transient temperature profiles with the 1D analytical solution (right).

The material parameters from [7, 8] are summarized in Table 2. The left panels of Fig. 5 present the simulated temperature field at $t = 10, 50$ and $200\,\mathrm{ms}$, while the corresponding comparisons between the analytical and numerical temperature profiles along the vertical axis y are shown in the right panels

These results were obtained using a coarse-mesh. The boundary conditions are identical to those of the benchmark case. The internal length parameter is set to $l = 0.5\,\mathrm{mm}$ and the geometry is discretized with quadrilateral elements of size $l/4$. Fig. 6 illustrates the predicted

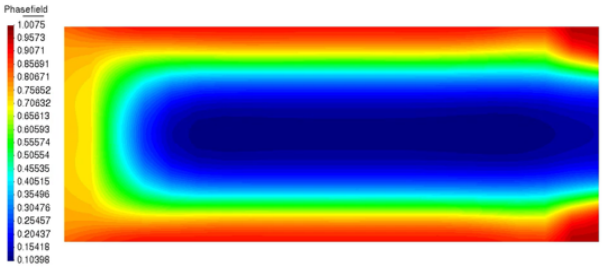

Figure 6: Phase-field solution at 200 ms

homogeneous phase-field distribution at $t = 200\,\mathrm{ms}$, where fracture region coincides with region undergoing sharp temperature gradients during the quenching process. The simulation with a fine-mesh is currently in progress (where a surface crack localization is emerging).

4 CONCLUSIONS

This study introduces a comprehensive coupled thermo-hydro-mechanical and phase-field model for water saturated porous materials. The model successfully captures interactions among mechanical stress, water pressure and thermal gradients, to predict crack formation. Validation against a mechanical tension test and a thermal shock benchmark shows the model ability and accuracy. The multiphysics framework advances the predictive modeling of cracks in complex porous environments, supporting future developments in material design and failure analysis under coupled loading conditions. Ongoing work focuses on extension to unsaturated conditions [9, 10], refining mesh resolution and extending applications to diverse real-world porous media systems.

Nomenclature

C_p	effective specific heat of porous medium [$\mathrm{Jkg^{-1}\,K^{-1}}$]
C_p^w	specific heat of liquid phase [$\mathrm{Jkg^{-1}\,K^{-1}}$]
C_p^s	specific heat of solid [$\mathrm{Jkg^{-1}\,K^{-1}}$]
$(\rho C_p)_{\mathrm{eff}}$	effective thermal capacity of porous medium [$\mathrm{JL^{-3}\,K^{-1}}$]
g	gravity acceleration [$\mathrm{ms^{-2}}$]
k	intrinsic permeability tensor [$\mathrm{m^2}$]
M_w	molar mass of water [$\mathrm{kg\ kmol^{-1}}$]
n	total porosity (pore volume/total volume) [-]
p^w	liquid water pressure [Pa]
T	absolute temperature [K]
t	time [s]
$\mathbf{u}$	displacement vector of solid matrix [m]
$\mathbf{E}$	Young modulus [Pa]
$\mathbf{v}$	Poisson ratio
α	Biot cofficient

Greek symbols

β_{sw}	combined (solid + liquid) cubic thermal expansion coefficient [$\mathrm{K^{-1}}$]
β_s	cubic thermal expansion coefficient of solid [$\mathrm{K^{-1}}$]

β_w	thermal expansion coefficient of liquid water [K^{-1}]
χ_{eff}	effective thermal conductivity of the porous medium [$\mathrm{Wm}^{-1}\mathrm{K}^{-1}$]
Δt	time step [s]
μ^w	water viscosity [$\mu\mathrm{Pas}$]
ρ	apparent density of porous medium [kgm^{-3}]
ρ^w	liquid phase density [kgm^{-3}]
ρ^s	density of the solid grains [kgm^{-3}]
σ	Cauchy stress tensor [Pa]
σ'	effective stress tensor [Pa]

Mathematical operators

Δ	Laplacian
$\nabla\cdot$	divergence
∇	gradient

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