COMSOL in a New Tensorial Formulation of Non-Isothermal Poroelasticity

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Abstract: The presence of a moving fluid in a porous rock modifies its mechanical response. Poroelasticity explains how the fluid inside the pores bears a portion of the total load supported by the rock. The remaining part of the load is supported by the elastic skeleton, which contains a laminar fluid coupled to the framework by equilibrium and continuity conditions. This work introduces an original tensorial formulation of Biot's theory and the experimental thermoporoelastic parameters that support the theory. By defining a 4-dimensional total stress tensor and three basic poroelastic coefficients, we deduce a system of differential equations coupling the bulk rock and the fluid. The inclusion of the fourth dimension allows extending the theory of solid linear elasticity to thermoporoelastic rocks, taking into account the effect of both the fluid phase and the Introducing three volumetric temperature. thermal dilation coefficients, one for the fluid and two for the skeleton, a complete set of parameters for geothermal poroelastic rocks are obtained.

Keywords: Poroelasticity, thermoporoelasticity, Biot's theory, finite elements.

1. Introduction

Several factors affect the geomechanical behavior of porous crustal rocks containing fluids: porosity, pressure, and temperature, characteristics of the fluids, fissures, and faults. Rocks in underground systems (aquifers, geothermal and hydrocarbon reservoirs) are porous, compressible, and elastic. The presence of a moving fluid in the porous rock modifies its mechanical response. Its elasticity is evidenced by the compression that results from the decline of the fluid pressure, which can shorten the pore volume. This reduction of the pore volume can be the principal source of fluid released from storage. A rock mechanics model is a group of equations capable of predicting the porous medium deformation under different internal and external forces. In this paper, we present an original four-dimensional tensorial formulation of linear thermo-poroelasticity theory. This formulation makes more comprehensible the linear Biot's theory, rendering the resulting equations more convenient to be solved using the Finite Element Method. To illustrate practical aspects of our model some classic applications are outlined and solved using the Earth Science Module of COMSOL-Multiphysics.

1.1 Experimental background

In classic elastic solids only the two Lamé moduli, (λ, G) or Young's elastic coefficient and Poisson's ratio (E, ν) , are sufficient to describe the relations between strains and stresses. In poroelasticity, we need five poroelastic moduli for the same relationships (Bundschuh and Suárez, 2009), but only three of these parameters are independent. The Biot's field variables for an isotropic porous rock are the stress σ acting in the rock, the bulk volumetric strain ε_B , the pore pressure p_f and the variation of fluid mass content ζ . The linear relations among these variables are the experimental foundations of Biot's poroelastic theory (Biot & Willis, 1957; Wang, 2000):

$$\varepsilon_{B} = \frac{\sigma}{K_{B}} + \frac{p_{f}}{H}, \quad \zeta = \frac{\sigma}{H} + \frac{p_{f}}{R}$$

$$\Leftrightarrow \begin{pmatrix} \varepsilon_{B} \\ \zeta \end{pmatrix} = \begin{pmatrix} C_{B} & H^{-1} \\ H^{-1} & R^{-1} \end{pmatrix} \cdot \begin{pmatrix} \sigma \\ p_{f} \end{pmatrix}$$
(1)

Where K_B , H, and R are poroelastic coefficients that are experimentally measured as follows (Wang, 2000):

$$\varepsilon_{B} = \frac{\Delta V_{B}}{V_{B}}, \quad C_{B} = \left(\frac{\Delta \varepsilon_{B}}{\Delta \sigma}\right)_{p_{f}}, \quad K_{B} = \frac{1}{C_{B}}$$

$$\frac{1}{H} = \left(\frac{\Delta \varepsilon_{B}}{\Delta p_{f}}\right)_{\sigma} = \left(\frac{\Delta \zeta}{\Delta \sigma}\right)_{p_{f}}, \quad \frac{1}{R} = \left(\frac{\Delta \zeta}{\Delta p_{f}}\right)_{\sigma}$$
⁽²⁾

The following figure (1) illustrates all the parts forming a poroelastic medium.



Figure 1. Skeleton of sandstone showing its pores and solid grains $(3 \times 3 \times 3 \text{ mm}^3)$. (Piri, 2003).

Here V_B is the bulk volume, consisting of the rock skeleton formed by the union of the volume of the pores V_{Φ} and the volume of the solid matrix $V_{\rm S}$ (Fig. 1). The control volume is ΔV_B . The drained coefficients K_B and C_B are the bulk modulus and the bulk compressibility of the rock, respectively; 1/H is a poroelastic expansion coefficient, which describes how much ΔV_B changes when p_f changes while keeping the applied stress σ constant; 1/H also measures the changes of ζ when σ changes and p_f remains constant. Finally 1/R is an unconstrained specific storage coefficient, which represents the changes of ζ when p_f changes. Inverting the matrix equation (1) and replacing the value of σ in ζ we obtain:

$$\sigma = K_B \varepsilon_B - \frac{K_B}{H} p_f \implies$$

$$\zeta = \frac{K_B}{H} \varepsilon_B + \left(\frac{1}{R} - \frac{K_B}{H^2}\right) p_f \qquad (3)$$

The sign conventions are stress $\sigma > 0$ in tension and $\sigma < 0$ in compression; the volumetric strain $\varepsilon_B > 0$ in expansion and $\varepsilon_B < 0$ in contraction; the fluid content $\zeta > 0$ if fluid is added to the control volume ΔV_B and $\zeta < 0$ if fluid is extracted from ΔV_B ; the pore pressure $p_f > 0$ if it is larger than the atmospheric pressure. Biot (1941) and (Biot & Willis, 1957) introduced three additional parameters, *b*, *M* and *C*, that are fundamental for the tensorial formulation herein presented. 1/M is called the constrained specific storage, which is equal to the change of ζ when p_f changes measured at constant strain. Both parameters *M* and *C* are expressed in terms of the three fundamental ones defined in equation (2):

$$\frac{1}{M} = \left(\frac{\Delta\zeta}{\Delta p_f}\right)_{\varepsilon_B} = \frac{1}{R} - \frac{K_B}{H^2} \implies$$

$$M = \frac{RH^2}{H^2 - K_B R}; \quad C = \frac{K_B}{H} M$$
(4)

Let $C_S = 1/K_S$ be the compressibility of the solid matrix. The Biot-Willis coefficient *b* is defined as the change of confining pressure p_k with respect to the fluid pressure change when the total volumetric strain remains constant:

$$b = \left(\frac{\partial p_k}{\partial p_f}\right)_{\varepsilon} = 1 - \frac{K_B}{K_S} = \frac{C}{M} = \frac{K_B}{H}$$
(5)

The coefficient *C* represents the coupling of deformations between the solid grains and the fluid. The coefficient *M* is the inverse of the constrained specific storage, measured at constant strain (Wang, 2000); this parameter characterizes the elastic properties of the fluid because it measures how the fluid pressure changes when ζ changes.

These three parameters b, M and C are at the core of the poroelastic partial differential equations we introduce herein (Bundschuh and Suárez, 2009).

2. Isothermal Poroelasticity Model

Let u_s and u_f be the displacements of the solid and fluid particles; let $u = u_f - u_s$ be the displacement of the fluid phase relative to the solid matrix respectively. Let ε_s , ε_f , φ_s , φ , V_s and V_f be the volumetric dilatations, porosities and volumes of each phase; $-\varepsilon_V$ is the volumetric deformation of the fluid phase relative to the solid phase. The mathematical expressions of these variables are:

$$\frac{\Delta V_S}{V_S} = \varepsilon_s = \vec{\nabla} \cdot \vec{u}_S; \quad \frac{\Delta V_f}{V_f} = \varepsilon_f = \vec{\nabla} \cdot \vec{u}_f$$
$$\varepsilon_V = \varepsilon_S - \varepsilon_f; \quad \vec{u} = \vec{u}_f - \vec{u}_S \implies -\varepsilon_V = (6)$$
$$-\vec{\nabla} \cdot \left(\vec{u}_S - \vec{u}_f\right) = \vec{\nabla} \cdot \vec{u} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}$$

Biot and Willis (1957) introduced the strain variable ζ (*u*, *t*), defined in equation (3), to describe the volumetric deformation of the fluid relative to the deformation of the solid with homogeneous porosity:

$$\zeta(\vec{u},t) = \varphi \vec{\nabla} \cdot \left(\vec{u}_s - \vec{u}_f\right) = \varphi \varepsilon_s - \varphi \varepsilon_f = \varphi \varepsilon_V \quad (7)$$

The function ζ represents the variation of fluid content in the pore during a poroelastic deformation. The total applied stresses in the porous rock are similar to the equations of classic elasticity. However, we need to couple the effect of the fluid in the pores. The linear components of the global stresses, deduced experimentally by Biot, (Biot, 1941; Biot and Willis, 1957; Wang, 2000) are:

$$\sigma_{ij} = \lambda_U \,\varepsilon_B \,\delta_{ij} + 2 G \,\varepsilon_{ij} - C \,\zeta \,\delta_{ij} \qquad (8)$$

Where:

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \ \delta_{ij} = \begin{cases} 1, \text{ if } i = j \\ 0, \text{ if } i \neq j \end{cases}$$
$$\lambda_U = \lambda + Cb; \text{ for } i, j = x, y, z$$

The fluid pressure is deduced from equation (3):

$$p_f = \frac{K_B R H^2}{H^2 - K_B R} \left[\frac{\zeta}{K_B} - \frac{\varepsilon_B}{H} \right]$$
(9)

We define a two-order tensor $\sigma_{T} = (\sigma_{ij})$ in four dimensions, which includes the bulk stress tensor σ_{B} acting in the porous rock and the fluid stress σ_{F} acting in the fluid inside the pores, positive in compression:

$$\sigma_T = \sigma_B + \sigma_F \implies$$

$$\sigma_{ij} = \left(\lambda_U \,\varepsilon_B - C\,\zeta\right) \delta_{ij} + 2\,G\,\varepsilon_{ij} \qquad (10)$$

$$\sigma_f = p_f = M\,\zeta - C\,\varepsilon_B; \ i, j = x, y, z$$

This tensorial equation becomes identical to the Hookean solids equation, when the rock has zero porosity and b = 0. From equations (8) and (9), we deduce that:

$$\sigma_{ij} = \tau_{ij} - b \, p_f \, \delta_{ij} \tag{11}$$

$$\tau_{ij} = \lambda \, e_B \, \delta_{ij} + 2 \, G \varepsilon_{ij} \tag{12}$$

Tensor τ_{ij} is called the Terzaghi (1943) effective stress that acts only in the solid matrix; bp_f is the pore-fluid pressure. Since there are no shear tensions in the fluid, the pore fluid pressure affects only the normal tensions σ_i (i = x, y, z). The functions σ_{ij} are the applied stresses acting in the porous rock saturated with fluid. The solid matrix (τ_{ij}) supports one portion of the total applied tensions in the rock and the fluid in the pores (bp_f) supports the other part. This is a maximum for soils, when $b \approx 1$ and is minimum for rocks with very low porosity where $b \approx 0$. For this reason, b is called the effective stress coefficient.

Inverting the matrices of equations (8) and (9), we arrive to the following tensorial form of the poroelastic strains:

$$\varepsilon_{ii} = \frac{\sigma_{ii}}{2G} - \frac{3\nu}{E}\sigma_M + \frac{p_f}{3H}; \ \varepsilon_{ij} = \frac{\sigma_{ij}}{2G}$$
 (13a)

$$\zeta = \frac{\sigma_M}{H} + \frac{p_f}{R} = \frac{C \sigma_M + K_U p_f}{M K_U - C^2}$$
(13b)

$$\sigma_{M} = \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3} = K_{B} \varepsilon_{B} - bM\zeta$$

$$K_{B} = \lambda + \frac{2}{3}G; \quad K_{U} = K_{B} + b^{2}M$$
(14)

The coefficient K_U is the undrained bulk modulus, which is related to the previous defined coefficients. Note that both tensorial equations (10) and (13) only need four basic poroelastic constants. The presence of fluid in the pores adds an extra tension due to the hydrostatic pressure, which is identified with the pore pressure, because it is supposed that all the pores are interconnected. This linear theory is appropriate for isothermal, homogeneous, and isotropic porous rocks.

3. ThermoPoroelasticity Model

The equations of non-isothermal poroelastic processes are deduced using the Gibbs thermoporoelastic potential or available enthalpy per unit volume and the energy dissipation function of the skeleton (Coussy, 1991).

Analytic expressions are constructed in terms of the stresses, the porosity, the pore pressure, and the density of entropy per unit volume of porous rock. As we did for the isothermal poroelasticity, we can write in a single fourdimensional tensor the thermoporoelastic equations relating stresses and strains. We have for the pore pressure:

$$p - p_0 = M \left(\zeta - \zeta_0\right) - C\varepsilon_B$$

- $M \varphi \left(\gamma_{\varphi} - \gamma_f\right) \left(T - T_0\right)$ (15)

The volumetric thermal dilatation coefficient γ_B [1/K] measures the dilatation of the skeleton and γ_{φ} [1/K] measures the dilatation of the pores:

$$\gamma_B = \frac{1}{V_B} \left(\frac{\partial V_B}{\partial T} \right)_{p_k} \quad \left[\frac{1}{\mathrm{K}} \right] \tag{16}$$

$$\gamma_{\varphi} = \frac{1}{V_{\varphi}} \left(\frac{\partial V_{\varphi}}{\partial T} \right)_{p_f} = \frac{1}{\varphi} \left(\frac{\partial \varphi}{\partial T} \right)_{p_f} \quad \left[\frac{1}{\mathrm{K}} \right] \quad (17)$$

The fluid bulk modulus K_f and the thermal expansivity of the fluid γ_f [1/K] are defined as follows:

$$\frac{1}{K_f} = C_f = \frac{1}{\rho_f} \left(\frac{\partial \rho_f}{\partial p} \right)_T$$
(18)

$$\gamma_f = \frac{1}{V_f} \left(\frac{\partial V_f}{\partial T} \right)_{p_f} = \frac{-1}{\rho_f} \left(\frac{\partial \rho_f}{\partial T} \right)_{p_f}$$
(19)

The term p_k is the confining pressure. Expanding the corresponding functions of the Gibbs potential and equating to zero the energy dissipation we obtain the 4D thermoporoelastic equations, which include the thermal tensions in the total stress tensor (Bundschuh and Suárez, 2009):

$$\sigma_{ij} - \sigma_{ij}^{0} = \left(\lambda \varepsilon_B - b\left(p - p_0\right)\right) \delta_{ij} + 2G \varepsilon_{ij} - K_B \gamma_B \left(T - T_0\right)$$
(20)

In this case, an initial reference temperature T_0 and an initial pore pressure p_0 are necessary because both thermodynamic variables T and pare going to change in non-isothermal processes occurring in porous rock. The fluid stress is deduced in a similar way:

$$\sigma_{f} = p_{f} = M \left(\zeta - \zeta_{0} \right) - C \varepsilon_{B} - M \varphi \left(\gamma_{\varphi} - \gamma_{f} \right) \left(T - T_{0} \right)$$
⁽²¹⁾

4. Dynamic Poroelastic Equations

The formulation we introduced herein is very convenient to be solved using the Finite Element Method. The fundamental poroelastic differential equation is the tensorial form of Newton's second law in continuum porous rock dynamics:

$$\vec{div} \, \vec{\sigma}_T + \vec{F} = \rho \frac{\partial^2 \vec{u}}{\partial t^2}; \ \vec{div} \, \vec{\sigma}_T = \mathbf{I}^T \cdot \vec{\sigma}_T$$
(22)
where : $\vec{\sigma}_T = C_B \cdot \vec{\varepsilon}_T; \ \vec{\varepsilon}_T = \mathbf{I} \cdot \vec{u}$

The terms σ_T and ε_T are the equivalent vectorial form of tensorial equations (20) and C_B is the matrix of poroelastic constants. While **F** is the body force acting on the rock and the tensor differential operator \mathcal{L} is given by:

$$\mathbf{I}^{T} = \begin{pmatrix} \partial_{x} & 0 & 0 & \partial_{y} & \partial_{z} & 0 & \partial_{x} \\ 0 & \partial_{y} & 0 & \partial_{x} & 0 & \partial_{z} & \partial_{y} \\ 0 & 0 & \partial_{z} & 0 & \partial_{x} & \partial_{y} & \partial_{z} \end{pmatrix}$$
(23)
$$\mathbf{I} \cdot \begin{pmatrix} u_{x} \\ u_{y} \\ u_{z} \end{pmatrix} = \vec{\varepsilon}_{T} = (\varepsilon_{x} \ \varepsilon_{y} \ \varepsilon_{z} \ \varepsilon_{xy} \ \varepsilon_{xz} \ \varepsilon_{yz} \ e_{r})$$

Where $u = (u_x, u_y, u_z)$ is the displacement vector of equation (6). Using the operator \mathbb{Z} in equation (22), the dynamic poroelastic equation becomes:

$$\left(\mathbb{I}^{T} \cdot \mathbb{C}_{B} \cdot \mathbb{I}\right) \cdot \vec{u} + \vec{F} = \rho \frac{\partial^{2} \vec{u}}{\partial t^{2}}$$
(24)

4.1 Solution of Thermoporoelastic Equations: The Finite Element Method

Equation (24) includes Biot's poroelastic theory. It can be formulated and numerically solved using the Finite Element Method (FEM). Let Ω be the bulk volume of the porous rock, and let $\partial\Omega$ be its boundary, \boldsymbol{u} is the set of admissible displacements in Eq. (22); \mathbf{f}_{b} is the volumetric force and \mathbf{f}_{s} is the force acting on the surface $\partial\Omega$. After doing some algebra we arrive to a FEM fundamental equation for every element V^{e} in the discretization:

$$\mathcal{K}^{e} \cdot \vec{d}^{e} + \mathcal{M}^{e} \cdot \frac{\partial^{2} \vec{d}^{e}}{\partial t^{2}} = \vec{F}^{e}; \ e = 1, M$$
(25)

 \mathbf{d}^{e} is a vector containing the displacements of the nodes in each V^{e} . Equation (25) approximates the displacement \boldsymbol{u} of the poroelastic rock. \mathbf{F}^{e} is the vector of total nodal forces. K^{e} and M^{e} are the stiffness and equivalent mass matrices for the finite element V^{e} . The mathematical definitions of both matrices are:

$$\mathcal{K}^{e} = \int_{V^{e}} \mathcal{B}^{T} \cdot \mathcal{C}_{B} \cdot \mathcal{B} \, \mathrm{d} \, \mathrm{V} \, ; \quad e = 1, M$$

$$\mathcal{B} = \mathcal{I} \cdot \mathcal{N} \, ; \quad \mathcal{M}^{e} = \int_{V^{e}} \rho \, \mathcal{N}^{T} \cdot \mathcal{N} \, \mathrm{d} \, \mathrm{V}$$
(26)

Where \mathbb{N} is the matrix of shape functions that interpolate the displacements (Liu and Quek, 2003). Matrix \mathbb{B} is called the strain poroelastic matrix.

5. Use of COMSOL Multiphysics

This section contains two brief illustrations of the deformation of an aquifer (Leake & Hsieh, 1997) and the form that a temperature change can affect its poroelastic deformation. In the first example, we assume cold water at 20° C (1000 kg/m³). After, we consider a temperature of 250° C (50 bar, 800.4 kg/m³). Results are shown in figures (4) to (9). To simplify the discussion we use the same model previously solved by COMSOL-Multiphysics and described in the Earth Science Module (COMSOL AB, 2006):

"Three sedimentary layers overlay impermeable bedrock in a basin where faulting creates a bedrock step (BS) near the mountain front (Fig. 2). The sediment stack totals 420 m at the deepest point of the basin (x = 0 m) but thins to 120 m above the step (x > 4000 m). The top two layers of the sequence are each 20 m thick. The first and third layers are aquifers; the middle layer is relatively impermeable to flow.



Figure 2. Simplified geometry of the aquifer and the impermeable bedrock in the basin. Initial state.



Figure 3. The mesh of the basin with 2967 elements.

As given by the problem statement, the materials here are homogeneous and isotropic within a layer. The flow field is initially at steady state, but pumping from the lower aquifer reduces hydraulic head by 6 m per year at the basin center (under isothermal conditions). The head drop moves fluid away from the step. The fluid supply in the upper reservoir is limitless. The period of interest is 10 years".

The corresponding FE mesh has 2967 elements excluding the bedrock step (Figure 3). The rock is Hookean, poroelastic and isothermal. In the first example we use the same data of the ES Module user's guide, except for the Biot-Willis coefficient we assume that b = 0.3.



Figure 4. Poroelastic deformation of the basin for the BS problem with cold water (20°C). Streamlines represent the fluid to porous rock coupling.



Figure 6. Vertical strain at the basin with a BS. Case of cold water (20°C).



Figure 8. Horizontal strain at the basin with a BS. Case of cold water (20°C).



Figure 5. Poroelastic deformation of the basin for the BS problem with hot water $(250^{\circ}C)$. Streamlines represent the fluid to porous rock coupling.



Figure 7. Vertical strain at the basin with a BS. Case of hot water (250°C).



Figure 9. Horizontal strain at the basin with a BS. Case of hot water $(250^{\circ}C)$.

6. Discussion of Results

The two examples presented herein were solved using COMSOL–Multiphysics for a wellknown problem of linked fluid flow and solid deformation near a bedrock step in a sedimentary basin described in the Earth Science module. The problem concerns the impact of pumping for a basin filled with sediments draping an impervious fault block. In the first example, we considered the water in the aquifer to be cold, at 20°C. In the second example, the water is hot, at 250°C. The basin is composed of three layers having a total depth of 500 m and is 5000 m long in both cases.

Figures (4) and (5) show simulation results for years 1, 2, 5, and 10, respectively. The difference here with the results of COMSOL Multiphysics is that we have performed the simulation of a thermoporoelastic - coupled deformation when the water in the aquifer corresponds to geothermal conditions (fluid density of 800.4 kg/m³, temperature of 250 °C, and pressure of 50 bar). Figures (6) and (7) compare the vertical strains and figures (8) and (9) compare the horizontal strains, in both cases respectively. Figures (8) and (9) also illustrate the evolution of lateral deformations that compensate for the changing surface elevation above the bedrock step. Note that vertical scales are different in both examples for clarity.

7. Conclusions

■ All crustal rocks forming geothermal reservoirs are poroelastic and the fluid presence inside the pores affects their geomechanical properties.

• The elasticity of aquifers and geothermal reservoirs is evidenced by the compression resulting from the decline of the fluid pressure, which can shorten the pore volume. This reduction of the pore volume can be the principal source of fluid released from storage

• The immediate physical experience shows that the supply or extraction of heat produces deformations in the rocks. Any variation of temperature induces a thermo-poroelastic behavior that influences the elastic response of porous rocks.

• We introduced herein a general tensorial thermoporoelastic model that takes into account

both the fluid and the temperature effects in linear porous rock deformations, and presenting two practical examples solved with COMSOL.

• The second example illustrates the influence of temperature changes on the poroelastic strains. For cold water, the estimated value of ε_z is about -1.5×10^{-4} , while for hot water ε_z is -7.5×10^{-4} . Therefore, the poroelastic deformations are much higher in geothermal reservoirs than in isothermal aquifers. In the first case the bulk modulus of water K_w = 0.45 GPa, corresponding to $T = 250^{\circ}$ C. For cold aquifers K_w = 2.5 GPa.

• Water bulk modulus affect other poroelastic coefficients, including the expansivity of rocks, which is relatively small, but its effects can produce severe structural damages in porous rocks subjected to strong temperature gradients, as happens during the injection of cold fluids.

8. References

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