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# A thermo-poro-mechanical constitutive and numerical model for deformation in sedimentary basins



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#### ABSTRACT

Comprehensive modeling of sedimentary basins should integrate the coupled nature of different phenomena such as sediment compaction, pore-fluid flow and heat transport. In this context, the thermal evolution of the basin plays an important role in the mechanical and chemo-mechanical deformation processes as heat modifies fluids viscosity and minerals physicochemical properties, thus affecting pore fluid expulsion and mineral stability. The present paper describes a three-dimensional constitutive and numerical model specifically devised for dealing with thermo-poromechanical deformation processes during diagenesis. The sedimentary basin is modeled as a fully saturated thermo-poro-elastoplastic-viscoplastic medium undergoing large strains. A key feature of the model is related to the evolution of the sediment material properties associated with temperature and large irreversible porosity changes. The computational model, which integrates both poroplastic and poroviscoplastic components of deformation at large strains, relies upon a parallel implementation of the finite element method with a shared memory multiprocessing interface. Numerical simulations of gravitational compaction during the sediment accretion phase as well as along geological period of pore pressure dissipation are performed in the context of oedometric setting. Special emphasis is given to temperature effects on the deformation history of the basin.

#### 1. Introduction

Relaying upon available or postulated geological scenario related to successive events that have affected the basin along its life cycle, modeling and simulation of a sedimentary basin seeks to primarily understanding the geological history and providing a relevant description of corresponding poromechanical state by reconstructing the deformation processes during diagenesis. Referring for intake to petroleum engineering activities, predicting the thermal evolution and porosity reduction histories of the basin, together with the evolution of fundamental poromechanical parameters, such as permeability distribution, is of major importance, as the combined effects of deformation and heat flow control reservoir formation and hydrocarbon generation. Nevertheless, the progress in basin modeling still remains a challenging issue in geosciences and formulation of a comprehensive thermo-poromechanical description of the geological material reveals a complex task, since it should integrate mechanical, geochemical, geophysical and geological aspects. Sedimentary basin form when an appreciable amount of waterborne sediments in shallow seas are deposited during geological time. As burial proceeds, deposited sediments experience several physical and chemical processes that modify their poromechanical properties. Heating, compaction and pore-fluid flow are fundamental aspects in the formation of sedimentary basins. Models devoted to basin simulation should therefore incorporate these coupled phenomena in order to properly capture essential aspects of diagenesis.

One of the major issues refers to the modeling of compaction process. From a mechanical viewpoint, deformation in sedimentary basins is controlled by two mechanisms: (1) purely mechanical compaction originated mainly from rearrangement of solid particles and subsequent pore fluid expulsion during burial, and (2) chemo-mechanical compaction resulting from Intergranular Pressure-Solution (IPS), generally induced by stress and temperature. Purely mechanical compaction prevails in the upper layers of the basin, whereas chemo-mechanical compaction dominates for deeper burial as stress and temperature increase. Depth and thickness of the transition zone located in between depends on the nature of sediment material as well as on field conditions. Along the transition

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zone, mechanical and chemo-mechanical deformations occur simultaneously as strongly interdependent processes (Angevine and Turcotte, 1983; Gutierrez and Wangen, 2005; Hedberg, 1936; Schmidt and McDonald, 1979; Schneider et al., 1996; Tada and Siever, 1989). Furthermore, deformation mechanisms in a sedimentary basin may be substantially affected by the thermal evolution of the basin, as heat modifies fluid viscosity and physicochemical properties of minerals, thus affecting fluid flow and mineral stability. Temperature increases with depth and depends on several factors such as mantle heat flow, radioactive processes and thermal conductivity of the porous material. The latter property evolves with compaction as the thermal conductivity of fluids and minerals may be significantly different (Bjorlykke, 2010; de Boer, 1977; Gosnold, 1990; Morgan and Gosnold, 1989; Niemeijer et al., 2002; Renard et al., 1999; Yang, 2000).

In this general context, the paper presents a three-dimensional thermo-poromechanical constitutive and numerical model for compaction in sedimentary basins. The approach extends the isothermal formulation developed in Brüch et al. (2016) to incorporate the temperature effects on the basin evolution analysis. Purely mechanical and chemo-mechanical deformations are respectively addressed by means of poroplastic and poroviscoplastic components in the macroscopic state equations (Maghous et al., 2013; Schneider and Hay, 2001; Zhang and Spiers, 2005). A key feature of the model refers to its ability to account for the evolution of sediment material properties associated with temperature and large irreversible porosity changes (Abdulagatova et al., 2009; Amir et al., 2008; Bernaud et al., 2002; Deudé et al., 2004; Dormieux and Maghous, 2000; Somerton, 1992; Vosteen and Schellschmidt, 2003; Waples and Waples, 2004). The basin simulator relies on a parallel finite element implementation of proposed constitutive model with shared memory multiprocessing interface. A specific numerical procedure is used to model the sediment accretion periods by progressive activation of gravity forces within a fictitious closed material system (Bernaud et al., 2006).

For illustrative purposes, an oceanic basin simulation is performed in the last part of the paper, considering a single column of elements intended to represent a horizontal infinite layer of sediments submitted to gravitational compaction under oedometric conditions. During accretion phase and subsequent basin evolution, several aspects of diagenesis are investigated by means of the numerical simulations. The evolution along geological time of local poromechanical state of the sediment material is analyzed in conjunction with the overall behavior of the sedimentary basin. The primary objective of the numerical simulation is to demonstrate the ability of the proposed approach to deal with complex multi-coupled geological processes involved in a basin lifecycle. Particular emphasis is dedicated to assess temperature effects on the deformation history of the basin.

#### 2. Theoretical aspects

As burial proceeds, compaction processes induce significant porosity reduction along the basin, reaching in some situations deformation levels as high as 50%. Appropriate predicting model for deformation in sedimentary basin requires therefore the constitutive behavior of the sediment material to be formulated within the context of large irreversible strains, incorporating both the geometric and physical nonlinearities at the state equations level (Bernaud et al., 2002, 2006; Brüch et al., 2016). The purpose of this section is to extend the poromechanical framework and concepts formulated in the previous works to account for the effects of heat transport on the deformation processes in sedimentary basins.

#### 2.1. State equations

The state equations of the sedimentary rock, modeled as a fully saturated porous material, are formulated at macroscopic scale. At this scale, the representative elementary volume (particle of the porous medium) is the superposition of two particles located at the same

geometrical point and remaining in thermal equilibrium at any instant of time (Coussy, 2004; Dormieux et al., 2006): a skeleton particle and a fluid particle associated with the fluid saturating the interconnected porous space. The skeleton is the macroscopic expression of the solid phase. Let  $d\Omega_0$  (resp.  $d\Omega_t$ ) denote the reference initial (resp. the current) configuration of the representative elementary volume of the porous medium. In any configuration, the amount of fluid content can be conveniently related to the Eulerian porosity  $\varphi = d\Omega_t^f/d\Omega_t$  defined as the pore-fluid volume in the considered configuration normalized by the total current volume. Alternatively, it is also convenient to normalize the pore-fluid volume by the total reference volume, yielding the so-called Lagrangian porosity  $\phi = d\Omega_t^f/d\Omega_0$ . These macroscopic quantities are connected through by relationship  $\phi = J\varphi$ , where  $J = d\Omega_t/d\Omega_0$  denotes the Jacobian of the transformation between  $d\Omega_0$  and  $d\Omega_t$ .

In the framework of finite poroplasticity, the constitutive behavior is defined by two state equations expressed in rate-type form, together with complementary relations specifying the flow rule structure (Dormieux and Maghous, 1999; Bernaud et al., 2002). In what follows, it is assumed that the reversible part of the deformation gradient of the skeleton particles remains infinitesimal, which implies that large strains involved in the compaction process are of irreversible nature. Furthermore, anisotropy of the thermo-poromechanical properties of the sediment material induced by the compaction process is disregarded. Extending the isothermal formulation provided in Brüch et al. (2016), the first state equation, relating the Cauchy total stress rate  $\dot{\underline{a}}$ , the pore-fluid pressure rate  $\dot{p}$  and temperature rate  $\dot{T}$  to the strain rate tensor  $\underline{d}$  defined as the symmetric part of the velocity gradient, reads

$$\frac{D_{J}\underline{\underline{\underline{\sigma}}}^{1le}}{Dt} = \underline{\dot{\underline{\sigma}}}^{1le} + \underline{\underline{\sigma}}^{1le} \cdot \underline{\underline{\Omega}} - \underline{\underline{\Omega}} \cdot \underline{\underline{\sigma}}^{1le} 
= \underline{\underline{C}} : (\underline{\underline{d}} - \underline{\underline{d}}^{ir}) + \underline{\dot{\underline{C}}} : \underline{\underline{\sigma}}^{1le}$$
(1)

where  $\underline{Q}$  is the spin rate tensor (skew-symmetric of the velocity gradient) that aims at taking the large rotation of the elementary volume into account, whereas the irreversible part of strain rate  $\underline{\underline{d}}^{ir} = \underline{\underline{d}}^p + \underline{\underline{d}}^{vp}$  is additively split into two contributions, namely the plastic component of strain  $\underline{\underline{d}}^p$  that accounts for purely mechanical compaction, and the viscoplastic component  $\underline{\underline{d}}^{vp}$  that represents creep compaction resulting from Intergranular Pressure-Solution. The fourth-order tensor  $\underline{C}$  is the material drained elastic stiffness moduli and expresses by virtue of isotropy assumption:

$$C = (K - 2\mu/3) \underline{\underline{1}} \otimes \underline{\underline{1}} + 2\mu \underline{1}$$
 (2)

Where K and  $\mu$  denote the bulk and shear modulus, respectively.  $\underline{\underline{1}}$  and  $\underline{1}$  refer to the second and fourth-order identity tensors. The state equation (1) involves:

A rotational time derivative  $D_J/Dt$  of the generalized Biot effective stress tensor  $\underline{\underline{\sigma}}^{te} = \underline{\underline{\sigma}} + bp \, \underline{\underline{1}} + 3K\alpha^s \Delta T \, \underline{\underline{1}}$ , where b is the Biot coefficient and  $\alpha^s$  the thermal dilation coefficient of the solid phase (Coussy, 2004);

An additional term related to the particulate derivative  $\dot{C}$  of the tensor of drained elastic moduli, which aims at capturing the evolution of the elastic properties with microstructural changes due to large irreversible strains (Dormieux and Maghous, 2000).

The second state equation relates the pore volume change rate  $\dot{\phi}$  to the pore-fluid pressure rate  $\dot{p}$ , temperature rate  $\dot{T}$  and to the strain rate d:

$$\dot{p} = M \left( -b \operatorname{tr} \left( \underline{\underline{d}} - \underline{\underline{d}}^{ir} \right) + \frac{\dot{\phi} - \dot{\phi}^{ir}}{J^{ir}} + 3\alpha^{\phi} \dot{T} \right)$$

$$+ \frac{\dot{M}}{M} p - M \dot{b} \operatorname{tr} \left( C^{-1} : \underline{\underline{\sigma}}^{ue} \right) + 3M \dot{\alpha}^{\phi} \Delta T$$
(3)

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