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Thermo coupled elastoplastic-viscoplastic solutions for compaction process in sedimentary basins

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Abstract. This work presents semianalytical solutions for the deformation induced by gravitational compaction in sedimentary basins. Formulated within the framework of thermo coupled plasticity–viscoplasticity at large strains, the modeling dedicates special emphasis to the effects of material densification associated with large irreversible porosity changes on the stiffness and hardening of the sediment material. The analysis is restricted to the fully drained setting in which excess pore-pressures are disregarded. In addition, the thermal problem is posed, formulating the thermal field with constant parameters. These solutions can be viewed as reference solutions for verification and benchmarks of basin simulators.

Keywords: sedimentary basin, large strains, thermo coupled elastoplasticity-viscoplasticity, semi-analytical approach.

1 Introduction

The sedimentary basins are natural geological structures with significant economical interest due to hydrocarbons, groundwater, and mineral reserves. Exploration of these resources need a understanding of the coupled phenomena that occur over timescale, and for this reason, the models (analytical and numerical) are of considerable importance as they permit to test different scenarios of a basin history.

The mechanical model used to describe compaction through time is one of the key aspects of basin simulation as tectonic subsidence and basin deformation are strongly coupled with fluid flow and thermal evolution. For example, in siliciclastic rocks two main types of compaction mechanisms can take place, the purely mechanical and chemo-mechanical compaction. The first prevails in the early stages of a newly deposited layer due to grain rearrangement and subsequent pore fluid expulsion, whereas the second progressively dominates as continuous burial increases sediments temperature and effective stresses resulting from dissolution, diffusion, and precipitation of minerals, known as intergranular pressure solution (IPS) (Schmidt and Mcdonald [1]).

Lemos et al. [2] presents the development of semianalytical solutions for the deformation induced by gravitational compaction in sedimentary basins. These solutions can be viewed as reference solutions for verification and benchmarks of basin simulators. The mechanical compaction is modeled with a plastic component, while for chemo-mechanical compaction a viscoplastic model is used. Formulated within the framework of coupled plasticity–viscoplasticity at large strains, the modeling dedicates special emphasis to the effects of material densification associated with large irreversible porosity changes on the stiffness and hardening of the sediment material.

Based on this model, the work presents the formulation of analytical and semianalytical reference solutions that describe the deformation and thermal processes in a sedimentary basin. This research corresponds to the initial results of the study of the thermal field and its effects on the behavior of the sedimentary basin.

2 Statement of the thermo-mechanical problem

The thermo-mechanical problem under consideration refers to the evaluation of stresses, strains and temperatures developing in a sedimentary basin under oedometric conditions during the formation phases by continuous accretion of sediment material. The analysis shall focus on deformation induced in the basin by purely mechanical and chemo-mechanical compaction processes.

While purely mechanical compaction originates mainly from rearrangement of the solid particles during burial and can thus be modeled in the framework of plasticity, chemo-mechanical compaction resulting from IPS phenomena is generally associated with creep-like deformation. In addition, compaction process in a sedimentary basin generally involves large strains, the reduction in porosity of the sediment material exceeding in many situations values as high as 50% (Houseknecht [3]). The theoretical framework of coupled elastoplasticity–viscoplasticity at finite strains appears therefore suitable for accurate description of the mechanics controlling the basin deformation.

The temperature of the sedimentary basins increases with depth. Therefore, the heat flow is upward, transported from the interior to the exterior of the Earth, where the heat source originates from radiogenic processes. In the asthenosphere this heat is carried mainly by convection, while in the lithosphere it is carried mainly by conduction. Although the water flow can also transport heat in the basins, the movement of the fluids is usually very slow, and it can be considered that in many cases the heat transport is controlled by conduction (Bethke [4]; Jessop and Majorowicz [5]; Bjørlykke [6]; Cloetingh et al. [7]).

For the purpose of formulate semianalytical solutions for the compaction process in sedimentary basins, a simplified configuration based on the following assumptions is adopted: (a) sedimentation occurs in oedometric conditions; (b) the sediment has homogeneous and isotropic mechanical properties in its reference state, that is, the instant it is deposited at the top of the basin; (c) the effect of pore pressure is disregarded in the analysis, which is equivalent to addressing the particular case of highly permeable sediment material (fully drained conditions); (d) mechanical evolution is decoupled from the thermal evolution of the basin, disregarding the effect of the thermal gradient on the material properties and strains; and (e) thermal evolution is decoupled from mechanical evolution, disregarding the effect of compaction on thermal properties.

The sedimentary basin undergoing compaction is modeled as an infinite layer, perpendicular to the $\underline{e}_3$ direction and lying on a rigid substratum along the plane $x_3 = 0$. Despising the tectonic activity, the gravitational field $\underline{g} = -g\underline{e}_3$ stands for the only external loading in the compaction process. Additionally, the anisotropy of constitutive properties of the material in its reference state and that induced by compaction processes are neglected in the analysis. In this simplified framework, the physical quantities involved in the problem only depend on time and the vertical coordinate x_3. The position of a material particle in the sedimentary layer at a time t is defined by coordinate as x_3, whereas the instant when the particle is deposited at the top of the layer is referred to as $T(x_3, t)$.

Due to the continuous deposition of sediments at the top of the basin, the sediment layer thickness is time dependent. Whereas the top of the layer remains horizontal, the position of the upper boundary is defined by the gravitational compaction law $x_3 = H(t)$ (see Fig. 1).

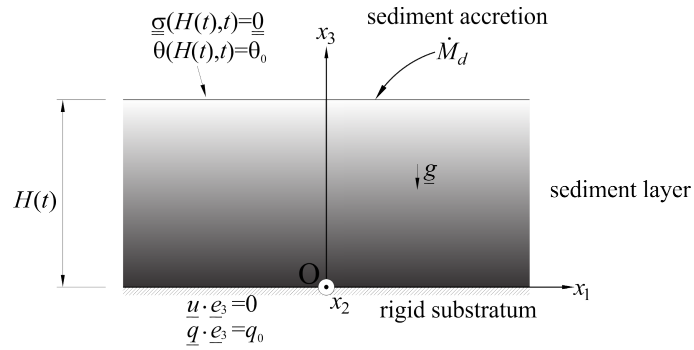


Figure 1. Geometry model for sedimentary basin and thermo-mechanical loading conditions

2.1 Field equations

From the mechanical point of view, the quasistatic BVP is defined by two field equations. The momentum balance equation (neglecting the inertial effects) and the mass balance equation (in the Eulerian and Lagrangian formulations) reads as follows:

$$\mathrm{div}\underline{\underline{\sigma}}(x_3,t) + \rho(x_3,t)\underline{g} = \underline{0}, \quad \frac{\partial\rho(x_3,t)}{\partial t} + \mathrm{div}\left(\rho(x_3,t)\,\underline{u}(x_3,t)\right) = 0 \quad \text{and} \quad \rho(x_3,t) = \frac{\rho_0}{J(x_3,t)}, \tag{1}$$

where $\underline{\underline{\sigma}}$ is the Cauchy stress tensor, ρ is the mass density of the sediment material, $\underline{u}$ is the Eulerian velocity field of the sediment particles, ρ_0 is the initial mass density and $J = d\Omega_t/d\Omega_0$ is the Jacobian of the transformation, that is, the ratio of the volume of a particle at the current configuration to the initial configuration.

The initial conditions of the physical quantities associated with the material particles seated at the top of the sedimentary basin (viewed as an open material system) and the boundary condition of the velocity field of the particles in contact with the rigid substrate are expressed by:

$$\underline{\underline{\sigma}}(H(t),t) = \underline{\underline{0}}, \quad J(H(t),t) = 1, \quad \rho(H(t),t) = \rho_0 \quad \text{and} \quad \underline{u}(0,t) \cdot \underline{e}_3 = 0. \tag{2}$$

In the context of oedometric compaction setting, which implicitly disregards the effects of plate tectonics, together with the disregard of loading induced anisotropy and the assumption of homogeneity of the deposited sediment material along the whole accretion period, the general form for the velocity and stress fields is expressed as

$$\underline{u}(x_3,t) = u_3(x_3,t)\underline{e}_3 \quad \text{and} \quad \underline{\underline{\sigma}} = \sigma_h(x_3,t)(\underline{e}_1 \otimes \underline{e}_1 + \underline{e}_2 \otimes \underline{e}_2) + \sigma_v(x_3,t)\underline{e}_3 \otimes \underline{e}_3. \tag{3}$$

From the thermal point of view, the heat conduction equation is written in Eulerian form as

$$\rho c \frac{d\theta(x_3,t)}{dt} + \text{div}\underline{q}(x_3,t) = r, \quad \text{with} \quad \underline{q}(x_3,t) = -\underline{\underline{K}} \cdot \underline{\nabla}\theta(x_3,t), \tag{4}$$

where c is the specific heat, θ is the temperature field, $\underline{q}$ is the heat flow vector (Fourier's law), r is the heat generation per unit volume and $\underline{\underline{K}}$ is the thermal condutivity tensor of the porous medium.

The thermal field has the following initial and boundary conditions:

$$\theta(H(t),t) = \theta_0 \quad \text{and} \quad \underline{q}(0,t) \cdot \underline{e}_3 = q_0, \tag{5}$$

where θ_0 is a constant prescribed value for the temperature field associated with the material particles seated at the top of sedimentary basin and q_0 is a constant prescribed value for the heat flow in the contact with the rigid substratum.

2.2 Loading and geometrical transformation

The magnitude of the loading applied to the sedimentary basin is characterized by the mass of sediments deposited per unit area $M_d(t)$ on the top of the basin during the time interval [0,t]:

$$M_d(t) = \int_0^{H(t)} \rho(x_3,t)dx_3. \tag{6}$$

The vertical stretch $\Lambda(x_3,t)$ defines the ratio between the height of a particle in the current configuration at time t and its height in the reference state at time $T(x_3,t)$ (see Fig. 2).

The gradient of the geometrical transformation of a particle between the reference and the current states under oedometric conditions takes the following form:

$$\underline{\underline{F}}(x_3,t) = \underline{e}_1 \otimes \underline{e}_1 + \underline{e}_2 \otimes \underline{e}_2 + \Lambda(x_3,t)\underline{e}_3 \otimes \underline{e}_3. \tag{7}$$

The Eulerian gradient of the velocity field $\underline{\underline{\nabla}}\ \underline{u}$ is related to $\underline{\underline{F}}$ according to $\underline{\underline{\nabla}}\ \underline{u} = \dot{\underline{\underline{F}}} \cdot \underline{\underline{F}}^{-1}$, which leads to the strain rate tensor $\underline{\underline{d}} = \frac{1}{2}(\underline{\underline{\nabla}}\ \underline{u} + {}^t\underline{\underline{\nabla}}\ \underline{u})$.

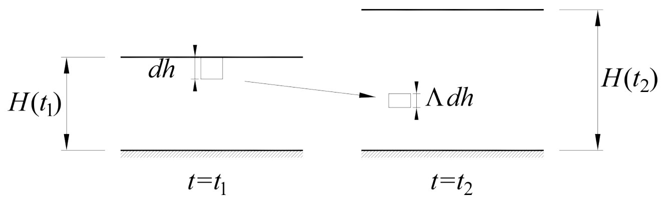


Figure 2. The particle vertical stretch

2.3 Constitutive equations, plastic and viscoplastic behavior

The sediment is modeled as an isotropic elastic–plastic–viscoplastic material that is subjected to large strains. The anisotropy induced by the compaction on the sediment mechanical properties is disregarded. In the geometric transformation, the elastic strains are assumed to remain infinitesimal, while large strains produced are irreversible nature.

Whereas the solid phase that constitutes the skeleton particle is incompressible, the solid mass balance implies that the Eulerian porosity (current pore volume fraction) is expressed as (Dormieux and Maghous [8])

$$\varphi(x_3,t) = 1 - \frac{1-\phi_0}{J(x_3,t)} \approx 1 - \frac{1-\phi_0}{J_{ir}(x_3,t)}, \tag{8}$$

where $\phi_0 = \varphi(H(t),t)$ refers to sediment porosity in the reference state and J_{ir} is the irreversible component of the Jacobian transformation, which is close to the total Jacobian $J_{ir} \approx J$ owing to the assumption of infinitesimal elastic strains.

The equation 8 relates current porosity to volumetric dilatation of the sediment material during burial. It is expected that the large porosity variation modifies the material elastic properties (Dormieux and Maghous [8]). The progressive reduction in porosity induces an increase in stiffness of the skeleton elastic modulus, which is modeled by the Hashin–Shtrikman upper bounds formulated for isotropic composite materials. These variational bounds coincide with the micromechanical estimates derived from Mori-Tanaka scheme (Maghous et al. [9]), which are known to reasonably model the elastic properties of isotropic porous media (Zaoui [10], Dormieux et al. [11]). The expressions for the bulk and shear moduli as a function of porosity are given by

$$K(\varphi) = \frac{4k^s\mu^s(1-\varphi)}{3k^s\varphi + 4\mu^s} \quad \text{and} \quad \mu(\varphi) = \frac{\mu^s(1-\varphi)(9k^s+8\mu^s)}{k^s(9+6\varphi)+\mu^s(8+12\varphi)}, \tag{9}$$

where k^s and μ^s are the bulk and shear moduli of the solid phase, which are assumed to be unaffected by compaction processes.

A strong coupling between elasticity and plastic-viscoplastic component of the constitutive behavior is introduced by equations 8 and 9. The state equations describing the stress–strain relationship can be formulated in rate-form as follows (Dormieux and Maghous [8]):

$$\dot{\underline{\underline{\sigma}}} = \underset{\sim}{C} : (\underline{\underline{d}} - \underline{\underline{d}}^{ir}) + \dot{\underset{\sim}{C}} : \underset{\sim}{C}^{-1} : \underline{\underline{\sigma}} = \underset{\sim}{C} : (\underline{\underline{d}} - \underline{\underline{d}}^{ir}) + \dot{J}_{ir}\frac{\partial \underset{\sim}{C}}{\partial J_{ir}} : \underset{\sim}{C}^{-1} : \underline{\underline{\sigma}}, \tag{10}$$

where $\dot{\underline{\underline{\sigma}}}$ is the Cauchy stress rate tensor, $\underline{\underline{d}}^{ir}$ is the irreversible part of the strain rate tensor, and the fourth-order tensor $\underset{\sim}{C}$ is the material elastic stiffness moduli, in which the expression under the assumption of isotropy is

$$\underset{\sim}{C}(\varphi) = (K(\varphi) - 2\mu(\varphi)/3)\underline{\underline{1}} \otimes \underline{\underline{1}} + 2\mu(\varphi)\underset{\sim}{1}, \tag{11}$$

where $\underline{\underline{1}}$ and $\underset{\sim}{1}$ refer respectively to the second-order and fourth-order identity tensors.

The term $\dot{\underset{\sim}{C}} : \underset{\sim}{C}^{-1} : \underline{\underline{\sigma}}$ in 10 represents the influence of large irreversible strains on elastic properties.

The plastic and viscoplastic strain components are additively related to the irreversible strain by $\underline{\underline{d}}^{ir} = \underline{\underline{d}}^{p} + \underline{\underline{d}}^{vp}$.

The purely mechanical compaction is represented by the plastic component of the constitutive model. To the plastic yield surface we resort to the concept of so-called "cap models" for the formulation of a simplified isotropic plastic criterion. Referring to the $p \times q$ plane, the yield surface is bounded in the dilation domain by a straight line that stands for the brittle failure regime (critical line), while the side corresponding to ductile failure and material hardening (contracting state) is also approximated in this analysis by an inclined straight line. For the plastic strain rate an associated flow rule was adopted. The plastic hardening law, that describes the evolution of the consolidation pressure (p_c) due to the irreversible material densification, is based on limit analysis and micromechanics (Barthélémy et al. [12], Brüch et al. [13]).

The chemo-mechanical compaction is represented by the viscoplastic component of the constitutive model. In a similar way than for plastic behavior the viscoplastic yield surface is defined resorting once again to the concept of "cap models". The generalized Perzyna's overstress theory (Perzyna [14]) bases the time-dependent component of the strain rate. The viscoplastic hardening law, that describes the evolution of the consolidation pressure (p_{vp}) due to the irreversible material densification, has been formulated (Brüch et al. [15]) and stems from the heuristic idea that similarity can be preserved between the plastic and viscoplastic models.

The plastic and viscoplastic yield criterion are described by

$$f^{\alpha}(\underline{\underline{\sigma}}, h) = -\frac{1}{3}\mathrm{tr}\underline{\underline{\sigma}} + a\sqrt{\frac{1}{2}\underline{\underline{s}} : \underline{\underline{s}}} - h = 0, \tag{12}$$

where $\alpha = p, vp$ for the plastic and viscoplastic yield criterion, $h = p_c, p_{vp}$ for the plastic and viscoplastic consolidation pressure (the hardening parameters in the model), while a is a positive scalar that controls the slope of the ductile part of yield surfaces.

The plastic and viscoplastic strain rate are defined by

$$\underline{\underline{d}}^{p} = \dot{\chi}\frac{\partial f^{p}}{\partial \underline{\underline{\sigma}}} \quad \text{and} \quad \underline{\underline{d}}^{vp} = \frac{\langle f^{vp} \rangle}{\eta_{vp}}\frac{\partial g^{vp}}{\partial \underline{\underline{\sigma}}}, \tag{13}$$

where $\dot{\chi}$ is the nonnegative plastic multiplier rate, $\langle\rangle$ is the Macaulay brackets, η_{vp} is the viscosity coefficient, and g^{vp} is the viscoplastic potential defining the direction of viscoplastic strain rate. An associated flow rule $g^{vp} = f^{vp}$ shall be assumed in the subsequent analysis.

3 Thermo-Mechanical formulation

As explained in Lemos et al. [2], the evolution of the sedimentary basin under compaction processes is divided into five consecutive phases, distinct from each other by the behavior ranges involved along the basin layers. Each domain of behavior in each phase is described by a first-order nonlinear partial differential system of equations given by:

$$\left\{ \begin{aligned} \frac{\partial \Lambda}{\partial x_3} &= \frac{\rho_0 g}{F^{\alpha}_{v1}} - \frac{F^{\alpha}_{v2}}{F^{\alpha}_{v1}}\Lambda\frac{\partial J_{ir}}{\partial x_3} \\ \frac{\partial \sigma_h}{\partial x_3} &= \frac{F^{\alpha}_{h1}}{\Lambda}\frac{\partial \Lambda}{\partial x_3} + F^{\alpha}_{h2}\frac{\partial J_{ir}}{\partial x_3} \\ \frac{\partial \sigma_v}{\partial x_3} &= \frac{\rho_0 g}{\Lambda} \\ \frac{\partial J_{ir}}{\partial x_3} &= -\frac{G^{\alpha}_1 J_{ir}}{\Lambda(1 + G^{\alpha}_2 J_{ir})}\frac{\partial \Lambda}{\partial x_3} \\ \frac{\partial u_3}{\partial x_3} &= \frac{-\dot{M}_d g}{F^{\alpha}_{v1} + F^{\alpha}_{v2}\Lambda\dfrac{\partial J_{ir}}{\partial x_3} \Big/ \dfrac{\partial \Lambda}{\partial x_3}} \end{aligned} \right. , \tag{14}$$

where $\alpha = e, p, vp, v$ for the elastic, elastoplastic, elastoplastic–viscoplastic and elasto-viscoplastic domains, $F^{\alpha}_{\beta\gamma}$ and G^{α}_{γ} ($\beta = h, v$ and $\gamma = 1, 2$) are mechanical functions explained in Lemos et al. [2].

This system relates the unknown fields $\Lambda,\ J_{ir},\ \sigma_h,\ \sigma_v,$ and u_3 of the problem. These equations are completed by the complementary constitutive relationships as well as by initial and boundary conditions. The solution of the mechanical problem is carried out incrementally, with the temporal discretization of the governing equations and with the reduction of the PDE system into an ODE system. The incremental scheme as well as the solution to the system of ordinary nonlinear differential equations is performed numerically using the MAPLE software. A finite difference technique with Richardson extrapolation is used to solve the BVP.

As previously explained, the model developed disregards the thermo-mechanical coupling. Additionally, thermal properties are considered constant throughout the analysis. The thermal field is obtained by Fourier's series, separating the stationary θ_1 and transient θ_2 response as

$$\theta(x_3,t) = \theta_1(x_3,t) + \theta_2(x_3,t) = \left((H(t)-x_3)\frac{q_0}{k} + \theta_0\right) + \left(\sum_{n=1}^{\infty} b_n(t)\phi_n(x_3)\right). \tag{15}$$

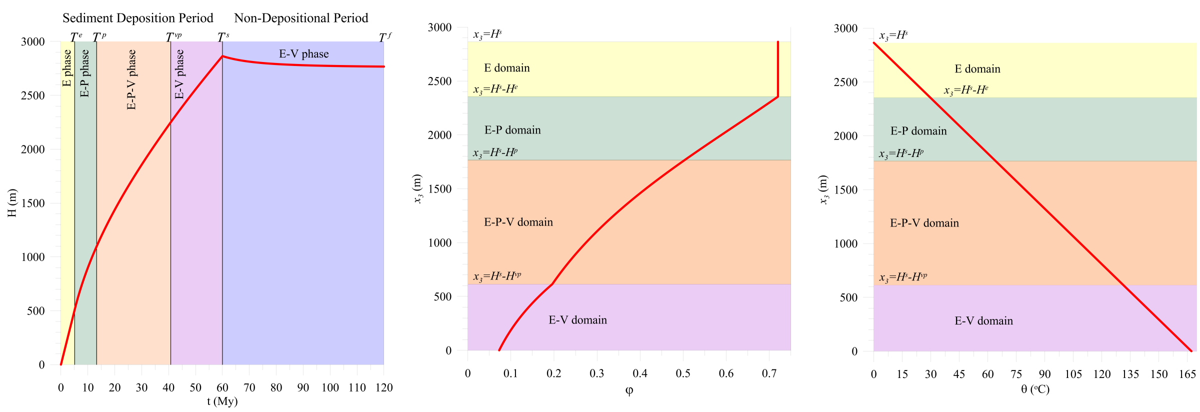
In this equation, the stationary response θ_1 appears as a function of the temporal variable t. However, the temporal dependence is only due to the compaction law $H(t)$, that determines the size of the material domain. The terms $b_n(t)$ and $\phi_n(x_3)$ in 15 are expressed as

$$b_n(t) = \alpha_n \mathrm{e}^{-\lambda_n{}^2 t} \quad \text{and} \quad \phi_n(x_3) = \cos(\lambda_n x_3), \tag{16}$$

where $\alpha_n = \dfrac{\int_0^{H(t)} \rho c\, \theta_1(x_3)\phi_n(x_3)dx_3}{\int_0^{H(t)} \rho c\, \phi_n(x_3)^2 dx_3}$ and $\lambda_n = \dfrac{(2n-1)\pi}{2H(t)}$.

4 Illustrative results

The problem description and data are presented in Lemos et al. [2]. Additionally, the thermal data used for modeling of sedimentary material are: specific heat capacity $c = 2.6 \times 10^3\ J/kg°C$, thermal conductivity coefficient $k = 1.2\ W/m°C$, mass density $\rho = \rho_0$, $\theta_0 = 0°C$ and $q_0 = 70\ mW/m^2$.



(a) (b) (c)

Figure 3. (a) gravitational compaction law of the sedimentary basin, (b) Eulerian porosity profile along basin thickness at $t = T^s$ and (c) temperature profile along basin thickness at $t = T^s$.

At the scale of basin, a main feature in sedimentary basin simulation refers to assessment of the compaction law $t \to H(t)$ (Fig. 3a). The level of basin compaction predicted by semianalytical solution at $t = T^s$ (end of the accretion phase) is 52.2%. In the postaccretion period, the compaction level exhibits a slight decrease to reach approximately 54% at $t = T^f$ (end of the analysis).

The Eulerian porosity $\varphi(x_3, T^s)$ is depicted in Fig. 3b. As expected, the material densification induced by compaction at large strains is reflected by the decrease of porosity with depth.

The temperature profile $\theta(x_3, T^s)$ is depicted in Fig. 3c. Some comments are made about the behavior of this variable: (a) the weak hypothesis of constant thermal properties for the sedimentary material (independent of the variation in porosity and temperature) produces a stationary response θ_1 with a constant associated gradient $\partial\theta/\partial x_3 = -q_0/k$ (as can be seen in eq. (15) and Fig. 3c); (b) the characteristic time of thermal diffusion $\tau =$

L^2/α, where L is the characteristic length and $\alpha = k/\rho c$, is small compared to the time scales of the sedimentary basin, which explains the stationary response in Fig. 3c; (c) the weak hypothesis about the disregard of the influence of the geothermal field on the mechanical evolution of the basin, which would have considerable influence on the viscoplastic viscosity coefficient, accelerating the deferred deformation processes.

5 Conclusion

This work presented the development of new features for the reference solutions of the compaction processes in sedimentary basins. Continuing the research presented in Lemos et al. [2], the work incorporated the thermal response to the model. Assumptions that simplify the model were adopted to facilitate obtaining an analytical response to the geothermal field, which will serve as a reference for the next steps of the research. From the thermal point of view, the main characteristics exhibited by the model were the constant geothermal gradient and the stationary response. From the mechanical point of view, the main characteristic was the absence of thermal effects on the mechanical response of the sedimentary basin. The next developments are the incorporation of thermal properties sensitive to the variation of porosity and temperature and the thermo-mechanical coupling of the deformation of the sedimentary basin.

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