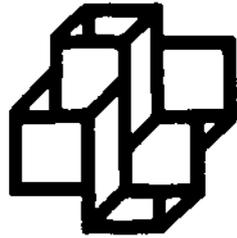


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A THERMODYNAMICALLY CONSISTENT
CONSTITUTIVE THEORY FOR A RIGID
SOLID-STOKESIAN FLUID MIXTURE

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ABSTRACT

This work is concerned with the modelling for the flow of a stokesian fluid through a rigid porous medium, using a Theory of Mixtures viewpoint. A systematic procedure to obtain constitutive relations that verify automatically the principle of objectivity and a local version of the second law of Thermodynamics is proposed. The prescription of two thermodynamic potentials for each constituent is sufficient to define a complete set of constitutive relations.

UMA TEORIA CONSTITUTIVA TERMODINAMICAMENTE CONSISTENTE PARA UMA MISTURA SÓLIDO RÍGIDO-FLUIDO STOKESIANO

RESUMO

O presente trabalho trata da modelagem do escoamento de um fluido stokesiano através de um meio poroso rígido, sob um ponto de vista de Teoria de Misturas. Propõe-se um procedimento sistemático para a obtenção de relações constitutivas verificando automaticamente o princípio de objetividade e uma versão local da segunda lei da Termodinâmica. A prescrição de dois potenciais termodinâmicos para cada constituinte é suficiente para definir um conjunto completo de relações constitutivas.

A THERMODYNAMICALLY CONSISTENT CONSTITUTIVE THEORY FOR A RIGID SOLID-STOKESIAN FLUID MIXTURE

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Introduction

The development of modern computers and numerical techniques for approximating the solution of non linear problems now permits the use of more complex (and realistic) constitutive equations in the Continuum Theory of Mixtures. This is very important in many industrial applications such as oil prospection and geothermal energy extraction. To set up a general constitutive theory it is necessary to consider aspects of the Second Law of Thermodynamics since dissipative phenomena must be taken into account. Besides, the constitutive equations must satisfy the principle of objectivity. This paper presents a systematic procedure to obtain a complete set of objective constitutive equations for a rigid solid-stokesian fluid mixture. The Second Law of Thermodynamics is automatically verified independently of the geometry, of the external actions and of the boundary conditions.

Basic Balance Equations for a Binary Mixture

In this section the local form of the basic governing equations of a solid-fluid mixture are presented. In the absence of chemical reactions and under suitable regularity assumptions, they may be expressed as [1], [2]:

Balance of mass:

$$\frac{\partial \rho_\alpha}{\partial t} + \text{div}(\rho_\alpha \mathbf{v}_\alpha) = 0 \quad \alpha = 1, 2 \quad (1)$$

Balance of linear momentum:

$$\rho_\alpha \frac{D^a \mathbf{v}_\alpha}{Dt} = \text{div} \mathbf{e}_\alpha + \mathbf{m}_\alpha + \rho_\alpha \mathbf{b}_\alpha \quad \alpha = 1, 2 ; \quad \sum_{\alpha=1}^2 \mathbf{m}_\alpha = 0 \quad (2)$$

Balance of energy:

$$\rho_\alpha \frac{D^\alpha e_\alpha}{Dt} = \rho_\alpha r_\alpha - \text{div } \underline{q}_\alpha + \psi_\alpha + \text{tr}[\underline{\sigma}_\alpha \underline{D}_\alpha] \quad \alpha = 1, 2 ; \quad \sum_{\alpha=1}^2 \psi_\alpha = 0 \quad (3)$$

Second law of thermodynamics (SLT):

$$d = \sum_{\alpha=1}^2 \left\{ \rho_\alpha \frac{D^\alpha s_\alpha}{Dt} + \text{div} \frac{\underline{q}_\alpha}{T_\alpha} - \rho_\alpha \frac{r_\alpha}{T_\alpha} \right\} \geq 0 \quad (4)$$

where the constituents 1 and 2 are, respectively, the solid and the fluid constituents, ρ_α is the density of C_α , the α -th constituent, \underline{v}_α its velocity, $\underline{\sigma}_\alpha$ is the partial stress tensor, \underline{m}_α is the interaction force, \underline{b}_α is the external body force, e_α is the internal energy of C_α , r_α , the energy generation per unit mass of C_α and \underline{q}_α the partial heat flux. The energy supplied to C_α to account for its thermal interaction with the remaining constituent is given by ψ_α , the tensor \underline{D}_α represents the symmetrical part of C_α velocity gradient and s_α is the entropy of C_α . Throughout this paper it will be assumed that the partial stress tensor is symmetric and, hence, the angular momentum conservation comes automatically.

The Second Law of Thermodynamics makes a distinction between possible processes ($d \geq 0$) and impossible ones ($d < 0$). The possible processes can be reversible (the dissipation d is always equal to zero) or not. The SLT may be written in another local form, by introducing equations (3) into (4):

$$d = \sum_{\alpha=1}^2 \left\{ \underline{\sigma}_\alpha \cdot \underline{D}_\alpha - \rho_\alpha \left(\frac{D^\alpha e_\alpha}{Dt} - T_\alpha \frac{D^\alpha s_\alpha}{Dt} \right) - \underline{q}_\alpha \cdot \underline{g}_\alpha \right\} \geq 0 ; \quad \underline{g}_\alpha = \frac{1}{T_\alpha} \text{grad} T_\alpha \quad (5)$$

An alternative local form for the Second Law of Thermodynamics, analogous to the Clausius-Dühen inequality in the classical Continuum Mechanics, may be obtained by introducing on equation (5) the definition of the free energy A_α :

$$A_\alpha = e_\alpha - T_\alpha s_\alpha \Rightarrow d = \sum_{\alpha=1}^2 \left\{ \underline{\sigma}_\alpha \cdot \underline{D}_\alpha - \rho_\alpha \left(\frac{D^\alpha A_\alpha}{Dt} + s_\alpha \frac{D^\alpha T_\alpha}{Dt} \right) - \underline{q}_\alpha \cdot \underline{g}_\alpha \right\} \geq 0 \quad (6)$$

Abstract Constitutive Theory for a Solid-Fluid Mixture

The balance equations (1) to (3) and the second law restriction (6) are valid for any kind of solid-fluid mixture. A complete modelling requires additional informations in order to characterize the behaviour of each kind of mixture. In this section, it is proposed a

constitutive theory for a rigid solid and a non-Newtonian fluid mixture. A systematic procedure to obtain a set of thermodynamically admissible constitutive equations that verify automatically the principle of objectivity, similarly to Costa Mattos [3], may be described by the steps below. In order to simplify the presentation, it will be restricted to incompressible fluid constituents.

H 1: It will be considered constituents for which the free energy A_α is a differentiable function of the temperature T_α :

$$A_\alpha = \hat{A}_\alpha(T_\alpha) \quad \alpha = 1, 2 \quad (7)$$

H 2: The following state law holds:

$$s_\alpha = -\frac{dA_\alpha}{dT_\alpha} \quad \alpha = 1, 2 \quad (8)$$

A consequence of the hypotheses 1 and 2 is that the dissipation d (see equation (6)) will always be equal to zero in equilibrium, i. e. when $\underline{v}_\alpha = 0$ and $gradT_\alpha = 0$.

H 3: The partial stress $\underline{\sigma}_\alpha$ is such that:

$$\underline{\sigma}_\alpha = -p_\alpha \underline{1} + \underline{\sigma}_\alpha^{IR} \quad \alpha = 1, 2 \quad (9)$$

where the pressure p_α is a Lagrange multiplier related to the incompressibility constraint and $\underline{\sigma}_\alpha^{IR}$ represents the partial stress tensor irreversible parcel.

Using the hypotheses H1, H2 and H3, the Second Law of Thermodynamics restriction, given by equation (6), can be reduced to:

$$d = \sum_{\alpha=1}^2 (d_\alpha^I + d_\alpha^T) \geq 0 \quad d_\alpha^I = \underline{\sigma}_\alpha^{IR} \cdot \underline{D}_\alpha \quad d_\alpha^T = -\underline{q}_\alpha \cdot \underline{g}_\alpha \quad (10)$$

where d_α^I and d_α^T are called, respectively, the internal dissipation and the thermal dissipation associated to the constituent α .

In order to characterize completely the behaviour of the constituent, additional informations about the partial stress irreversible part $\underline{\sigma}_\alpha^{IR}$ and about the partial heat flux vector \underline{q}_α must be given. In this theory, the additional informations are obtained from two potentials $\Phi_\alpha^I(\underline{D}_\alpha)$ and $\Phi_\alpha^T(\underline{g}_\alpha)$, which are called internal dissipation potential and thermal dissipation potential, respectively.

H 4: There exists two objective and differentiable potentials $\Phi_\alpha^I(\underline{D}_\alpha)$ and $\Phi_\alpha^T(\underline{g}_\alpha)$, such that:

$$\underline{\sigma}_\alpha^{IR} = \frac{\partial \Phi_\alpha^I}{\partial \underline{D}_\alpha} \quad \underline{q}_\alpha = -\frac{\partial \Phi_\alpha^T}{\partial (\underline{g}_\alpha)} \quad \alpha = 1, 2 \quad (11)$$

The definition of the potentials A_α , Φ_α^I and Φ_α^T is motivated by experimental observation in simple tests. Therefore, the constitutive equations (8), (9) and (11) may eventually allow some thermodynamically impossible processes. In order to assure that the local version of the second law (10) will always be satisfied, independently of the geometry, of the external actions and of the boundary conditions, it is sufficient to restrict the choice of Φ_α^I and Φ_α^T in the following way:

H 5: $\Phi_\alpha^I(\underline{D}_\alpha)$ and $\Phi_\alpha^T(\underline{g}_\alpha)$ are nonnegative convex functions such that:

$$\Phi_\alpha^I(\underline{0}) = \Phi_\alpha^T(\underline{0}) = 0 \quad (12)$$

The demonstration that equation (10) is verified if hypothesis 5 holds is done by using the following classical result of the Convex Analysis:

"Let X and Y be elements of a vector space V with an internal product $(X.Y)$. If $\Phi : V \rightarrow [0, +\infty)$ it is a convex and differentiable function such that $\Phi(0) = 0$, then $(X.Y) \geq \Phi(X) \geq 0$ if $Y = \frac{d\Phi}{dX}$ "

Taking $X = \underline{D}_\alpha$, $Y = \underline{g}_\alpha^{IR}$ and $(X.Y) = \underline{D}_\alpha \cdot \underline{g}_\alpha^{IR}$ it is easy to verify that $d_\alpha^I = \underline{g}_\alpha^{IR} \cdot \underline{D}_\alpha \geq 0$ if $\underline{g}_\alpha^{IR} = \frac{\partial \Phi_\alpha^I}{\partial \underline{D}_\alpha}$. Similarly, taking $X = \underline{g}_\alpha$, $Y = -\underline{g}_\alpha$ and $(X.Y) = -\underline{g}_\alpha \cdot \underline{g}_\alpha$ it is easy to verify that $d_\alpha^T = -\underline{g}_\alpha \cdot \underline{g}_\alpha \geq 0$ if $\underline{g}_\alpha = \frac{\partial \Phi_\alpha^T}{\partial \underline{g}_\alpha}$. Hence, $d = \sum_{i=1}^a (d_\alpha^I + d_\alpha^T) \geq 0$, if hypothesis 5 holds. //

It is important to remark that this demonstration can be easily extended if other variables are taken as independent parameters in Φ_α^I and Φ_α^T , as, for instance the temperature T_α and the diffusive velocity ($\underline{v}_{\alpha\beta} = \underline{v}_\alpha - \underline{v}_\beta$).

$$\Phi_\alpha^I = \hat{\Phi}_\alpha^I(\underline{D}_\alpha; T_\alpha, \underline{v}_{\alpha\beta}) \quad \Phi_\alpha^T = \hat{\Phi}_\alpha^T(\underline{g}_\alpha; T_\alpha, \underline{v}_{\alpha\beta}) \quad (13)$$

It is also interesting to note that, in this theory, the Second Law inequality does not impose restrictions on the constitutive expressions for the interaction force \underline{m}_α and the energy generation function ψ_α . In this paper, the theory is restricted to a mixture of a rigid solid constituent and a stokesian fluid constituent.

Definition: the solid constituent will be called rigid and the fluid constituent will be called stokesian if:

$$\Phi_1^I \equiv 0 ; \quad \Phi_2^I = \hat{\Phi}_2^I(J_2, T_2) \quad (14)$$

where $J_2 = (\underline{D}_2 \cdot \underline{D}_2)$. In this case, it is easy to conclude from equation (11) that $\underline{g}_1^{IR} \equiv 0$.

For a mixture which satisfies the hypothesis H1 to H5 and the definition (14), it is reasonable to suppose that the interaction force $\underline{m}_1 = -\underline{m}_2$ and the energy generation $\psi_1 = -\psi_2$ are functions of the diffusive velocity and of the temperatures.

$$\underline{m}_2 = -\underline{m}_1 = \hat{m}(\underline{v}_{21}, T_F, T_S) \quad \psi_2 = -\psi_1 = \hat{\psi}(\|\underline{v}_{21}\|, T_F, T_S) \quad (15)$$

If A_α , Φ_α^I , Φ_α^T , \hat{m} and $\hat{\psi}$ are known, equations (8), (9), (11) and (15) form a complete set of objective and thermodynamically admissible constitutive equations, provided the hypothesis H5 and the definition (14) are verified.

Analysis of the Thermomechanical Couplings

An alternative local form of the first law of thermodynamics (the energy balance equation) can be obtained by introducing the constitutive relations obtained in the third section in the equation (3). Initially, using the definition (6)₁ of the free energy A_α and the state law (8), the following alternative expression may be obtained for the first law of thermodynamics:

$$-\text{div} \underline{q}_\alpha - \rho_\alpha c_\alpha \frac{D^\alpha T_\alpha}{Dt} + \rho r = \underline{\sigma}_\alpha \cdot \underline{D}_\alpha + \psi_\alpha \quad ; \quad c_\alpha = - \left[\frac{d^2 A_\alpha}{dT^2} T_\alpha \right] \quad (16)$$

Finally, using the constitutive relations (9) and (11), the following expression is obtained:

$$-\text{div} \underline{q}_\alpha - \rho_\alpha c_\alpha \frac{D^\alpha T_\alpha}{Dt} + \rho r = \frac{\partial \Phi_\alpha^I}{\partial \underline{D}_\alpha} \cdot \underline{D}_\alpha + \psi_\alpha \quad (17)$$

The terms in the right side of equation (17) are responsible for the thermomechanical couplings: the temperature evolution on both constituents is coupled, due to the term $\psi_\alpha(\|\underline{v}_{21}\|, T_1, T_2)$ and the mechanical evolution of the mixture is coupled to the thermic evolution due to the term $\frac{\partial \Phi_\alpha^I}{\partial \underline{D}_\alpha} \cdot \underline{D}_\alpha$.

Rigid Solid Matrix and Ostwald-de Waele Fluid

In a binary mixture composed by a rigid solid constituent and an Ostwald-de Waele incompressible fluid, which is a particular kind of stokesian fluid, the free energy, the intrinsic and thermal dissipation potentials, the interaction force and the energy generation function, for the solid and the fluid constituents are defined as:

$$A_\alpha = \int_{T_0}^{T_\alpha} a_\alpha \log \xi d\xi - \frac{1}{2} b_\alpha T_\alpha^2 \quad \alpha = 1, 2 \quad (18)$$

$$\Phi_1^I \equiv 0 \quad \Phi_2^I \equiv \frac{1}{n+1} \beta(T_2) (\underline{D}_2 \cdot \underline{D}_2)^{n+1} \quad ; \quad \beta(T_2) = \mu_0 \exp \left[\gamma \left(\frac{1}{T_2} - \frac{1}{T_2^0} \right) \right] \quad (19)$$

$$\Phi_\alpha^T = \frac{1}{2} T_\alpha \left[\underline{k}_\alpha(T_\alpha, \|\underline{v}_{21}\|) \cdot \underline{g}_\alpha \right] \cdot \underline{g}_\alpha \quad (20)$$

$$\underline{m}_2 = -\underline{m}_1 = -d \|\underline{v}_{21}\|^{2n} \underline{v}_{21} \quad \psi_2 = -\psi_1 = R_{FS} (1 + \delta \|\underline{v}_{21}\|) (T_1 - T_2) \quad (21)$$

where $a_1, b_1, a_2, b_2, \mu_0, \gamma$ and T_2^0 are positive constants of the mixture and n is a constant. $\underline{k}_\alpha(T_\alpha, \|\underline{v}_{12}\|)$; $\alpha = 1, 2$ are symmetric and positive definite tensors and d, R_{FS} and δ are positive valued parameters which depend on both constituents thermal properties and on the internal structure of the mixture [2].

Under these hypotheses and using equations (8), (9) and (11), the constitutive equations for the mixture are:

$$s_\alpha = a_\alpha [\log T_\alpha - \log T_\alpha^0] + b_\alpha T_\alpha \quad \underline{q}_\alpha = -\underline{k}_\alpha \text{grad} T_\alpha \quad \alpha = 1, 2 \quad (22)$$

$$\underline{\sigma}_1 = -p_1 \underline{1} \quad \underline{\sigma}_2 = -p_2 \underline{1} + 2\mu \underline{D}_2 \quad ; \quad \mu = \frac{\partial \Phi_2^I}{\partial J_2} = \beta(T_2) (\underline{D}_2 \cdot \underline{D}_2)^n \quad (23)$$

where μ is the dynamical viscosity. Considering the constant γ in equation (19) equal to zero, the fluid constituent is called thermically insensitive and the equation (23)₃ is reduced to:

$$\mu = \mu_0 (\underline{D}_2 \cdot \underline{D}_2)^n \quad (29)$$

If $n = 0$ the fluid is called newtonian and if $n = -1$ the fluid has a plastic behaviour.

It is important to remark that the material constants $a_1, b_1, a_2, b_2, \mu_0, \gamma, T_2^0$ and n must be obtained from experiments using a Theory of Mixtures viewpoint. Hence, although the constitutive equation for the partial stress in the fluid constituent is similar to the constitutive equation for the stress in the fluid, regarded as a continuum, the material constants are not necessarily the same.

If the mentioned constants, for each constituent of the mixture, are not available it is possible to relate some of them with the constants of the solid matrix and of the fluid, regarded as continua. Using the results presented by Williams [4], Martins Costa, Sampaio and Saldanha da Gama [2] and Saldanha da Gama and Sampaio [5], it may be written:

$$p_2 = \varphi p \quad \mu_0 = \lambda \varphi^2 \eta_0 \quad (25)$$

$$\underline{k}_1 = \lambda k_S (1 - \varphi) \underline{1} \quad ; \quad \underline{k}_2 = \lambda k_F \varphi \underline{1} \quad (26)$$

$$d = \frac{\varphi^2 \eta_0}{K} \left[\left(\frac{4n+3}{2n+1} \right)^{2n+1} \frac{1}{3} \left(\frac{\varphi}{6K} \right)^n \right] \quad (27)$$

where φ is the fluid fraction, coincident to the porosity in saturated flows; p is the pressure acting on the mixture as a whole; λ is a positive-valued factor, accounting for the solid matrix structure, η_0 is the viscosity parameter related to the thermally insensitive Ostwald-de Waele fluid ($\underline{\sigma} = -\varphi p \underline{1} + 2\eta_0(\underline{D} \cdot \underline{D})^n \underline{D}$), whose value is found in the literature; k_F and k_S are, respectively, the fluid and the solid matrix thermal conductivities; A is an always positive parameter, which may depend on both the internal structure and the porous matrix permeability.

Finally, considering the basic balance equations shown in section 2 and the constitutive equations (21) and (25) to (27) discussed in this section, the governing equations to describe the flow of an Ostwald-de Waele fluid in a rigid solid matrix and the heat transfer process are automatically obtained.

Final Remarks

The systematic procedure to obtain constitutive relations that verify automatically the principle of objectivity and the second law of thermodynamics proposed in this paper is a promising tool in the modelling of rigid solid-fluid mixtures. Interesting works can be made by analysing the dependence of the constitutive equations on both constituents temperatures and the resulting thermomechanical couplings. Numerical simulations using the proposed set of constitutive equations can be found in [6].

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