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the Assumptions and Thermodynamics,
Updated**

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Flow and Deformation: Understanding the Assumptions and Thermodynamics, Updated

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Abstract

Coupling flow and deformation is of interest when modeling settling due to pumping water or oil, compaction due to construction, or, in other fields, modeling soft tissue, bones, or man-made porous materials. The modeling usually combines the Conservation of Mass equations for all phases, Darcy's law for flow, the Terzaghi's principal of effective stress, and a stress-strain relation. Here we discuss the assumptions and thermodynamic framework underlying this formulation for single-phase flow and discuss the need to generalize the traditional model.

1 Introduction

Combining flow and deformation is of critical importance for such problems as: land subsidence due to extraction of groundwater or oil; compaction of soils due to construction of buildings, bridges, or roads; and bio-tissue modeling. The modeling of flow and deformation individually has been modeled separately and is well-understood. However most people involved with flow or transport are not familiar with the deformation problem and vice versa. The purpose of this manuscript is to give a brief overview of the simplest flow and deformation model and provide the thermodynamic assumptions underlying

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this model. The intent is that once the simplest model is well-understood then extensions to these models can be made in a physically meaningful manner.

Throughout we assume isothermal conditions and that the material is non-swelling, i.e. that the liquid phase has the same properties (density, viscosity, etc) in the porous material as without.

2 Conservation of Mass and Linear Momentum

For either the flow or deformation problem, the conservation of mass and momentum for each phase must be considered. If $\alpha = l, s$ where l denotes the liquid and s denotes the solid phase, then the conservation of mass (or continuity equation) is given by

$$\frac{\partial(\varepsilon^\alpha \rho^\alpha)}{\partial t} + \nabla \cdot (\varepsilon^\alpha \rho^\alpha \mathbf{v}^\alpha) = 0, \quad \alpha = l, s \quad (1)$$

where ε^α is the volume fraction of phase α in the Representative Elementary Volume (REV) [1] so that $\varepsilon^l + \varepsilon^s = 1$, ρ^α is the (true) density of phase α (mass of α per volume of α), and \mathbf{v}^α is the velocity of phase α (length per unit time). This equation may be derived by volume averaging the corresponding equations at the microscale [2,3] and then assuming there is no mass transfer between phases. If one wants to incorporate chemical reactions then one needs a continuity equation for each species and the right-hand side must include terms accounting for the rate of chemical reactions. Likewise if one wants to incorporate phase transformation, a term on the right-hand side must be added to account for this as well.

If one phase is considered incompressible, then the corresponding mathematical constraint is:

$$\frac{D^\alpha \rho^\alpha}{Dt} = 0, \quad \alpha = l, s, \quad (2)$$

where $\frac{D^\alpha}{Dt} = \frac{\partial}{\partial t} + \mathbf{v}^\alpha \cdot \nabla$ is the material time derivative with respect to phase α [4]. This states that as one follows the material, the density does not change.

One form of the conservation of linear momentum for phase α is

$$\varepsilon^\alpha \rho^\alpha \frac{D^\alpha \mathbf{v}^\alpha}{Dt} - \nabla \cdot (\varepsilon^\alpha \mathbf{t}^\alpha) - \varepsilon^\alpha \rho^\alpha \mathbf{g} = \varepsilon^\alpha \rho^\alpha \widehat{\mathbf{T}}_\beta^\alpha, \quad \alpha = l, s, \quad (3)$$

where \mathbf{t}^α is the partial Cauchy stress tensor, \mathbf{g} is gravity, and $\varepsilon^\alpha \rho^\alpha \widehat{\mathbf{T}}_\beta^\alpha$ represents the rate momentum is transferred from phase β ($\beta = l, s \neq \alpha$) to phase α [3]. The constraint that $\varepsilon^l \rho^l \widehat{\mathbf{T}}_s^l + \varepsilon^s \rho^s \widehat{\mathbf{T}}_l^s = \mathbf{0}$ states that the momentum equation must hold for the entire porous material.

3 Flow

In this section we review the assumptions typically considered for modeling slow flow of a single liquid phase through a homogeneous porous solid.

To begin, one usually neglects the solid phase (thus one has only the continuity and conservation of linear momentum for the fluid phase). Thus at this point we have 2 equations and 4 unknowns: ε^l , ρ^l , \mathbf{t}^l , and $\widehat{\mathbf{T}}_s^l$. To close the system we need two more equations, termed *constitutive equations* (any equation which is not a conservation equation is termed a constitutive equation and these equations have coefficients which must be determined experimentally).

One constitutive equation is that the liquid phase stress tensor is isotropic and is given by: $\mathbf{t}^l = -p^l \mathbf{I}$. This is a simplified version of the Stokes assumption that $\mathbf{t}^l = -p^l \mathbf{I} + \nu^l \left((\nabla \mathbf{v}^l)^T + \nabla \mathbf{v}^l \right)$, where ν^l is the viscosity of the liquid phase, which is the form of the constitutive equation used to derive the Navier Stokes equation. Thus in assuming $\mathbf{t}^l = -p^l \mathbf{I}$ viscosity has been neglected, which is normally valid for slow enough flows (incorporating viscosity is usually necessary when modeling the faster flow of air through a porous material and is called the Brinkman correction factor). Now we've replaced the need for a constitutive equation for \mathbf{t}^l by a constitutive equation for p^l . The constitutive equation for p^l is termed an *equation of state* (the equation holds whether one is at equilibrium or not - it applies in all situations). The usual equation of state for p^l is that $p^l = p^l(\rho^l)$ (i.e. the liquid pressure is not a function of anything other than density), or the system is closed by assuming the liquid phase is incompressible, in which case p^l becomes an unknown determined from the boundary conditions [5].

The second *constitutive equation is for the rate of exchange of momenta*: and for this the constitutive equation can be derived using thermodynamical arguments [6,7] and is: $\varepsilon^l \rho^l \widehat{\mathbf{T}}_s^l = p^l \nabla \varepsilon^l - (\varepsilon^l)^2 \mathbf{R} \cdot \mathbf{v}^{l,s}$ where $\mathbf{v}^{l,s} = \mathbf{v}^l - \mathbf{v}^s$ and where in general \mathbf{R} is a second-order tensor which can be a function of the liquid phase density, volume fraction, relative velocities, etc., but for the simplest case it is assumed to be a function of the liquid phase viscosity. The volume fraction is put in so that \mathbf{R} corresponds to what hydrologists term the *resistivity tensor*. Thermodynamically it can be shown to be invertible [7,8], and we denote its inverse as the *hydraulic conductivity tensor*, \mathbf{K} . Assuming

further that the *inertial* term, $\frac{D^l \mathbf{v}^l}{Dt}$, is negligible (which is valid if the flow is slow enough) then the momentum equation for the liquid phase with the constitutive equations mentioned above becomes:

$$\varepsilon^l \mathbf{v}^{l,s} = -\mathbf{K} \cdot (\nabla p^l - \rho^l \mathbf{g}) \quad (4)$$

which is known as *Darcy's Law*, developed empirically in the 1850's by Henri Darcy [9,10]. The usefulness of this relation has withstood time; this law has been in use for over a century. The exact value of the hydraulic conductivity must be determined experimentally, but is usually considered constant for an isotropic, homogeneous porous material.

Given the assumptions listed above then, the equations governing the flow through a non-deforming porous material for a spatially homogeneous porous media include: (1) *for an incompressible liquid fluid*,

$$\rho^l \frac{\partial \varepsilon^l}{\partial t} + \rho^l \nabla \cdot (\varepsilon^l \mathbf{v}^l) \approx \rho^l \nabla \cdot (\varepsilon^l \mathbf{v}^l) = 0 \quad (5)$$

$$\varepsilon^l \mathbf{v}^{l,s} = -\mathbf{K}(\varepsilon^l, \nu^l) \cdot (\nabla p^l - \rho^l \mathbf{g}) \quad (6)$$

where the unknowns are the pressure, p^l and the liquid flux, $\varepsilon^l \mathbf{v}^{l,s}$; and (2) *for a compressible liquid fluid*,

$$\frac{\partial(\varepsilon^l \rho^l)}{\partial t} + \nabla \cdot (\varepsilon^l \rho^l \mathbf{v}^l) = 0, \quad (7)$$

$$\varepsilon^l \mathbf{v}^{l,s} = -\mathbf{K}(\varepsilon^l, \nu^l) \cdot (\nabla p^l - \rho^l \mathbf{g}), \quad (8)$$

$$p^l = p^l(\rho^l) \quad (9)$$

where the unknowns to be solved for are ρ^l , p^l , and $\varepsilon^l \mathbf{v}^{l,s}$. In general, ε^l is considered fixed in time (which is equivalent to assuming an incompressible solid with the solid-phase velocity being zero via the solid continuity equation) and spatially known.

4 Deformation

The equation corresponding to Darcy's equation for deformation is the Terzaghi stress principle, and understanding the assumptions going into this principle and how it helps complete the system of equations is the goal of this section. Most of this material is from a recently published book by Herbert F. Wang [11].

To arrive at the Terzaghi stress principle, the assumption is made that the change in total volume δV , is a function of two of the three pressures, p , p^l , and p^s . For experimental reasons, the two independent pressures are: the liquid pressure, p^l , and the difference between the total pressure and liquid pressure, $p - p^l$, i.e.

$$\delta V = \delta V(p^l, p - p^l). \quad (10)$$

Thus the total differential is:

$$\begin{aligned} dV &= \left. \frac{\partial V}{\partial p^l} \right|_{p-p^l} dp^l + \left. \frac{\partial V}{\partial (p-p^l)} \right|_{p^l} d(p-p^l) \\ &= \left. \frac{\partial V}{\partial p^l} \right|_{p-p^l} dp^l + \left. \frac{\partial V}{\partial p} \right|_{p^l} d(p-p^l). \end{aligned} \quad (11)$$

Defining theunjacketed modulus, K^s , and the jacketed (or drained) modulus, K to be

$$K^s = -V \left. \frac{\partial p^l}{\partial V} \right|_{p-p^l} \quad K = -V \left. \frac{\partial p}{\partial V} \right|_{p^l} \quad (12)$$

then (11) can be re-written as:

$$-\frac{dV}{V} = \frac{1}{K^s} dp^l + \frac{1}{K} d(p-p^l). \quad (13)$$

Equation (13) is the general starting point for deriving the Terzaghi stress principle [12,13,11].

The coefficients K^s and K are generally assumed to be constant, and this appears to be reasonable for sandstone, but not for fractured porous material (see [13] and references cited therein). The jacketed and unjacketed moduli are measured in a deformation experiment set up as in Figure 1. In this experiment, typically p^l and p are varied under a variety of conditions and volumetric changes and the amount of liquid entering/exiting the system can be measured. To obtain K , the jacketed (or drained) modulus, the liquid pressure is held fixed (typically at atmospheric pressure, hence allowing the liquid to drain freely) and the *confining pressure* or overburden pressure, p , is methodically changed and the volumetric changes recorded. To obtain K^s , the liquid pressure and confining pressure are kept the same (i.e. $p = p^l$), which can be done by letting the liquid escape into confining liquid (thus the system is jacketed). Then the pressure versus deformation is determined under these

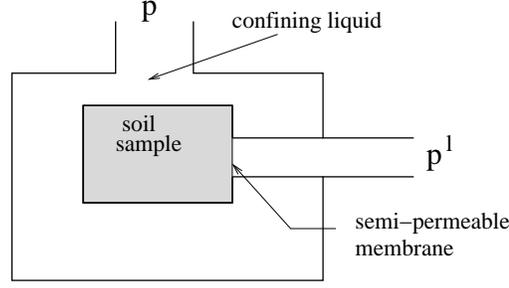


Fig. 1. Experimental setup for measuring compressibilities: varying the total or liquid pressure and measuring volumetric changes

conditions. The jacketed and unjacketed coefficients are defined so that they are positive quantities.

Define α to be $1 - K/K^s$. Then (13) can be re-written as

$$-\frac{dV}{V} = \frac{1}{K} (dp - \alpha dp^l). \quad (14)$$

Solving for dp and approximating $dp \approx p - p_0 = p$ and $dp^l \approx p^l - p_0^l = p^l$ we get

$$p = -K \frac{dV}{V} + \alpha p^l. \quad (15)$$

The Terzaghi stress principle is the generalization of the above equation - replacing p with the total stress, $-\mathbf{t}$, and denoting $K \frac{dV}{V}$ as the constitutive equation for an *effective stress tensor*, we get

$$\mathbf{t} = \mathbf{t}' - \alpha p^l \mathbf{I}. \quad (16)$$

The effective stress is constitutively assumed (and experimentally validated by a wide range of soils) to be linearly related to the strain of the material, so that a linear stress-strain relationship (such as what is used in linear elasticity) is assumed:

$$\mathbf{t}' = \lambda \text{tr}(\mathbf{e}) \mathbf{I} + 2\mu \mathbf{e} \quad (17)$$

where \mathbf{e} is the strain tensor, tr is the trace operator, λ is an experimentally measurable Lamé coefficient, and μ is an experimentally measurable coefficient called the shear modulus of elasticity (see a text on solid mechanics such as Malvern [4]). Note that $p = -1/3 \text{tr}(\mathbf{t})$ and for small deformations (small strains), $dV/V \approx \text{tr}(\mathbf{e})$. Thus taking 1/3 of the trace of equation (17) we get

$$-\frac{1}{3}\text{tr}(\mathbf{t}') = -(\lambda + \frac{2}{3}\mu)\text{tr}(\mathbf{e}) \approx -(\lambda + \frac{2}{3}\mu)\frac{dV}{V} \quad (18)$$

and comparing this with (15) we obtain that $K = (\lambda + (2/3)\mu)$.

The constitutive relationship for the effective stress is what makes the Terzaghi stress principle so useful: under a wide range of liquid pressures and overburden stresses the effective stress (and not the total stress) has the same (linear) constitutive relationship.

Originally the effective stress was defined for $\alpha = 1$ by Terzaghi [14,15], and the principle more concretely formulated by Fillunger [16]. It states that the constitutive equation for the stress may be formulated only for the excess over the (weighted) pore water pressure. Thus the effective pressure has the same constitutive relationship as the dry sample. The liquid pressure is assumed to not affect the shearing strain so that μ can be determined directly from a dry sample shearing test.

In this section we have presented a rough thermodynamical derivation of the Terzaghi stress principle. Others begin with slightly different formulations, such as choosing as independent variables p and ξ , the *increment of water volume per unit volume of soil* [17]. Biot's initial assumption is that there exists an energy density, $u = u(\epsilon, \xi)$, for which

$$p = -\frac{\partial u}{\partial \epsilon} \quad p^l = -\frac{\partial u}{\partial \xi}, \quad (19)$$

i.e. $du = -pd\epsilon - p^l d\xi$ where ϵ is dV/V , the change in total volume over volume ($\frac{1}{3}$ the trace of the porous material strain tensor), and the units of ξ must be volume of liquid per volume of porous material (i.e., the same dimensions as the liquid phase volume fraction). The exact definition of ξ is not precise. Biot and Willis, [18], expressed the increment of fluid content as $\xi = -\epsilon^l \nabla \cdot \mathbf{u}^{l,s}$ where $\mathbf{u}^{l,s}$ is the relative (average) displacement of the fluid to the solid phase (so that $\nabla \cdot \mathbf{u}^{l,s}$ is a volumetric measurement). On the other hand, Rice and Cleary, [19], defined it to be $\xi = (\epsilon^l \rho^l - \epsilon_0^l \rho_0^l) / \rho_0^l$ where ϵ_0^l and ρ_0^l are the volume fraction and liquid density at some reference configuration, respectively. This latter definition is likely more practical as it can be determined by measuring the change in mass (as oppose to volume) of liquid in the porous material. Note that the volume of liquid in the porous material may be slightly different than the volume of the same liquid outside of the porous material due to the interaction of the liquid and solid.

Noting that if we assume u has enough continuity, the second-order partials commute and we get:

$$\left. \frac{\partial p^l}{\partial \epsilon} \right|_{\xi} = \left. \frac{\partial p}{\partial \xi} \right|_{\epsilon} \quad (20)$$

so that the coefficient denoting the change in liquid pressure while changing the porous material volume (while keeping the liquid content fixed) is the same as the change in confining pressure with respect to liquid pressure while keeping the porous material volume fixed.

While this latter framework is more appealing than the former (it is in terms of intensive variables), the relationship between the formulation and the Terzaghi stress principle is not as straight forward. In either case, the main assumption is that there are only two independent variables which can describe the system.

5 Flow and Deformation

We now combine the equations for flow and deformation in a physically meaningful manner. Begin by assuming the solid phase is incompressible, so that the continuity of the solid phase, (1), is

$$\frac{\partial \epsilon^s}{\partial t} + \nabla \cdot (\epsilon^s \mathbf{v}^s) = 0. \quad (21)$$

The equation of state for the liquid is usually assumed to be

$$\rho^l = \rho_0^l \exp(C^l(p^l - p_0^l)), \quad (22)$$

which is derived by assuming the compressibility, $C^l = \frac{1}{\rho^l} \frac{\partial \rho^l}{\partial p^l}$, is constant.

Eliminating ρ^l in the continuity equation for the liquid phase, (1), using the equation of state, (22), one gets:

$$\frac{\partial \epsilon^l}{\partial t} + \epsilon^l C^l \frac{\partial p^l}{\partial t} + \nabla \cdot (\epsilon^l \mathbf{v}^l) = 0, \quad (23)$$

where we assume that the term with $\nabla \rho^l / \rho^l$ is negligible relative to the others (i.e. that the density of the liquid phase is approximately constant, though it is not incompressible, which is a reasonable assumption).

Next we combine (23) with (21) to eliminate the time derivative of volume fraction, $\frac{\partial \epsilon^l}{\partial t}$. In addition we note that $\nabla \cdot \mathbf{u}^s = \epsilon$ where ϵ is the volumetric strain (see a continuum mechanics text such as [4]) so that

$$\begin{aligned}\nabla \cdot \mathbf{v}^s &= \nabla \cdot \left(\frac{D^s \mathbf{u}^s}{Dt} \right) = \nabla \cdot \left[\frac{\partial \mathbf{u}^s}{\partial t} + \mathbf{v}^s \cdot \nabla \mathbf{u}^s \right] = \frac{\partial}{\partial t} (\nabla \cdot \mathbf{u}^s) + \nabla \cdot (\mathbf{v}^s \cdot \nabla \mathbf{u}^s) \\ &\approx \frac{\partial \epsilon}{\partial t}.\end{aligned}$$

This then results in being able to express the combined continuity equations as:

$$\varepsilon^l C^l \frac{\partial p^l}{\partial t} + \nabla \cdot (\varepsilon^l \mathbf{v}^{l,s}) + \frac{\partial \epsilon}{\partial t} = 0, \quad (24)$$

which is sometimes referred to as the *storage equation*. So now we have two of the three governing equations, (24) and Darcy's law, (4).

The third governing equation is obtained by combining the momenta equations, (3), with the Terzaghi effective stress principle. Neglecting the inertial (acceleration) terms for both the liquid and solid phase, the momentum equation for the porous material (obtained by adding the momenta equations for the liquid and solid phase) is:

$$\nabla \cdot \mathbf{t} + \rho \mathbf{g} = \mathbf{0}, \quad (25)$$

where, because the inertial terms have been neglected, this is sometimes referred to as the *equilibrium equation*. Recalling that the strain of the porous material, \mathbf{e} , is related to displacement (sometimes referred to as the *compatibility equation*) as $\mathbf{e} = \frac{1}{2} (\nabla \mathbf{u}^s + (\nabla \mathbf{u}^s)^T)$ [20]. For small deformation gradients [4], the constitutive equation for the effective stress tensor, (17), can be written as

$$\mathbf{t}' = \lambda \nabla \cdot \mathbf{u}^s \mathbf{I} + \mu [\nabla \mathbf{u}^s + (\nabla \mathbf{u}^s)^T]. \quad (26)$$

Substituting this expression into the Terzaghi stress principle, (16), and then using this expression to eliminate \mathbf{t} in (25) results in

$$(\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}^s) + \mu \nabla \cdot \nabla \mathbf{u}^s = \alpha \nabla p^l - \rho \mathbf{g}. \quad (27)$$

Thus we have the system of equations: the storage equation, (24), Darcy's law, (4), and the equilibrium equation combined with the Terzaghi stress principle and a constitutive equation for the effective stress, (27), along with the unknowns: $\varepsilon^l \mathbf{v}^{l,s}$, p^l , and \mathbf{u}^s .

6 Conclusion

The derivation of Darcy's law (and hence the flow part of the governing equations) has been derived theoretically from many perspectives - mixture theoretic (as is summarized here), averaging, and homogenization. Extensions to Darcy's law include adding a Forchheimer term (representing the exchange of momenta term in the momentum equation (3) as a linear term in relative velocity plus a quadratic term) [1,21]:

$$\varepsilon^l \mathbf{v}^{l,s} + a |\mathbf{v}^{l,s}| \mathbf{v}^{l,s} = -\mathbf{K}(\varepsilon^l, \nu^l) \cdot (\nabla p^l + \rho^l \mathbf{g}), \quad (28)$$

where a is the Forchheimer coefficient (extensions of this may include a cubic term in the liquid flux). Another extension is the Brinkman term, which incorporates the fluid viscosity times the rate of deformation in the liquid stress tensor [22]:

$$\varepsilon^l \mathbf{v}^{l,s} = -\mathbf{K}(\varepsilon^l, \nu^l) \cdot (\nabla p^l + \rho^l \mathbf{g}) + \nu \nabla \cdot \nabla (\varepsilon^l \mathbf{v}^{l,s}), \quad (29)$$

where ν is the Brinkman coefficient or effective viscosity. And finally other extensions not used as often are the incorporation of the inertial term (acceleration in the momentum equation), and a swelling potential term used for swelling materials such as montmorillonite clay [20].

On the other hand the deformation equations have a more fuzzy derivation. Extensions to Terzhaghi stress include a non-constant compressibility coefficients, α . Part of the problem is that only two independent variables are used when there are actually three. For example, by summing the momenta equations for the liquid and solid phase one gets $\mathbf{t} = \varepsilon^l \mathbf{t}^l + \varepsilon^s \mathbf{t}^s$, so that by taking the trace of the above equation one gets: $p = \varepsilon^l p^l + \varepsilon^s p^s$. By assuming the independent variables include p^l and p one is neglecting the dependence on volume fraction or solid phase pressure. Extending this theory to three independent variables is not straight forward because the volume fraction is an internal variable and is not directly measurable; as Figure 1 indicates, only two independent variables are practically measurable. However if this theory is to be extended to porous materials other than sandstone-like materials (such as swelling polymers and bio-tissue), it would be valuable to have a clear theoretical foundation for the development, and to understand exactly what is being neglected.

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