Phase coexistence in consolidating porous media

Emilio N.M. Cirillo,1,∗ Nicoletta Ianniro,1,† and Giulio Sciarra2,‡

1Dipartimento Me. Mo. Mat., Università degli Studi di Roma “La Sapienza,” via A. Scarpa 16, 00161 Roma, Italy
2Dipartimento di Ingegneria Chimica Materiali Ambiente, Università degli Studi di Roma “La Sapienza,” via Eudossiana 18, 00184 Roma, Italy

The appearance of the fluid–rich phase in saturated porous media under the effect of an external pressure is investigated. For this purpose we introduce a two field second gradient model allowing the complete description of the phenomenon. We study the coexistence profile between poor and rich fluid phases and we show that for a suitable choice of the parameters non-monotonic interfaces show up at coexistence.

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I. INTRODUCTION

When a porous medium is plunged in an infinite fluid reservoir, the solid matrix absorbs fluid until an equilibrium state is reached. Many interesting features of this swelling phenomenon have been demonstrated experimentally. The amount of swelled fluid can be controlled depending on the external pressure acting on the porous material, phases differing in fluid content are observed. This problem has been addressed by the authors in particular a first gradient model; the existence of two different phases and the formation of critical droplets, if any, of one phase into the other.

The adopted approach in modeling the behavior of porous continua is essentially based on a pure solid Lagrangian description of motion, referring kinematics to the reference configuration of the porous skeleton (see Section II).

The constitutive model is purely phenomenological, which means that the overall potential energy, regarded as a function of the strain of the skeleton and the fluid mass density (per unit volume, in the solid reference configuration), is built up in such a way to describe the existence of two states of equilibrium: the solid–rich and the fluid–rich phase. Thus no refined description of solid grain connectivity, as well as connection among regions with different porosity is available in such a model. Conversely the constitutive state parameters are selected so as to describe the showing up of the fluid–rich phase, which is possibly associated to the occurrence of fluid segregation.

II. THE POROMECHANICS SETUP

Let $B_s \subset \mathbb{R}$ be the reference configurations for the solid and fluid components. The solid placement is a $C^2$–diffeomorphism $\chi_s(\cdot, t) : B_s \to \mathbb{R}$ such that $\chi_s(X_s, t)$ is the position occupied at time $t$ by the solid particle $X_s$ in the reference configuration $B_s$. Consider $\phi(\cdot, t) : B_s \to \mathbb{R}$ such that $\phi(X_s, t)$ is the fluid particle which at time $t$ occupies the same position of the solid particle $X_s$. Assume also $\phi(\cdot, t)$ to be a $C^2$–diffeomorphism, thus the map $\phi(\cdot, t)$ associate univocally a solid particle to a fluid one and vice versa. The fluid placement map $\chi_f(\cdot, t) : \mathbb{R} \to \mathbb{R}$, giving the position of a fluid particle $X_f$, is defined as $\chi_f(X_f, t) := \chi_s(\phi^{-1}(X_f), t)$. The current configuration $\chi_s(B_s, t)$ at time $t$ is the set of positions of the superposed solid and fluid particles.

Let $J_s(X_s, t) := |\partial_x \chi_s(X_s, t)/\partial X_s|$ be the Jacobian of the placement map $\chi_s(\cdot, t)$ measuring the ratio between current and reference volumes of the solid component; we let $\varepsilon(X_s, t) := (J_s(X_s, t)^2 - 1)/2$ be the strain field. Let $\varrho_{s, \alpha}(X_s)$ with $\alpha = s, f$, be the solid and fluid reference densities; we define the fluid mass density field $m(X_s, t) := \varrho_{s, f}(\phi(X_s, t)) \partial \phi(X_s, t)/\partial X_s$. Assuming that the mass is conserved, it is not difficult to prove that the field $m$ can be interpreted as the fluid mass density measured w.r.t. (with respect to) the solid reference volume.

Assume, now, that the Lagrangian density $\mathcal{L}(\chi_s, \phi, \chi_s''', \phi'', \chi'_s, \phi', \chi_s, \phi)$ of the system is in the form

$$\mathcal{L} = T(\dot{x}, \dot{\phi}, \chi_s, \phi) - \Phi(\chi_s''', \phi'', \chi'_s, \phi', \chi_s, \phi)$$

where $T$ is the kinetic energy density and $\Phi$ is the overall potential energy density accounting for both the internal and the external forces. In (1) we have denoted with the dot the derivative taken w.r.t. time and with the prime the derivative w.r.t. the solid reference space variable. The equation of motion for the two fields $\chi_s$ and $\phi$ can be derived assuming that the possible motions of the system in an interval of time $(t_1, t_2) \subset \mathbb{R}$ are those such that the fields $\chi_s$ and $\phi$ are extremals for the action functional

$$A(\chi_s, \ldots, \phi) := \int_{B_s} \! dX_s \int_{t_1}^{t_2} \! dt \mathcal{L}(\chi_s, \ldots, \phi)$$
in correspondence of the independent variations of the two fields $\chi_s$ and $\phi$ on $B_s \times \{(t_1, t_2)\}$. In other words any possible motion of the system in the considered interval is a solution of the Euler–Lagrange equations associated to the variational principle $\delta \lambda = 0$.

If one is interested to find equilibrium profiles $\chi_s(X_s)$ and $\phi(X_s)$ of the system, namely, the solutions of the equations of motion independent of time, since the kinetic energy associated to those profiles is equal to zero, the Lagrangian reduces to minus the potential energy density $\Phi$.

The variational principle associated to such an action time integral gives a not essential multiplicative constant, and the variational principle associated to such an action gives the sought for equilibrium profiles.

Assume, now, that the effect of the internal forces exchanged by the solid and fluid particles and that of the conservative external fields can be described via a potential energy density $\Phi(m', \epsilon', m, \epsilon)$ depending on the kinematic fields $\chi_s$ and $\phi$ only through the strain and the fluid mass density fields. Note that the strain depends only on $\chi_s$ and the fluid mass density only on $\phi$, hence the independent variations of those profiles reflect on independent variations of $\epsilon$ and $m$. Thus, limiting the study to boundary value problems expressed in terms of the fields $\epsilon$ and $m$, we can treat the fields $\epsilon$ and $m$ as primitive, consider their independent variations and look for the equilibrium profiles $\epsilon(X_s)$ and $m(X_s)$ starting from the variational principle

$$\delta \int_{B_s} dX_s \Phi(m'(X_s), \epsilon'(X_s), m(X_s), \epsilon(X_s)) = 0 \quad (3)$$

Finally, we can derive, starting from (3), the equations governing the equilibrium profiles $\epsilon$ and $m$. By computing the variation of the action functional on $B_s = (t_1, t_2)$, with $t_1, t_2 \in \mathbb{R}$, we get the Euler–Lagrange equations

$$\frac{\partial \Phi}{\partial \epsilon} - \frac{d}{dX_s} \epsilon \frac{\partial \Phi}{\partial \epsilon'} = 0 \quad \text{and} \quad \frac{\partial \Phi}{\partial m} - \frac{d}{dX_s} \frac{\partial \Phi}{\partial m'} = 0 \quad (4)$$

with boundary conditions ensuring that

$$\left[ \frac{\partial \Phi}{\partial \epsilon} \frac{\partial \Phi}{\partial \epsilon'} + \frac{\partial \Phi}{\partial m} \frac{\partial \Phi}{\partial m'} \right]_{t_1}^{t_2} = 0 \quad (5)$$

where $\delta \epsilon$ and $\delta m$ are, respectively, the variations of the strain and fluid mass density fields. For instance Dirichelet boundary conditions would do the job, since we would have $\delta \epsilon(t_1) = \delta \epsilon(t_2) = 0$ and $\delta m(t_1) = \delta m(t_2) = 0$. But for potential energy densities $\Phi$ at least quadratic in the derivatives $\epsilon'$ and $m'$ even Neumann boundary conditions would be acceptable. In the sequel we shall refer to any solution of the Euler–Lagrange equations (4) with suitable boundary conditions as an equilibrium profile of the system corresponding to the chosen boundary conditions.

The model (3) is called a first gradient model if the potential energy density $\Phi$ does not depend on the first derivatives of the strain and of the liquid density, otherwise the model is said a second gradient model. This way of classifying the models is related to the fact that both $\epsilon$ and $m$ depends, by definition, on the gradient of the primitive kinetic fields $\chi_s$ and $\phi$.

Second gradient theories are suitable to be developed for modeling stress/strain concentration due, for instance, to the presence of geometrical singularities (crack propagation in fracture mechanics\textsuperscript{9}) or phase transitions as in the case of wetting\textsuperscript{10,11}. In particular second gradient poromechanics has been recently formulated\textsuperscript{8,12} extending the standard arguments of the Biot theory\textsuperscript{13}. Such a model addresses the description of those deformation phenomena which occur at the same length scale as that where high gradients in deformation can be detected. Classical poromechanics\textsuperscript{7} is not able to describe these phenomena; the macroscopic model is regarded in that case as the average of a microscopic one where a kind of stationarity assumption\textsuperscript{14} (spatial ergodicity) on the random field which characterizes the microscopic mechanical properties of the material has been formulated. This allows for replacing ensemble averages with volume averages insofar as the characteristic size of the heterogeneities is much smaller than the typical length scale of the reference volume element (RVE). If this is no more the case, the classical assumptions of uniform strain (stress) or periodic boundary conditions, for every reference volume, are no more valid, but, conversely, macroscopic strain gradient plays a crucial role in specifying the state of stress/strain inside the RVE itself.

The goal, here, is to formulate a second gradient poromechanical model for describing the transition from the standard Biot–like equilibrium, associated to a compacted solid, versus the fluid–segregated phase describing duct thinning in the matrix and, consequently, fluid mass concentration in the pores. Thus, we consider a model with total potential energy density in the form

$$\Phi(m', \epsilon', m, \epsilon) = K(m', \epsilon', m, \epsilon) + \Psi(m, \epsilon) \quad (6)$$

where $K$ is a polynomial quadratic function of $\epsilon'$ and $m'$, $\Psi$ is a differentiable function positively diverging along any radial direction in the plane $\epsilon-m$, having at least a local minimum, and whose stationary points are isolated. Since $K$ is quadratic, we have that a constant solution of the Euler–Lagrange problem (4) must necessarily satisfy the equations $\Psi_{\epsilon} = 0$ and $\Psi_{m} = 0$; in other words a constant profile must be constantly equal to an extremal point of the first gradient part $\Psi$ of the total potential energy.

We then let a phase of the model to be a constant equilibrium profile equal to one of the local minima of the function $\Psi$.

Note that the Euler–Lagrange problem (4) and (5) for the first gradient model associated to (6), namely the one obtained for $K = 0$, is the system of algebraic equations $\Psi_{m} = 0$ and $\Psi_{\epsilon} = 0$. Since the stationary points of the two variable function $\Psi$ are isolated, we have that the equilibrium profiles for such a model are necessarily constant functions of $X_s \in B_s$ equal to the values of the stationary points of $\Psi$. 
Hence, in the case of a first gradient model it is not possible to discuss phase coexistence, since there exist only continuous constant equilibrium profiles. On the other hand, in second gradient models, different (not constant) equilibrium profiles can exist. This fact allows us to pose the problem of the coexistence of two existing phases. Suppose that the model exhibits the two phases \((m_1, \varepsilon_1)\) and \((m_2, \varepsilon_2)\); a connection \(^{15}\) between those phases is an equilibrium profile \(m, \varepsilon\) of the action functional on \(B_\varepsilon = (-\infty, +\infty)\) satisfying the boundary conditions \(m(-\infty) = m_1, m(+\infty) = m_2, \varepsilon(-\infty) = \varepsilon_1, \) and \(\varepsilon(+\infty) = \varepsilon_2.\) We say that the two considered phases coexist if and only if a connection does exist.

III. THE MODEL

We study, now, a particular poroelastic model and in that framework we discuss the existence of the consolidation phase transition and prove the coexistence of the two phases for a particular value of the external pressure. More precisely we consider the poroelastic system with overall potential energy density \((6)\) with

\[
K(m', \varepsilon') := \frac{1}{2}k_1(\varepsilon')^2 + 2k_2\varepsilon'm' + k_3(m')^2 \tag{7}
\]

with \(k_1, k_3 > 0, k_2 \in \mathbb{R}\) such that \(k_1k_3 - k_2^2 \geq 0,\) and

\[
\Psi(m, \varepsilon, p) := \frac{\alpha}{12}m^3(3m^2 - 8\varepsilon m + 6b^2\varepsilon^2) + \Psi_B(m, \varepsilon, p) \tag{8}
\]

where

\[
\Psi_B(m, \varepsilon; p) := p\varepsilon - \frac{1}{2}\varepsilon^2 + \frac{1}{2}a(m - \varepsilon b)^2 \tag{9}
\]

is the Biot potential energy density \(^{13}\), \(a > 0\) is the ratio between the fluid and the solid rigidity, \(b > 0\) is a coupling between the fluid and the solid component, \(p > 0\) is the external pressure, and \(\varepsilon > 0\) is a material parameter responsible for the showing up of the additional equilibrium. We remark that the condition \(k_1k_3 - k_2^2 \geq 0\) ensures that the second gradient part \(K\) of the overall potential energy density is convex. Under this assumption there exists a minimizer for the action functional

\[
\int_{f_1}^{f_2} dx \Phi(m', \varepsilon', m, \varepsilon)
\]

on a bounded domain. As we will see later to ensure the existence of a connection profile, which is a Dirichlet problem on an unbounded domain, it will be necessary to assume \(k_1k_3 - k_2^2 > 0;\) in the limiting case \(k_1k_3 - k_2^2 = 0\) the existence of the connection will depend on the choice of the parameter \(k_1, k_2,\) and \(k_3.\)

We have already studied\(^*\) the associated first gradient model with overall potential energy density \(\Psi\) and we have proven the existence of a phase transition driven by the external pressure \(p.\) More precisely it has been shown that there exists a critical pressure \(p_c = p_c(a, a, b)\) such that for \(0 < p \leq p_c\) the system admits the single standard phase \((m_s(p), \varepsilon_s(p)),\) while a second fluid–rich phase \((m_f(p), \varepsilon_f(p)),\) appears for \(p > p_c.\) The standard phase is similar to the unique phase described by the model with potential energy density \(^{13}\) \(\Psi_B.\) In FIG. 1 the standard and the fluid–rich phases are depicted for \(p \geq p_c\) and for a particular choice of the physical parameters \(\alpha, a, b.\)

IV. COEXISTENCE

The second gradient model has the same phases as the associated first gradient model. The main result of this paper is the existence of \(p_{co} = p_{co}(a, a, b) > p_c,\) called coexistence pressure, such that the standard and the fluid–rich phases coexist at the pressure \(p = p_{co}\) and do not coexist at \(p > p_c\) and \(p \neq p_{co}.\) The proof will be achieved in two steps: first we shall show that there exist a unique value of the pressure such that the total potential energy densities evaluated at the two phases are equal; the second step will consist in proving the existence of the connection, that is the equilibrium profile connecting the two phases.

A. Coexistence pressure

We first review some of the results in the previous paper\(^*\) there we have studied the equations \(\Psi_\varepsilon = 0\) and \(\Psi_m = 0\) looking for the minima of the function \(\Psi.\)

We have shown that the standard phase \((m_s(p), \varepsilon_s(p))\) is the solution of the two equations \(m = \varepsilon b\) and \(p = f_1(\varepsilon),\) for any \(p > 0,\) where \(f_1(\varepsilon) := -\varepsilon - ab^4\varepsilon^3/3.\)

On the other hand the fluid–rich phase \((m_f(p), \varepsilon_f(p))\) is the solution, with the smallest value of \(\varepsilon,\) of the two equations \(m = m_+(\varepsilon)\) and \(p = f_+(\varepsilon),\) where

\[
m_+(\varepsilon) = \frac{b}{2} \left[ 1 + \sqrt{\varepsilon^2 - \frac{4a}{ab^2}} \right]
\]
and 
\[ f_+ (\varepsilon) := -\varepsilon + ab [m_+ (\varepsilon) - \varepsilon] - ab^2 \varepsilon m_+^2 (\varepsilon) + \frac{2}{3} abm_+^3 (\varepsilon) \]

For \( \varepsilon \leq -2 / (b \sqrt{\alpha / a}) \) the function \( f_+ (\varepsilon) \) is positive, diverging to \( +\infty \) for \( \varepsilon \to -\infty \), and has a minimum at \( \varepsilon_c \) such that \( f_+ (\varepsilon_c) = p_c \); this explains why the fluidized phase is seen only for \( p > p_c \). Moreover it has been proven that for any \( p > p_c \), the point \( (m_1 (p), \varepsilon_1 (p)) \) is a minimum of the two variable potential energy \( \Psi (m, \varepsilon, p) \) with \( p \) fixed, while it is a saddle point for \( p = p_c \).

We now prove the first step of the above stated coexistence result. For any \( p > p_c \), we let \( \Psi_s (p) := \Psi (m_1 (p), \varepsilon_1 (p), p) \) and \( \Psi_t (p) := \Psi (m_1 (p), \varepsilon_1 (p), p) \) and prove that

\[
\begin{align*}
\Psi_s (p) &> \Psi_t (p) \quad \text{for } p > p_{co} \\
\Psi_s (p) &= \Psi_t (p) \quad \text{for } p = p_{co} \\
\Psi_s (p) &< \Psi_t (p) \quad \text{for } p_{co} > p \geq p_c
\end{align*}
\]

(10)

that is the overall potential energy density of the standard and the fluid–rich phases are equal only at the coexistence pressure. This statement has been tested on numerical grounds, see FIG. 2 where the graphs of the functions \( \Psi_s (p) \) and \( \Psi_t (p) \) are depicted for a given set of physical parameters.

In order to prove (10) we first compute the derivative of the two functions \( \Psi_s (p) \) and \( \Psi_t (p) \) (with respect to \( p \)); by using (8), the chain rule, and the fact that \( \Psi_s (m, \varepsilon, p) = 0 \) and \( \Psi_t (m, \varepsilon, p) = 0 \), we have that \( \Psi_s' (p) = \varepsilon_1 (p), \Psi_t' (p) = \varepsilon_1 (p), \Psi_s'' (p) = \varepsilon_1'' (p), \) and \( \Psi_t'' (p) = \varepsilon_1'' (p) \).

Now, since \( \varepsilon_1 (p) \) and \( \varepsilon_1 (p) \) are negative functions of the pressure, we have that both \( \Psi_s (p) \) and \( \Psi_t (p) \) are decreasing functions of the pressure on the interval \((p_c, +\infty)\). Moreover, noted that both \( f_1 \) and \( f_+ \) are decreasing functions of \( -\infty, \varepsilon_c \), we have that \( \varepsilon_1 (p) \) and \( \varepsilon_1 (p) \) decrease when \( p \) increases. It then follows that \( \varepsilon_1'' (p) \) and \( \varepsilon_1'' (p) \) are negative and therefore \( \Psi_s (p) \) and \( \Psi_t (p) \) are concave on the interval \((p_c, +\infty)\).

Since the two functions \( \Psi_s (p) \) and \( \Psi_t (p) \) are decreasing concave functions on the interval \((p_c, +\infty)\), in order to prove (10) it is sufficient to show that \( \Psi_s (p_c) < \Psi_t (p_c) \) and \( \Psi_s (p) > \Psi_t (p) \) for some \( p \) sufficiently large. The proof of the first remark is easy: at \( p = p_c \) the two variable function \( \Psi (m, \varepsilon, p_c) \) has just the two stationary points \( (m_1 (p_c), \varepsilon_1 (p_c)) \) and \( (m_1 (p_c), \varepsilon_1 (p_c)) \). Since \( (m_1 (p_c), \varepsilon_1 (p_c)) \) is a local minimum of \( \Psi (m, \varepsilon, p_c) \), which tends to \( +\infty \) along every direction on the plane \( m, \varepsilon \), the single local minimum must be the absolute minimum; hence, \( \Psi_s (p_c) < \Psi_t (p_c) \). The second remark follows from the asymptotic behavior of the two functions \( \Psi_s (p) \) and \( \Psi_t (p) \); as proven in the Appendix A, for \( p \to \infty \) we have

\[
\Psi_s (p) = -\frac{3}{4} 3^{1/3} \left( \frac{1}{ab^2} \right) p^{4/3} + O(p^{2/3})
\]

(11)

and

\[
\Psi_t (p) = \frac{1}{1 + ab^2} p^2 + \frac{1}{2(1 + ab^2)} p^2 + O(p)
\]

(12)

By comparing the two asymptotic formulas (11) and (12) we get immediately that for \( p \) large enough \( \Psi_s (p) > \Psi_t (p) \).

B. Connection profile

It is worth remarking that the variational problem (3) for profiles with fixed values at the end points \( \ell_1 \) and \( \ell_2 \) of the interval \( B_s \), is nothing but the Hamilton principle for a two degree of freedom mechanical system with Lagrangian coordinates \( \varepsilon \) and \( m \), kinetic energy \( T \) and potential energy \( U \) respectively given by

\[
T(m', \varepsilon') = \frac{1}{2} [k_1 (\varepsilon')^2 + 2k_2 \varepsilon' m' + k_3 (m')^2]
\]

(13)

and

\[
U(m, \varepsilon) = -\Psi (m, \varepsilon)
\]

(14)

and the space variable \( X_s \) interpreted as time. In other words the function \( \Phi \) defined by (6), (7), and (8) is the Lagrangian for such a two degree of freedom equivalent mechanical system.

It is important to remark that the mechanical interpretation is correct only when \( T \) is a positive definite quadratic form. It is easy to prove that this is the case provided \( k_1 k_3 - k_2^2 > 0 \). In the limiting case \( k_1 k_3 - k_2^2 = 0 \) the form \( T \) is positive semidefinite, indeed if we substitute \( k_1 = k_2^2 / k_3 \) in (13) the function \( T \) becomes

\[
T(m', \varepsilon') = K(m', \varepsilon') = \frac{1}{2} k_3 (k \varepsilon' + m')^2
\]

(15)

where we have set \( k := k_2 / k_3 \), and is equal to zero when \( k \varepsilon' + m' = 0 \).
We study now the case $k_1k_3 - k_2^2 > 0$ and postpone the degenerate $k_1k_3 - k_2^2 = 0$ to the following section. Let us denote $X_s$ by $t$ and the derivative taken with respect to $t$ by the dot. By using (4) with $\Phi = T - U$ and recalling (13), we have that the equations of motion are

$$k_2\ddot{m} + k_1\ddot{\varepsilon} = -\frac{\partial U}{\partial \varepsilon} \quad \text{and} \quad k_2\ddot{m} + k_2\ddot{\varepsilon} = \frac{\partial U}{\partial m} \quad (16)$$

We note that the mechanical energy of the associated mechanical problem $E(m, \varepsilon, m, \varepsilon) := T(\dot{m}, \dot{\varepsilon}) + U(m, \varepsilon)$ is a constant of the motion.

First note that the two points $(m_s(p), \varepsilon_s(p))$ and $(m_t(p), \varepsilon_t(p))$, with $p > p_c$, are maxima of the potential energy $U(m, \varepsilon)$ of the equivalent mechanical system. The problem of the existence of a connection between the standard and the fluid–rich phase can be rephrased as follows: look for a solution of the equations (16), namely, a motion $(m_p(t), \varepsilon_p(t))$ of the equivalent mechanical system, on $\mathbb{R}$ connecting the phase space point $(m_p(-\infty), \varepsilon_p(-\infty)) = (m_s(p), \varepsilon_s(p))$ and $(m_p(-\infty), \varepsilon_p(-\infty)) = (0, 0)$ to the phase space point $(m_p(+\infty), \varepsilon_p(+\infty)) = (m_t(p), \varepsilon_t(p))$ and $(m_p(+\infty), \varepsilon_p(+\infty)) = (0, 0)$. The connection we are seeking for is an heteroclinic solution of the equation of motion tending to two fixed points in the phase space for $t \rightarrow -\infty$ and $t \rightarrow +\infty$.

Recall that the mechanical energy $E$ is a constant of the motion and remark that at the equilibrium points it is equal only for $p > p_c$, those two energies are equal only for $p = p_c$. This remark yields that for any $p > p_c$ and $p \neq p_c$ the standard and the fluid–rich phases do not coexist.

We are left with the case $p = p_c$. In principle an heteroclinic solution can exist, but to prove its existence is an highly not trivial problem which has been solved, under suitable hypotheses on the potential energy, in the recent paper\cite{15} whose main results have been summarized in the Appendix B. Since in the not degenerate case the form $T$ is positive definite, it is possible to find an orthogonal transformation of the coordinates in the plane $m-\varepsilon$ which diagonalize the form itself. Then, performing this transformation and subtracting to the potential energy $U$ of the equivalent mechanical system the constant term $U(m_s(p_c), \varepsilon_s(p_c)) = U(m_t(p_c), \varepsilon_t(p_c))$, the problem of finding a connection between the standard and fluid–rich phase is transformed in a problem in the form (B1) with $n = 2$ and $W$ replaced by $-[U - U(m_s(p_c), \varepsilon_s(p_c))]$. Since this function satisfies the hypotheses of the Theorem 3.6 by Allikakos and Fusco\cite{15} (see the Appendix B) we can then conclude that in the case $p = p_c$ there exists a connection between the standard and the fluid–rich phase and hence the two phases coexist.

V. THE DEGENERATE CASE

Consider the case $k_2 = \pm \sqrt{k_1k_3}$ and the change of variables

$$x := \frac{m + k\varepsilon}{\sqrt{1 + k^2}} \quad \text{and} \quad y := \frac{-km + \varepsilon}{\sqrt{1 + k^2}}$$

where we recall $k = k_2/k_3 = \pm \sqrt{k_1/k_3}$, which amounts to perform a rotation of the cartesian reference system in the plane $m-\varepsilon$. Using the new variables the two functions $T$ and $U$ become respectively

$$K(\dot{x}, \dot{y}) = T(\dot{m}(\dot{x}, \dot{y}), \dot{\varepsilon}(\dot{x}, \dot{y})) = \frac{1}{2}k_3(1 + k^2)\dot{x}^2 \quad (17)$$

and

$$V(x, y) = U(m(x, y), \varepsilon(x, y)) \quad (18)$$

where we have used (15) and (14) with

$$m = \frac{x - ky}{\sqrt{1 + k^2}} \quad \text{and} \quad \varepsilon = \frac{kx + y}{\sqrt{1 + k^2}}$$

The expression (18) of $V$ is awful, but this will not be a problem since $V$ is precisely the two variable functions $-\Psi$, which we have already deeply studied\cite{5}, written via a rotation of the cartesian reference system.

We apply, now, the variational principle (3) to the total poroelastic potential energy density $\mathcal{L}(\dot{x}, \dot{y}, x, y) := K(\dot{x}, \dot{y}) - V(x, y)$ and get the analogous (indeed it is a particularization) of the equations (4)

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} = 0 \quad \text{and} \quad \frac{\partial \mathcal{L}}{\partial y} = 0 \quad (19)$$
The function \( V(x, y(x)) \) in the case \( a = 0.5, b = 1, \alpha = 100, k_3 = 1, k = 1, \) and \( p = p_{\text{co}} = 0.24218 \).

Since \( (m_a(p), \varepsilon_a(p)) \) and \( (m_t(p), \varepsilon_t(p)) \) satisfy the equations \( \Psi_m(m, \varepsilon) = 0 \) and \( \Psi_t(m, \varepsilon) = 0 \), we have that the two points \( (x_a(p, y_a(p))) \) and \( (x_t(p, y_t(p))) \) are solutions of the constraint equation \( \partial V(x, y)/\partial y = 0 \) and hence they belong to the constraint curve.

We consider, now, the case in which at \( p = p_{\text{co}} \) the two points above fall on the same maximal component of the constraint equation (see FIG. 3 and 4). Using the conservation of the mechanical energy of the equivalent one dimensional conservative system allows for reducing the computation of the coexistence profile (heteroclinic) to the evaluation of a definite integral. Since the function \( V \) has two isolated absolute maximum points which, by hypothesis, belong to the same maximal component of the constraint curve, we have that the function \( V(x, y(x)) \) of the real function \( x \) has two absolute isolated maxima in \( x_a(p_{\text{co}}) \) and \( x_t(p_{\text{co}}) \) (see FIG. 5). Consider the motion of the equivalent one dimensional system corresponding to the energy level \( V_{\text{max}} := V(x_a(p_{\text{co}}), y_a(p_{\text{co}})) \). The conservation of the mechanical energy implies

\[
\frac{1}{2}k_3(1 + k^2)\dot{x}^2 + V(x, y(x)) = V_{\text{max}}
\]

Hence, the heteroclinic connecting the two maxima is given by

\[
t = \int_{x_0}^{x} \sqrt{\frac{k_3(1 + k^2)}{2[V_{\text{max}} - V(x', y(x'))]}} \, dx'
\]

for any \( x \in (\min\{x_a(p_{\text{co}}), x_t(p_{\text{co}})\}, \max\{x_a(p_{\text{co}}), x_t(p_{\text{co}})\}) \) and for some fixed \( x_0 \) in the same interval. By changing \( x_0 \) it is found a family of heteroclinic orbits which are the same curve up to a time translation.

Results are depicted in the FIG. 6. The \( \varepsilon \) coexistence profile shows a bump\(^{17,18} \) close both to the standard and the fluid–rich phase. This behavior is due to the two–dimensionality of the problem: in FIG. 7 we have depicted the heteroclinic on the graph of the function.
$U(m,\varepsilon) = -\Psi(m,\varepsilon)$. From the picture it is clear that the optimal path climbs the two hills going around the hills themselves. In other words the existence of the bump in the connecting $\varepsilon$–profile is due to the shape of the constraint curve in the plane $m$–$\varepsilon$. Since the problem has been reduced to the computation of the heteroclinic of a one dimensional conservative mechanical system in the $x$ variable, it is obvious that no bump can exist in the $x$–profile. On the other hand by looking closely at the picture in FIG. 3 and 4, it emerges that the constraint curve is monotonic w.r.t. $y$ and $m$; this implies the monotonicity of the $y$ and $m$–profiles. However, it is possible to find values of the parameters such that the $y$–profile presents a bump.

In Section VA we have proven that in the not degenerate case the connecting profile does exist for any proper choice of the parameters. A similar result does not hold true in the degenerate case, indeed it is possible to find the connection if and only if the two maxima of the function $U$ lie on the same maximal component of the constraint curve. We have that this is not the case for $k > 0$ large enough, see the dashed curve in FIG. 8 which is associated to the value $k = 1.9$. It is immediate to remark that the two maxima do not lie on the same connected component, hence in this case it is not possible to find a connection between the fluid–rich and the standard phase. It is worth remarking that no evidence of this patologic behavior is found in the case $k < 0$; see FIG. 9 where the constraint curve and the stationary point of $U$ are depicted for $a = 0.5$, $b = 1$, $\alpha = 100$, $k_3 = 1$, $k = 1$, and $p = p_{co} = 0.24218$. This case is the most interesting one from the physical point of view, indeed for $k_2 < 0$ the coupling between $\varepsilon'$ and $m'$ is negative, hence the preferred states are such that the two fields $\varepsilon(X_s)$ and $m(X_s)$ are both increasing or decreasing.
can be found, see FIG. 10, by computing the integral

\[ t = \pm \int_{\bar{x}}^{x} \sqrt{\frac{k_3(1 + k_2)}{2[V(\bar{x}, y(\bar{x})) - V(x', y(x'))]}} \, dx' \]  \hspace{1cm} (22)

for any \( x \in (\min\{\bar{x}, \bar{x}\}, \max\{\bar{x}, \bar{x}\}) \) with \( \bar{x} \) the unique (inversion) point in the interval \( (\min\{x_s, x_f\}, \max\{x_s, x_f\}) \) such that \( V(\bar{x}, y(\bar{x})) = V(x', y(x')) \).

The homoclinic solution corresponding to the lowest maximum is often interpreted as a “critical nucleus.” In the sense that, if a dynamic evolution would be taken into account, one would expect that an initial condition close to the critical nucleus would evolve into the standard or the fluid–rich phase (subcritical and supercritical behavior). This behavior depends on the size of the droplet in the neighborhood of \( t = 0 \). Indeed in \( t = 0 \) the profile has the value \( \bar{x} \) which, for \( p \) close to \( p_{\text{co}} \), is a good approximation of the phase corresponding to the largest maximum of the function \( V \). In other words the critical nucleus can be seen as a droplet of the phase correspondig to the smallest value of the potential energy \( \Psi \) plunged into the other phase.

VI. CONCLUSIONS

In conclusion we have studied the phase transition between the fluid poor and rich phases in the context of consolidating completely fluid saturated porous media. A second gradient model to study the existence of such a transition has been proposed. Moreover, coexistence between the two phases at the pressure \( p_{\text{co}} \), defined as the pressure such that the total potential energy of the two phases is the same, has been established. We have also shown that at different values of the pressure the two phases cannot coexist. For a particular choice of the parameters of the model it is possible to reduce the problem of finding the coexistence profile to the computation of a definite integral. We have studied the coexistence profile for different values of the physical parameters of the model and shown that non–monotonic interfaces exist.

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APPENDIX A: ASYMPTOTIC BEHAVIOR OF POTENTIAL ENERGY

In this appendix we discuss the asymptotic behavior of the two functions \( \Psi_s(p) \) and \( \Psi_f(p) \), see Section IV A, for \( p \) large and, in particular, prove the equations (11) and (12). We first note that by using \( m_s(p) = b \epsilon_s(p) \), we get

\[ \Psi_s(p) = p \epsilon_s(p) + \frac{1}{2}(\epsilon_s(p))^2 + \frac{1}{12}a b^4 (\epsilon_s(p))^4 \]
The equation $f_1(\epsilon) = p$ is a cubic equation in the form $\epsilon^3 + \lambda \epsilon + \lambda p = 0$, with $\lambda = 3/(\alpha b^4)$; by Cardano's formula, since $D := (\lambda/3)^3 + (\lambda p/2)^2 > 0$, there exists a single real solution given by

$$\epsilon_+(p) = \left[ -\frac{1}{2} \lambda p + \sqrt{D} \right]^{1/3} + \left[ -\frac{1}{2} \lambda p - \sqrt{D} \right]^{1/3}$$

+ \left[ -\frac{1}{2} \lambda b^2 p - \sqrt{\left(\frac{1}{3} \lambda b^2 p\right)^3 + \left(\frac{1}{3} \lambda b^2 p\right)^2} \right]^{1/3}

By using the Taylor series $(1 + x)^n = \sum_{n=0}^{\infty} C_n(\alpha)x^n$, with $C_n(\alpha) = \alpha(\alpha - 1) \cdots (\alpha - n + 1)/n!$ being the binomial coefficient, which is convergent for $-1 < x < +1$, it is not difficult to prove that $\epsilon_+(p) = - \left(3/(\alpha b^4)\right)^{1/3} + (3/\alpha b^2)^{2/3}(1/p)^{1/3} + O(p^{-5/3})$ for $p$ large. By inserting this expression in the expansion for $\Psi_s$, we get equation (11).

We can perform a similar computation for $\Psi_f(\epsilon)$. Accounting in particular for the qualitative of $\epsilon_f(p)$, which tends to $-\infty$ when $p$ is increased, we shall study the asymptotic behavior of $m_+(\epsilon)$ for $\epsilon \to -\infty$ and that of $\epsilon_f(p)$ which is the solution of the equation $f_+(\epsilon) = p$ when $p \to \infty$. The result of this analysis will provide us with the asymptotic behavior of $\Psi_f(p)$. First of all we note that

$$m_+(\epsilon) = \frac{1}{2} \epsilon \left[ \frac{2a}{\alpha b^2 \epsilon} + \frac{2a^2}{\alpha^2 b^4 \epsilon^3} + O(\epsilon^{-6}) \right]$$

for $\epsilon \to -\infty$. By using (8) we then have

$$\Psi_f(p) = p \epsilon_f(p) + \frac{1}{2} \left(1 + ab^2\right)\epsilon_f(p)^2 - \frac{a^2}{2a} + O\left(\epsilon_f(p)^{-2}\right)$$

for $p \to \infty$, where we have used that $\epsilon_f(p) \to -\infty$ for $p \to \infty$. The function $\epsilon_f(p)$ is implicitly defined by the equation $f_+(\epsilon) = p$ which is pretty complicated. By expanding $f_+$ for $\epsilon \to -\infty$ the equation becomes $-\epsilon(1 + ab^2) + h(\epsilon) = p$ with $h(\epsilon)$ a function having limit 0 for $\epsilon \to -\infty$. Suppose $p$ is large enough and let $\epsilon_f(p)$ be the solution of the equation above; by the qualitative study we get that $\epsilon_f(p) \to -\infty$ for $p \to \infty$. It is then easy to show that $g(p) := \epsilon_f(p) - \left(1/(1 + ab^2)\right)$ tends to zero for $p \to \infty$, indeed, since $\epsilon_f(p)$ is the solution of the equation above, we have that

$$g(p) = \frac{(1 + ab^2)\epsilon_f(p) + p}{1 + ab^2} = \frac{h(\epsilon_f(p))}{1 + ab^2} \to 0$$

for $p \to \infty$, where we have used that $h(\epsilon) \to 0$ for $\epsilon \to -\infty$ and $\epsilon_f(p) \to -\infty$ for $p \to \infty$. By inserting the obtained expression of $\epsilon_f(p)$ in the above expansion of $\Psi_f(p)$ we get equation (12).

**APPENDIX B: GENERAL RESULT ON THE EXISTENCE OF CONNECTIONS**

In this appendix we briefly review the main results by Alikakos and Fusco on the existence of connections.
Let \( W : \mathbb{R}^n \to \mathbb{R} \), with \( n \geq 1 \), be a \( C^2(\mathbb{R}^n) \) positive function satisfying the following hypotheses: (1) \( W \) has two distinct local minima \( a_-, a_+ \in \mathbb{R}^n \) such that \( W(a_-) = W(a_+) = 0 \), (2) \( W(u) > 0 \) for any \( u \neq a_-, a_+ \), (3) \( \lim \inf_{|u|\to\infty} W(|u|) > 0 \), (4) there exists \( r_0 \) in the open interval \((0, |a_- - a_+|)\) such that for any \( \xi \in \mathbb{R}^n \) such that \( |\xi| = 1 \) the two maps \( r \mapsto W(a_+ + r_0 \xi) \) have a strictly positive derivative for every \( r \in (0, r_0) \). Conditions (1) – (3) are quite natural and physically obvious; condition (4) is a mild technical requirement allowing for potential energies with \( C^\infty \) contact at zeroes.

Consider the ordinary differential equation problem
\[
\begin{align*}
 u_{xx} &= \nabla W(u) \\
 u(-\infty) &= a_- \quad \text{and} \quad u(+\infty) = a_+ 
\end{align*}
\] (B1)
where \( u : \mathbb{R} \to \mathbb{R}^n \). Solutions to the problem (B1) are known in the literature as heteroclinic motions of the mechanical system or connection solutions in the context of phase transitions. The Theorem 3.6 by Alikakos and Fusco states that, under the hypotheses discussed above, the problem (B1) admits a solution. In other words the theorem states the existence of a connection under very general and mild requirements on the potential \( W \). The proof of the theorem is based on a direct variational computation. More precisely the authors prove the existence of a critical profile of the action functional
\[
A(u) := \int_{-\infty}^{\infty} \left[ \frac{1}{2} |\dot{u}(x)|^2 + W(u(x)) \right] \, dx
\]
on the Sobolev space \( W^{1,2}_{\text{loc}}(\mathbb{R}, \mathbb{R}^n) \) of functions \( u : \mathbb{R} \to \mathbb{R}^n \) such that \( u \) and its weak derivative are in \( L^2(\Omega, \mathbb{R}^n) \) for any bounded subsets \( \Omega \subset \mathbb{R} \). Such a critical profile is the solution of the ordinary differential equation problem (B1).

Compared to the standard variational calculus, see for instance the paragraph 8.2 in Evan’s classical book\(^\dagger\), the authors have to face the lack of compactess due to the infinite domain \( \mathbb{R} \) on which the solution of the variational problem is defined. This problem is overcome by using suitable constraints that are successively removed. It is also worth noting that in the Theorem 3.7 the authors state that the connection is a minimizer of the action functional \( A(u) \).

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\(*\) Electronic address: cirillo@dmmm.uniroma1.it

1 Electronic address: ianiro@dmmm.uniroma1.it


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