Constitutive modelling of Hydro-Mechanical coupling in double porosity media based on Mixture Coupling Theory

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Abstract: Modelling of fluids in deformable geoformation media has gained great attention in the past decades due to significant applications such as groundwater prediction, shale gas and carbon capture and storage. However, considerable research has been focused on the porous media concept, and dual network (fracture and pores) multiphysics coupled modelling has remained a challenge due to the lack of a systemic theory to bridge the physical deformation of the media (e.g., rocks) and the interaction of water flow in pores and fractures. This paper adopts the non-equilibrium thermodynamics-based approach, the Mixture Coupling Theory, to develop a thermodynamics consistency constitutive model for the fully coupled Hydro-Mechanical behavior in double porosity formation. The energy dispassion due to fluid flow in matrix pore and fracture is given through non-equilibrium thermodynamics, and the relationship between the solid and fluid is linked through Helmholtz free energy. The dynamic evolution of stress, porosity change of the matrix pores and fracture, are derived with respect to mechanical strain, pore pressure, and fracture pressure to account for the flow-deformation interaction. The developed constitutive equations are then solved numerically to show the hydraulic and mechanical behavior of double porosity formation, as well as their sensitivity to parameters.

Keywords: double porosity; nonequilibrium thermodynamics; hydraulic-mechanical

Introduction

The ubiquity of double porosity media and its completely different characteristics compared to porous media give rise to the importance of studies on water flow in fractured soil or rock in groundwater sources evaluation, underground construction, groundwater contamination, petroleum and shale gas exploitation, underground gas storage, geothermal reservoir (Berkowitz 2002, Rutqvist and Stephansson 2003, Gupta and Yadav 2020). Water flow in the subsurface is driven by both hydraulic gradient and rock mechanical field. The interaction between water flow and the deformation of the solid results in a more complex process in groundwater flow (Segura and Carol 2008, Tsang et al. 2015), making it difficult for mathematical modelling.

The early modelling work toward the Hydro-Mechanical coupling are the ones by Terzaghi (1943) and Biot (1962), Biot (1972), then followed extensively by many other researchers (Lewis and Schrefler 1987, Vardoulakis et al. 1996, Rutqvist and Tsang 2002, Laloui et al. 2003, Rajagopal and Tao 2005, Tarantino and Tombolato 2005, Wong and Mašín 2014, Zhou and Sheng 2015). In these studies, the porous media is assumed to be homogeneous with single porosity. However, many geomaterials have two scales of void space: the matrix pores and the fracture (Borja and Koliji 2009), as illustrated in Fig. 1.

The distinctive fluid transport and pressure distribution in the fracture and matrix pores are quite different from those in the single porosity situation, so that the classic Biot equations fail to capture the feature of the double porosity situation.

To describe the coupled hydro-mechanical behavior of the double porosity material, the material is often viewed to be composed of two distinct but overlapping media: one consisting of the porous matrix, in which there are the solid matrix and matrix pores, and the other is the fracture (Barenblatt et al. 1960, Warren and Root 1963), see Fig. 1. The two media can exchange water mass as the porous matrix holds a large storage capacity and low permeability, while the fracture has high permeability and low storability (Song et al. 2019). Based on the above concept, various mathematical formulations representing the fluid flow or hydro-mechanical coupling have been developed by different approaches with different degrees of sophistication.

The early double porosity model (Barenblatt et al. 1960, Warren and Root 1963, Aifantis 1980) explored the fluid transport behavior but failed to explore the mechanical deformation and its coupling with fluid. In these research, the coupling between the fluids in the matrix pores and the fracture is achieved by the fluid exchange between the two regions; the flow is assumed to be independent of deformation. Later models (Wilson and Aifantis 1982, Khaled et al. 1984, Beskos and Aifantis 1986, Zhang et al. 2003, Zhang and Roegiers 2005) incorporated the fluid pressure into the strain equation and the strain influence on the fluid transport to achieve the coupling between flow and deformation. However, these models made no progress in the coupling between the fluids in the matrix pores and the fracture, as they only considered the mass exchange. The fact is that the fracture fluid acting on the porous matrix must lead to the change of fracture volume and matrix pore volume, and further influence the fluid transport in the matrix pore, and vice versa. Such a phenomenon is then incorporated in the new fully coupled Hydro-Mechanical models proposed by Khalili (2003), Khalili (2008).

The mathematical models are developed by different approaches. There is no certain classification of the approaches for modelling the double porosity problem. Different categories of approaches can be found in (Chen and Teufel 2000, Gelet et al. 2012, Boutin and Royer 2015). Among all the approaches, two noticeable ones are the conventional mechanics approach and the mixture theory approach. Some remarkable mathematic models have been developed by the mechanics approach (Elsworth and Bai 1992, Khalili and Valliappan 1996, Pao and Lewis 2002, Khalili 2003, Khalili 2008) and by the mixture theory approach (Aifantis 1977, Aifantis 1979, Aifantis 1980, Wilson and Aifantis 1982, Beskos and Aifantis 1986, Bai et al. 1993, Bai et al. 1993, Borja and Koliji 2009) and following further work (Wilson and Aifantis 1982, Khaled et al. 1984, Beskos and Aifantis 1986, Berryman and Wang 1995).

The mechanics approach is straightforward and simple, but it often requires ad hoc assumptions, and it lacks the ability of systemic self-development (Laloui et al. 2003). For the mixture theory approach, as pointed out by Heidug and Wong (1996), since it maintains the individuality of the solid and fluid phase, it highly relies on the phase interaction information that is very difficult to obtain. Physical intuition and specific assumptions must be required to form the coupling between phases. This may bring difficulties for this approach and restrict the application.

In this paper, a non-equilibrium thermodynamics-based approach, the mixture coupling theory, is adopted to develop the fully coupled governing equations for the hydro-mechanical behavior of double porosity media saturated with single-phase flow. This theory origins from Heidug's research for single porosity media with swelling effects (Heidug and Wong 1996). It is modified from the mixture theory by viewing the solid-fluid mixture as a single continuum without explicitly discriminating between the solid and fluid phases, therefore, this theory is more like a hybrid of the Biot poroelasticity view and the mixture theory. Unlike the mixture theory adopting the momentum conservation equation, mixture coupling theory directly works on the free energy conservation, making it easier. This theory provides a rigorous framework to study the coupling effects between multi-physics and multi-phases and has been applied to different couplings in porous media (Chen 2013, Chen et al. 2013, Chen et al. 2016, Chen et al. 2018, Ma et al. 2020), and it is the first attempt to apply the theory to the double porosity media to develop the fully coupled Hydro-Mechanical model.

By using mixture coupling theory, the very general evolution equation of stress, the porosity of the matrix pores and fracture are obtained with respect to the pore water pressure and fracture water pressure as well as coupling with mechanical strain. The final governing equations are restricted within the small strain and elastic conditions, and are the same as the model proposed by Khalili (2003) through the mechanics approach. The developed mathematical models are solved by the finite element method to illustrate the coupling phenomenon in double porosity media and the sensitivity of parameters.

Balance equation

Basic definitions and relationships

In a double porosity model, water can pass through the boundary via the porous matrix and the fracture, so that two water flux, namely, porous matrix flux $\mathbf{I}^{Mw}$ and fracture flux $\mathbf{I}^{Fw}$, are defined

$$\mathbf{I}^{Mw} = \rho^{Mw}\left(\mathbf{v}^{Mw} - \mathbf{v}^{s}\right),\ \mathbf{I}^{Fw} = \rho^{Fw}\left(\mathbf{v}^{Fw} - \mathbf{v}^{s}\right) \tag{1}$$

where the subscripts M_w, F_w, s represent the water in the matrix pore, water in fracture and the solid phase. ρ^{Mw} and ρ^{Fw} are the density of porous water and fracture water, which are relative to the volume of the whole mixture system. $\mathbf{v}^{Mw}$, $\mathbf{v}^{Fw}$, $\mathbf{v}^{s}$ are the velocity of porous water, fracture water and the solid.

ρ^{Mw} and ρ^{Fw} are related to the true mass density (relative to the volume of porous water and fracture water) ρ_t^{Mw} and ρ_t^{Fw} through

$$\rho^{Mw} = \phi^{Mw}\rho_t^{Mw}\ ,\ \rho^{Fw} = \phi^{Fw}\rho_t^{Fw} \tag{2}$$

where ϕ^{Mw}, ϕ^{Fw} are the porosity of porous matrix and fracture, and they are the volume of the matrix pore and fracture against the volume of the whole mixture.

The Darcy velocity for porous water and fracture water are

$$\mathbf{u}^{Mw} = \phi^{Mw}\left(\mathbf{v}^{Mw} - \mathbf{v}^{s}\right),\ \mathbf{u}^{Fw} = \phi^{Fw}\left(\mathbf{v}^{Fw} - \mathbf{v}^{s}\right) \tag{3}$$

Balance equation

An arbitrary domain V with a boundary S attached to its surface is selected. The domain includes all phases and the double porosity feature. Water flow can pass through the boundary while the solid cannot.

<u>1. Balance equation for Helmholtz free energy</u>

In the double porosity model, the Helmholtz free energy change involves four parts: the mechanical energy, the energy change by porous water flow, the energy change by fracture water flow and the entropy part, the balance equation writes as

$$\frac{D}{Dt}\int_V \psi dV = \int_S \boldsymbol{\sigma}\mathbf{n}\cdot\mathbf{v}^s dS - \int_S \mu^{Mw}\mathbf{I}^{Mw}\cdot\mathbf{n}dS - \int_S \mu^{Fw}\mathbf{I}^{Fw}\cdot\mathbf{n}dS - T\int_V \gamma dV \tag{4}$$

where: ψ is Helmholtz free energy density, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, μ^{Mw}, μ^{Fw} are the chemical potential of porous water and fracture water, respectively. T is the temperature, which is regarded as constant in this paper; γ is the entropy produced per unit volume of the mixture.

The material time derivative is $\frac{D}{Dt} = \partial_t + \mathbf{v}^s \cdot \nabla$, where ∂_t is the time derivative and ∇ the gradient, then the derivative version of the balance equation (4) for the Helmholtz free energy is

$$\dot{\psi} + \psi \nabla \cdot \mathbf{v}^s - \nabla \cdot \left(\boldsymbol{\sigma} \mathbf{v}^s \right) + \nabla \cdot \left(\mu^{Mw} \mathbf{I}^{Mw} \right) + \nabla \cdot \left(\mu^{Fw} \mathbf{I}^{Fw} \right) = -T\gamma \le 0 \tag{5}$$

2. Balance equation for water mass

Water in the matrix pore (fracture) changes in two ways: 1. Water flow $\mathbf{I}^{Mw}$ ($\mathbf{I}^{Fw}$) passes through the boundary and exchanges with the surroundings; 2. Water exchanges between the matrix pore and the fracture. The balance equation for water in the matrix pore and the fracture are

$$\frac{D}{Dt}\left(\int_V \rho^{Mw} dV \right) = -\int_S \mathbf{I}^{Mw} \cdot \mathbf{n} dS - \int_V r_{ex} dV \tag{6}$$

$$\frac{D}{Dt}\left(\int_V \rho^{Fw} dV \right) = -\int_S \mathbf{I}^{Fw} \cdot \mathbf{n} dS + \int_V r_{ex} dV \tag{7}$$

where r_{ex} is the exchange rate of fluid mass between the fracture and matrix pore.

The time derivative versions of the water balance equations are

$$\dot{\rho}^{Mw} + \rho^{Mw} \nabla \cdot \mathbf{v}^s + \nabla \cdot \mathbf{I}^{Mw} + r_{ex} = 0 \tag{8}$$

$$\dot{\rho}^{Fw} + \rho^{Fw} \nabla \cdot \mathbf{v}^s + \nabla \cdot \mathbf{I}^{Fw} - r_{ex} = 0 \tag{9}$$

Entropy production and transport law

Entropy production

During irreversible processes, such as heat and mass transfer, entropy will be produced. The entropy production can be expressed in terms of thermodynamic flows and thermodynamic forces (Kondepudi and Prigogine 2014). The quantification of entropy production through non-equilibrium thermodynamics is the core of the Mixture Coupling Theory.

During water transport in double porosity media, the entropy is generated from one mechanism, i.e., the friction between the solid and water boundary, which consists of three parts: 1. the friction of porous water ϑ_{Mw} ; 2. the friction of fracture water ϑ_{Fw} ; 3. the friction generated when water exchange between the matrix pore and the fracture networks ϑ_{ex} . From non-equilibrium thermodynamics (Katchalsky and Curran 1965), there is

$$\vartheta_{Mw} = -\mathbf{I}^{Mw} \cdot \nabla \mu^{Mw} \text{ , } \vartheta_{Fw} = -\mathbf{I}^{Fw} \cdot \nabla \mu^{Fw} \tag{10}$$

According to Gelet et al. (2012) and Coussy (2004), ϑ_{ex} can be expressed as

$$\vartheta_{ex} = r_{ex}\left(\mu^{Mw} - \mu^{Fw}\right) \tag{11}$$

Then, the overall entropy production of the mixture system can be written as

$$0 \le T\gamma = -\mathbf{I}^{Mw} \cdot \nabla \mu^{Mw} - \mathbf{I}^{Fw} \cdot \nabla \mu^{Fw} + r_{ex}\left(\mu^{Mw} - \mu^{Fw}\right) \tag{12}$$

In equation (12), $\mathbf{I}^{Mw}$, $\mathbf{I}^{Fw}$, r_{ex} are the thermodynamic flows, and $-\nabla \mu^{Mw}$, $-\nabla \mu^{Fw}$, $\left(\mu^{Mw} - \mu^{Fw}\right)$ are the corresponding thermodynamic forces that drive the transport processes.

The quantification of the entropy production (12) and the following substitution of $T\gamma$ term in the free energy equation (5) (like what has been done leading to equation (14)) are the key features of the Mixture Coupling Theory, distinguishing it from other thermodynamics approaches, such as the ones by Coussy (2004), Gelet et al. (2012), Nakshatrala et al. (2018). The advantages of the two features have been presented in Ma et al. (2022) when dealing with the dissolution process.

Transport Law

The entropy production in section 3.1, on the one hand, can be used to develop the transport law, like what has been done in Chen et al. (2018). This paper focuses on the coupling between the flow and deformation. To simplify the discussion, the fluid flow is assumed to obey the Darcy's law. The Darcy's law for porous water and the fracture water can be derived through the entropy production, Gibbs-Duhem equation and phenomenological equation, as (Chen 2013)

$$\mathbf{u}^{Mw} = -\frac{k^{Mw}}{\nu^{w}}\nabla p^{Mw}\ , \quad \mathbf{u}^{Fw} = -\frac{k^{Fw}}{\nu^{w}}\nabla p^{Fw} \tag{13}$$

where k^{Mw} , k^{Fw} are the intrinsic permeability for porous matrix and fracture, p^{Mw} and p^{Fw} correspond to the porous water pressure and fracture water pressure, respectively, ν^{w} is the water viscosity.

Constitutive equation

Basic equation for deformation

Assuming the material maintains mechanical equilibrium so that there is $\nabla\cdot\boldsymbol{\sigma} = \mathbf{0}$. Substituting the entropy production (12) into the Helmholtz free energy balance equation (5), the Helmholtz free energy change of the mixture system can be written as

$$\dot{\psi} + \psi\nabla\cdot\mathbf{v}^{s} - \nabla\cdot\left(\boldsymbol{\sigma}\mathbf{v}^{s}\right) + \mu^{Mw}\nabla\cdot\mathbf{I}^{Mw} + \mu^{Fw}\nabla\cdot\mathbf{I}^{Fw} + r_{ex}\left(\mu^{Mw} - \mu^{Fw}\right) = 0 \tag{14}$$

Equation (14) gets rid of the entropy term in equation (5), and enables us to explore the Helmholtz free energy change through the mass flux $\mathbf{I}^{Mw}$, $\mathbf{I}^{Fw}$ and r_{ex} . Multiplying μ^{Mw} , μ^{Fw} on both sides of equation (8), (9), and substituting the corresponding results into equation (14), the Helmholtz free energy change becomes

$$\dot{\psi} + \psi\nabla\cdot\mathbf{v}^{s} = \nabla\cdot\left(\boldsymbol{\sigma}\mathbf{v}^{s}\right) + \mu^{Mw}\left(\dot{\rho}^{Mw} + \rho^{Mw}\nabla\cdot\mathbf{v}^{s}\right) + \mu^{Fw}\left(\dot{\rho}^{Fw} + \rho^{Fw}\nabla\cdot\mathbf{v}^{s}\right) \tag{15}$$

In equation (15), the term $\dot{\rho}^{Mw} + \rho^{Mw}\nabla\cdot\mathbf{v}^{s}$ is the pore water mass change in the mixture, and therefore $\mu^{Mw}\left(\dot{\rho}^{Mw} + \rho^{Mw}\nabla\cdot\mathbf{v}^{s}\right)$ represents the free energy change due to pore water mass change. Equation (15) indicating that the free energy change of the system is the result of the mechanical energy and the mass energy.

Next, classic continuum mechanics method is adopted to measure the deformation state. Some basic relationships are required (Wriggers 2008)

$$\mathbf{F}=\frac{\partial \mathbf{x}}{\partial \mathbf{X}}(\mathbf{X},t)\ ,\ \mathbf{E}=\frac{1}{2}\left(\mathbf{F}^{\mathrm{T}}\mathbf{F}-\mathbf{I}\right),\mathbf{T}=J\mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{F}^{-T} \quad (16)$$

where $\mathbf{X}$ is an arbitrary reference configuration, $\mathbf{x}$ is the position, $\mathbf{E}$ represents Green strain, $\mathbf{F}$ is the deformation gradient, $\mathbf{T}$ and $\boldsymbol{\sigma}$ are the second Piola-Kirchhoff stress and Cauchy stress. J is the Jacobian of $\mathbf{F}$ ($J=\det\mathbf{F}$), and satisfies $J=\dfrac{dV}{dV_0}$ (V , V_0 are the volume in the current and reference configuration.)

The time derivation of J satisfies the Euler's formula

$$\dot{J}=Jdivv_s \quad (17)$$

From equation (15), with the relationships (16) and (17), the Helmholtz free energy equation (15) can be switched into the reference configuration as

$$\dot{\Psi}=tr\left(\mathbf{T}\dot{\mathbf{E}}\right)+\mu^{Mw}\dot{m}^{Mw}+\mu^{Fw}\dot{m}^{Fw} \quad (18)$$

in which: $\Psi=J\psi$ is the Helmholtz free energy in the reference configuration, $m^{Mw}=J\rho^{Mw}$, $m^{Fw}=J\rho^{Fw}$ are the mass density of porous water and fracture water in the reference configuration.

Helmholtz free energy density of porous/fracture water

According to classical thermodynamics, the free energy density of porous matrix water and fracture water can be written as

$$\psi_{porous}=-p^{Mw}+\rho_t^{Mw}\mu^{Mw} \quad (19)$$

$$\psi_{fracture}=-p^{Fw}+\rho_t^{Fw}\mu^{Fw} \quad (20)$$

Using the Gibbs-Duhem equation for porous water and fracture water, it leads to

$$\dot{p}^{Mw}=\rho_t^{Mw}\dot{\mu}^{Mw} \quad (21)$$

$$\dot{p}^{Fw}=\rho_t^{Fw}\dot{\mu}^{Fw} \quad (22)$$

Invoking equation (21), (22) into the time derivation of equation(19), (20), the following relationships can be obtained

$$\dot{\psi}_{porous}=\dot{\rho}_t^{Mw}\mu^{Mw} \quad (23)$$

$$\dot{\psi}_{fracture} = \dot{\rho}_t^{Fw} \mu^{Fw} \tag{24}$$

Free energy density of the solid matrix

The free energy of the solid-porous-fracture mixture system consists of three parts: the free energy of the porous water, the free energy of the fracture water and the free energy of the solid matrix. By subtracting the free energy of the porous water and fracture water from the free energy of the mixture system, the free energy of the solid matrix can be obtained.

From equation (18), (23), (24) and using the density relationship (2), the free energy of the solid matrix is

$$\left(\Psi - J\phi^{Mw}\psi_{porous} - J\phi^{Fw}\psi_{fracture}\right)^{\cdot} = tr\left(\mathbf{T}\dot{\mathbf{E}}\right) + \dot{\upsilon}^{Mw} p^{Mw} + \dot{\upsilon}^{Fw} p^{Fw} \tag{25}$$

where $\upsilon^{Mw} = J\phi^{Mw}$, $\upsilon^{Fw} = J\phi^{Fw}$ are the porosity of porous matrix and fracture in the reference configuration.

Subtracting the contribution of porous water pressure and fracture water pressure, that is

$$W = \left(\Psi - \phi^{Mw}\psi_{porous} - J\phi^{Fw}\psi_{fracture}\right) - \upsilon^{Mw} p^{Mw} - \upsilon^{Fw} p^{Fw} \tag{26}$$

Substituting equation (25) into the time derivation of the equation (26), the evolution of W can be obtained as below, enabling us to use the pressure $\dot{p}^{Mw}$ and $\dot{p}^{Fw}$ as variables

$$\dot{W} = tr\left(\mathbf{T}\dot{\mathbf{E}}\right) - \upsilon^{Mw}\dot{p}^{Mw} - \upsilon^{Fw}\dot{p}^{Fw} \tag{27}$$

where W is a function of $\mathbf{E}$, p^{Mw} and p^{Fw}.

From equation (27), there must be

$$T_{ij} = \left(\frac{\partial W}{\partial E_{ij}}\right)_{p^{Mw}, p^{Fw}}, \upsilon^{Mw} = -\left(\frac{\partial W}{\partial p^{Mw}}\right)_{E_{ij}, p^{Fw}}, \upsilon^{Fw} = -\left(\frac{\partial W}{\partial p^{Fw}}\right)_{E_{ij}, p^{Mw}} \tag{28}$$

So that

$$\dot{W}(\mathbf{E}, p^{Mw}, p^{Fw}) = \left(\frac{\partial W}{\partial E_{ij}}\right)_{p^{Mw}, p^{Fw}} \dot{E}_{ij} + \left(\frac{\partial W}{\partial p^{Mw}}\right)_{E_{ij}, p^{Fw}} \dot{p}^{Mw} + \left(\frac{\partial W}{\partial p^{Fw}}\right)_{E_{ij}, p^{Mw}} \dot{p}^{Fw} \tag{29}$$

Differentiating equation (28), with the help of equation (29), the evolution of stress, porosity matrix porosity and fracture porosity can be obtained.

$$\dot{T}_{ij} = L_{ijkl}\dot{E}_{kl} - M_{ij}\dot{p}^{Mw} - S_{ij}\dot{p}^{Fw} \tag{30}$$

$$\dot{\upsilon}^{Mw} = M_{ij}\dot{E}_{ij} + Q\dot{p}^{Mw} + B\dot{p}^{Fw} \tag{31}$$

$$\dot{\upsilon}^{Fw} = S_{ij}\dot{E}_{ij} + B\dot{p}^{Mw} + Z\dot{p}^{Fw} \tag{32}$$

where the parameters L_{ijkl}, M_{ij}, S_{ij}, H_{ij}, B, Q, Z, are as following group equations

$$L_{ijkl} = \left(\frac{\partial T_{ij}}{\partial E_{kl}}\right)_{p^{Mw},p^{Fw}} = \left(\frac{\partial T_{kl}}{\partial E_{ij}}\right)_{p^{Mw},p^{Fw}},\ M_{ij} = -\left(\frac{\partial T_{ij}}{\partial p^{Mw}}\right)_{E_{ij},p^{Fw}} = \left(\frac{\partial \upsilon^{Mw}}{\partial E_{ij}}\right)_{E_{ij},p^{Fw}}$$

$$S_{ij} = -\left(\frac{\partial T_{ij}}{\partial p^{Fw}}\right)_{E_{ij},p^{Mw}} = \left(\frac{\partial \upsilon^{Fw}}{\partial E_{ij}}\right)_{E_{ij},p^{Mw}},\ Z = \left(\frac{\partial \upsilon^{Fw}}{\partial p^{Fw}}\right)_{E_{ij},p^{Mw}} \tag{33}$$

$$B = \left(\frac{\partial \upsilon^{Fw}}{\partial p^{Mw}}\right)_{E_{ij},p^{Fw}} = \left(\frac{\partial \upsilon^{Mw}}{\partial p^{Fw}}\right)_{E_{ij},p^{Mw}},\ Q = \left(\frac{\partial \upsilon^{Mw}}{\partial p^{Mw}}\right)_{E_{ij},p^{Fw}}$$

Coupled hydro-mechanical governing equations

Assumptions and simplifications

Equations (30), (31), (32) are the general coupled equations for stress, strain, porous/fracture pressure and porous/fracture porosity, they allow us to explore the Hydro-Mechanical coupling in a broad way including anisotropy, large deformation, et.al. This paper forms the final governing equations in a simple elastic-isotropy cases, therefore, some simplifications and assumptions are made below.

1. The mechanical behavior is restricted to small strain condition, therefore the Green Strain tensor E_{ij} and Piola-Kirchhoff stress T_{ij} can be replaced by strain tensor ε_{ij} and Cauchy stress σ_{ij}.

2. Although many double porosity formations show the features of anisotropic and heterogeneous, following some other research (e.g. Berryman and Wang (1995)), it is roughly assumed that the material is isotropic. Therefore, material-dependent constants M_{ij}, S_{ij} can be substituted by a form of scalar multiplied by Kronecker delta.

$$M_{ij} = \zeta^{Mw}\delta_{ij}\ ,\ S_{ij} = \zeta^{Fw}\delta_{ij} \tag{34}$$

and considering only the elasticity, the elastic stiffness L_{ijkl} can be a fourth-order isotropic tensor

$$L_{ijkl} = G\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + \left(K - \frac{2G}{3}\right)\delta_{ij}\delta_{kl} \tag{35}$$

in which G and K denote the shear modulus and bulk modulus of the material.

According to equations (34), (35) and assumption (1), the stress evolution equation (30) can be simplified to

$$\dot{\sigma}_{ij} = \left(K - \frac{2G}{3}\right)\dot{\varepsilon}_{kk}\delta_{ij} + 2G\dot{\varepsilon}_{ij} - \zeta^{Mw}\dot{p}^{Mw}\delta_{ij} - \zeta^{Fw}\dot{p}^{Fw}\delta_{ij} \tag{36}$$

With assumption 1, 2, the porosity evolution equations (31) and (32) can be simplified as

$$\dot{\upsilon}^{Mw} = \zeta^{Mw}\dot{\varepsilon}_{ii} + Q\dot{p}^{Mw} + B\dot{p}^{Fw} \tag{37}$$

$$\dot{\upsilon}^{Fw} = \zeta^{Fw}\dot{\varepsilon}_{ii} + B\dot{p}^{Mw} + Z\dot{p}^{Fw} \tag{38}$$

Parameter identification

Identification of ζ^{Mw} and ζ^{Fw}

Consider a situation where the porous matrix block is blocked from the fracture, which means that there is no mass exchange between the matrix pores and the fracture. In this situation, the porous matrix block can be viewed as a non-porous material. The stress/strain change is purely induced by fracture water. This situation is the same as the traditional single porosity research as the porous block can be viewed as solid grain and the fracture become the pores.

In this situation, the incremental relationship between stress and pore fluid pressure is

$$\dot{\sigma}_{ij} = -\dot{p}^{Fw}\delta_{ij} \tag{39}$$

strain rate is related to the fracture water pressure through

$$\dot{\varepsilon}_{ij} = -\frac{\dot{p}^{Fw}}{3K_{pb}}\delta_{ij} \tag{40}$$

where K_{pb} is the bulk modulus of the porous matrix block.

Substituting equation (39) and (40) into equation (36) for the above situation

$$-\dot{p}^{Fw}\delta_{ij} = \left(K-\frac{2G}{3}\right)\left(-\frac{\dot{p}^{Fw}}{K_{pb}}\delta_{ij}\right)+2G\left(-\frac{\dot{p}^{Fw}}{3K_{pb}}\delta_{ij}\right)-\zeta^{Fw}\dot{p}^{Fw}\delta_{kl} \tag{41}$$

From equation (41), the expression of ζ^{Fw} can be obtained as

$$\zeta^{Fw} = 1-\frac{K}{K_{pb}} \tag{42}$$

Next, to identify the parameter ζ^{Mw}, a second situation is assumed where the porous water pressure and fracture water pressure change in the same way by $\dot{p}^{\Delta}$. In this situation, there is no discrimination between matrix pores and fracture, they are all viewed as the void space in the system. The incremental relationship between the stress and fluid pressure, and the strain response are

$$\dot{\sigma}_{ij} = -\dot{p}^{\Delta}\delta_{ij} \;,\; \dot{\varepsilon}_{ij} = -\frac{\dot{p}^{\Delta}}{3K_s}\delta_{ij} \tag{43}$$

Invoking equation (43) into equation (36) for the second situation, it's easy to obtain

$$\zeta^{Mw}+\zeta^{Fw} = 1-\frac{K}{K_s} \tag{44}$$

Then, with equation (42), the expression of ζ^{Mw} can be obtained

$$\zeta^{Mw} = \frac{K}{K_{pb}}-\frac{K}{K_s} \tag{45}$$

Identification of Q***,*** B ***and*** Z

In the first situation considered in section 5.2.1, the fracture volume fraction change is related to fracture water pressure through

$$\dot{\upsilon}^{Fw} = -\phi^{Fw}\frac{\dot{p}^{Fw}}{K_{pb}} \tag{46}$$

Invoking (46), (40) and the expression for ζ^{Fw} into equation (38) for the first situation leads to

$$-\phi^{Fw}\frac{\dot{p}^{Fw}}{K_{pb}} = \left(1-\frac{K}{K_{pb}}\right)\left(-\frac{\dot{p}^{Fw}}{K_{pb}}\right)+Z\dot{p}^{Fw} \tag{47}$$

The expression of Z can be derived as

$$Z = \frac{1}{K_{pb}}\left(1 - \frac{K}{K_{pb}} - \phi^{Fw}\right) \tag{48}$$

Then, in the second situation in section 5.2.1, the fracture volume change is

$$\dot{\upsilon}^{Fw} = -\phi^{Fw}\frac{\dot{p}^{\Delta}}{K_s} \tag{49}$$

With equation (49), (43), (48), equation (38) for the second situation can be written as

$$-\phi^{Fw}\frac{\dot{p}^{\Delta}}{K_s} = \left(1 - \frac{K}{K_{pb}}\right)\left(-\frac{\dot{p}^{\Delta}}{K_s}\right) + B\dot{p}^{\Delta} + \frac{1}{K_{pb}}\left(1 - \frac{K}{K_{pb}} - \phi^{Fw}\right)\dot{p}^{\Delta} \tag{50}$$

Then, the expression B can be obtained as

$$B = \left(1 - \frac{K}{K_{pb}} - \phi^{Fw}\right)\left(\frac{1}{K_s} - \frac{1}{K_{pb}}\right) \tag{51}$$

Applying the second situation to equation (37), with the strain and porosity evolution equations

$$\dot{\varepsilon}_{ij} = -\frac{\dot{p}^{\Delta}}{3K_s}\delta_{ij}, \quad \dot{\upsilon}^{Mw} = -\phi^{Mw}\frac{\dot{p}^{\Delta}}{K_s} \tag{52}$$

It leads to

$$-\phi^{Mw}\frac{\dot{p}^{\Delta}}{K_s} = \zeta^{Mw}\left(-\frac{\dot{p}^{\Delta}}{K_s}\right) + Q\dot{p}^{\Delta} + \left(1 - \frac{K}{K_{pb}} - \phi^{Fw}\right)\left(\frac{1}{K_s} - \frac{1}{K_{pb}}\right)\dot{p}^{\Delta} \tag{53}$$

So that the expression for Q can be obtained as

$$Q = \left(\frac{1}{K_{pb}} - \frac{1}{K_s}\right)\left(1 - \frac{K}{K_{pb}} + \frac{K}{K_s} - \phi^{Fw}\right) - \frac{\phi^{Mw}}{K_s} \tag{54}$$

Governing equations

Effective stress and mechanical equation

With the expression of ζ^{Mw} and ζ^{Fw}, equation (36) can be written as

$$\dot{\sigma}_{ij} = \left(K - \frac{2G}{3}\right)\dot{\varepsilon}_{kk}\delta_{ij} + 2G\dot{\varepsilon}_{ij} - \zeta^{Mw}\dot{p}^{Mw}\delta_{ij} - \zeta^{Fw}\dot{p}^{Fw}\delta_{ij} \tag{55}$$

From which the effective stress can be written as

$$\dot{\sigma}_{ij} = \dot{\sigma}'_{ij} - \zeta^{Mw}\dot{p}^{Mw}\delta_{ij} - \zeta^{Fw}\dot{p}^{Fw}\delta_{ij} \tag{56}$$

where σ'_{ij} is the effective stress.

The proposed effective stress includes the influence of matrix water pressure p^{Mw} and fracture water pressure p^{Fw} through the coefficient ζ^{Mw} and ζ^{Fw}. It is the same as the one proposed by Callari and Federico (2000) and the one by Khalili et al. (2005), Khalili (2008) reduced for saturated condition. When there is no fracture, the effective stress can be reduced to the effective stress in porous media by regarding $K = K_{pb}$.

Assuming the mechanical equilibrium condition $\partial\sigma_{ij} / \partial x_j = 0$, and using displacement variables $d_i (i = 1,2,3)$ through $\varepsilon_{ij} = \frac{1}{2}(d_{i,j} + d_{j,i})$, it leads to

$$G\nabla^2\dot{\mathbf{d}} + \left(\frac{G}{1-2\theta}\right)\nabla\left(\nabla\cdot\dot{\mathbf{d}}\right) - \zeta^{Mw}\nabla\dot{p}^{Mw} - \zeta^{Fw}\nabla\dot{p}^{Fw} = 0 \tag{57}$$

in which θ is Poisson's ratio

Hydraulic behavior

According to the parameters identified in section 5.2, the porosity change equation (37) and (38) can now be quantitated as

$$\dot{\upsilon}^{Mw} = \zeta^{Mw}\dot{\varepsilon}_{ii} + \left[\frac{\zeta^{Mw}}{K}\left(1-\zeta^{Mw}-\phi^{Fw}\right) - \frac{\phi^{Mw}}{K_s}\right]\dot{p}^{Mw} + \left[-\frac{\zeta^{Mw}}{K}\left(\zeta^{Fw}-\phi^{Fw}\right)\right]\dot{p}^{Fw} \tag{58}$$

$$\dot{\upsilon}^{Fw} = \zeta^{Fw}\dot{\varepsilon}_{ii} + \left(\zeta^{Fw}-\phi^{Fw}\right)\left(\frac{1}{K_s} - \frac{1}{K_{pb}}\right)\dot{p}^{Mw} + \frac{1}{K_{pb}}\left(\zeta^{Fw}-\phi^{Fw}\right)\dot{p}^{Fw} \tag{59}$$

The two equations represent the pore and fracture porosity change with respect to the volumetric strain, the porous water pressure and the fracture water pressure in a fully coupled way, which are the same as the porosity change equation in Khalili (2003).

1. Porous matrix water

From water partial mass equation (8), water density relationship (2), Darcy velocity equation (3), water flux equation (1) and Euler identity, the conservation equation of water can be written as

$$\left(\upsilon^{Mw}\rho_t^{Mw}\right)^{\square}+\nabla\cdot\left(\rho_t^{Mw}\mathbf{u}^{Mw}\right)+r_{ex}=0 \tag{60}$$

Expanding the first term in equation (60) and considering the variation of true density as

$$\dot{\rho}_t^{Mw}=\rho_t^{Mw}\left(\frac{1}{\rho_t^{Mw}}\frac{\partial\rho_t^{Mw}}{\partial p^{Mw}}\right)\frac{\partial p^{Mw}}{\partial t}=\rho_t^{Mw}\frac{1}{K_w}\dot{p}^{Mw} \tag{61}$$

where K_w is the compressibility of water.

With equation (61), equation (60) becomes

$$\dot{\upsilon}^{Mw}\rho_t^{Mw}+\upsilon^{Mw}\rho_t^{Mw}\frac{1}{K_w}\dot{p}^{Mw}+\nabla\cdot\left(\rho_t^{Mw}\mathbf{u}^{Mw}\right)+r_{ex}=0 \tag{62}$$

Invoking the porous volume fraction evolution equation (37) and Darcy's law (13), the governing equation for porous matrix water transport is

$$\zeta^{Mw}\nabla\cdot\dot{\mathbf{d}}+\left(Q+\frac{\upsilon^{Mw}}{K_w}\right)\dot{p}^{Mw}+B\dot{p}^{Fw}+r_{ex}=\frac{k^{Mw}}{\nu^{w}}\nabla^2 p^{Mw} \tag{63}$$

with $\zeta^{Mw}=\frac{K}{K_{pb}}-\frac{K}{K_s}$, $Q=\frac{\zeta^{Mw}}{K}\left(1-\zeta^{Mw}-\phi^{Fw}\right)-\frac{\phi^{Mw}}{K_s}$, $B=-\frac{\zeta^{Mw}}{K}\left(1-\frac{K}{K_{pb}}-\phi^{Fw}\right)$.

<u>*2. Fracture water*</u>

Similar to the above steps, the governing equation for the fracture water transport can be obtained as

$$\zeta^{Fw}\nabla\cdot\dot{\mathbf{d}}+B\dot{p}^{Mw}+\left(Z+\frac{\upsilon^{Fw}}{K_w}\right)\dot{p}^{Fw}-r_{ex}=\frac{k^{Fw}}{\nu^{w}}\nabla^2 p^{Fw} \tag{64}$$

with $\zeta^{Fw}=1-\frac{K}{K_{pb}}$, $B=\left(\zeta^{Fw}-\phi^{Fw}\right)\left(\frac{1}{K_s}-\frac{1}{K_{pb}}\right)$, $Z=\frac{1}{K_{pb}}\left(\zeta^{Fw}-\phi^{Fw}\right)$.

Verification and discussion

Equations (30)-(32) provide very general coupled formulations for the coupled evolution of PK-2 stress, porous matrix porosity and fracture porosity, along with the dynamic change of porous water pressure and fracture water pressure, and Green strain. These formulations are for general cases like large deformation, isotropic and anisotropic. With the assumption of small deformation and isotropic, the governing equations (57), (63), (64) derived in this paper are the same as the ones proposed based on the mechanics approach, such as Khalili et al. (1999), Khalili (2003) or the ones by Pao and Lewis (2002), Khalili (2008) reduced for saturated condition which have been verified by comparing with experimental data (Khalili 2003) and further verified through comparing with different double porosity models (Ashworth and Doster 2019). This indicates that the governing equations developed by mechanics approaches are only specific cases of the general constitutive equations by using mixture coupling theory.

Additionally, the mixture coupling theory framework developed in this paper is more rigorous and realistic, with the least assumptions. For example, in the mechanics approach, the assumptions (e.g. isotropic) were made at the very beginning of the derivation process, therefore, restricting its following derivation process, limiting any possibility of extension to other conditions, for example, anisotropic. In other words, the mechanics approach can only obtain the constitutive relations for a specific case. However, through the mixture coupling theory adopted in this paper, no specific assumptions are required at the beginning, so that the general constitutive relations (i.e. equation (30),(31),(32)) can be obtained. Such a relationship applies to many conditions, e.g., large deformation, isotropic/anisotropic. Following the general constitutive relations, elasticity and isotropy conditions are selected to obtain the final governing equations. It can thus be concluded that the mixture coupling theory approach is more flexible and widely applicable.

The key research object of Mixture Coupling Theory is the Helmholtz free energy change of the system, i.e., equation (15) and (25), which are achieved through the mass and energy balance, as well as the entropy production and the Gibbs-Duhem equation. Since many dynamics processes can be described through energy dispassion, Mixture Coupling Theory can be used in a lot of fields, such as thermo-hydro-mechanical-chemical coupling (Ma et al. 2022), swelling (Chen et al. 2016), dissolution (Ma et al. 2022), or potentially wave propagation as wave is mainly a movement of energy through a medium (Kumar et al. 2021, Rajak et al. 2022), or other fields like biological tissue. However, all the aforementioned research topics are mainly for porous media. This paper is the first attempt to develop the fully coupled equations for the double porosity media. It is noticed that Aghighi et al. (2021) used a similar approach to study the sorption in double porosity media, but their equations are not presented in a fully coupled way as the pore water pressure influence is missing in the mechanical or transport equation.

Numerical Simulation

A simple numerical simulation is presented in this section to illustrate the mechanical and hydraulic behavior in the double-porosity formation. The mechanical deformation and hydraulic pressure change are given, as well as the porosity and permeability change. The sensitivity of fracture spacing and permeability is analyzed.

Porosity, permeability and exchange rate

1.Porosity

The matrix and fracture porosity change equation have been derived as equation (31) and (32), which are further reduced to equation (37) and (38) according to the assumptions in section 5.1. From the parameters identified in section 5.2, the matrix and fracture porosity equation are solved in incremental form as

$$\Delta\upsilon^{Mw} = \zeta^{Mw}\Delta\varepsilon_{ii} + Q\Delta p^{Mw} + B\Delta p^{Fw} \tag{65}$$

$$\Delta\upsilon^{Fw} = \zeta^{Fw}\Delta\varepsilon_{ii} + B\Delta p^{Mw} + Z\Delta p^{Fw} \tag{66}$$

2.Permeability

The permeability change is related to porosity through the Kozeny-Carman's law as (Zheng and Samper 2008)

$$\frac{k^{Mw}}{k_0^{Mw}} = \left(\frac{\upsilon^{Mw}}{\upsilon_0^{Mw}}\right)^3 \left(\frac{1-\upsilon_0^{Mw}}{1-\upsilon^{Mw}}\right)^2 \tag{67}$$

in which the subscript '0' denotes the initial value.

This relationship is normally for porous matrix, for fracture, although there is no evidence to support this relationship, it is roughly assumed that the fracture permeability also follows equation (67).

3. Exchange rate

The exchange rate can be described by

$$r_{ex} = \frac{\chi k^{Mw}}{\nu^{w}}\left(p^{Mw} - p^{Fw}\right) \tag{68}$$

where χ is the shape factor. There have been some different expressions for χ proposed by different researchers (Warren and Root 1963, Kazemi et al. 1976), a summary can be found in Ranjbar and Hassanzadeh (2011). In this paper, the expression of χ developed by Warren and Root (1963) is adopted as

$$\chi = \frac{4N\left(N+2\right)}{L^2} \tag{69}$$

where N ($N = 1,2,3$) represents the dimension of the porous matrix block. L is the fracture spacing.

Geometry and boundary condition

A double porosity geoformation, with 20m length and 1m height (Fig. 2), is selected. The formation initially contains water at pressure of 30MPa. At the beginning of the simulation, the pressure at the right boundary drops to 5MPa due to external disturbance while maintaining 30MPa at the left boundary. By setting the right side to be permeable, water can flow out. The formation is initially at mechanical equilibrium with no effective stress. To explore the mechanical behavior when the pressure changes, the left boundary is allowed to move while the other boundaries are constrained.

One observation line and three observation points A, B, C are selected.

Parameters adopted in this simulation are listed in Table 1 (Abousleiman and Nguyen 2005, Nair et al. 2005, Gelet et al. 2012)

Numerical results

1. Hydraulic and mechanical behavior

The evolution of matrix pressure and fracture pressure along the observation line is presented in Fig. 3 and Fig. 4. Because of a pressure gradient generated at the beginning, water will flow from the left to the right, as time goes by, the pressure within the domain decreases and trends to reach equilibrium (Fig. 3, 4). Comparing Fig. 3 and Fig. 4, the pressure change in the fracture is quicker thanthat in the matrix pore, this is mainly because of a greater permeability of the larger permeability in the fracture zone. Fig. 5 shows the pressure change with time at observation points A, B, C, from which it is clearer that the fracture pressure changes quicker than the pore pressure, but finally, the pressure in the fracture and pore reaches the same as what has been set to be the boundary condition.

The domain is initially at mechanical equilibrium with no effective stress, indicating that the external loading is born by the water pressure. Because of the loss of water pressure through the right boundary, the external loading will be taken by both water pressure and solid matrix, therefore, effective stress and displacement generate correspondingly (Fig. 6 and 7). Since water pressure losses more near the right boundary, effective stress generates more on the right side (Fig. 6). As the solid matrix bears external loading, consolidation happens and displacement occurs on the free left boundary (Fig. 7).

The pressure difference in the fracture and matrix results in the exchange of water mass. The exchange rate is shown in Fig. 8. At the early time, the pressure difference between the fracture and pore is very significant, thus the exchange rate is great. As time goes by, the pressure difference becomes smaller and smaller, so that the exchange rate decreases.

2. Porosity and permeability

The matrix and fracture porosity distribution along the observation line are presented in Fig. 9 and Fig. 10. The Figs show up to a 5% decrease in matrix porosity and a 8% decrease in fracture porosity. Since the pressure change and strain change on the right part of the domain are more significant than those on the left part, and the porosity change shows similar distribution. As the permeability is related to porosity through equation (67), permeability change has a similar trend with porosity change, as shown in Fig. 11 and 12.

Sensitivity analysis of fracture spacing

An important part of the double porosity model is the exchange of water from the porous matrix to fracture. A greater exchange rate will help the porous water pressure change quicker. From equation (69), the exchange rate is inversely proportional to the fracture spacing L. Different values of L ($L = 0.1,\ 0.5,\ 1,\ 5,\ 10$) are chosen to explore the sensitivity dependence of hydraulic and mechanical behavior on L. The results are presented in Fig. 13-16.

From Fig. 13, the exchange rate in low L value is much higher than that in big L value. A lower L value means a high 'fracture density', so that water can be transferred quicker between porous block and fracture. In the simulated case, at a certain time or space, the matrix pressure is mostly greater than fracture pressure, so that matrix water flows into the fracture space. The lower L value is, the quicker matrix water lose to fracture, therefore, the matrix pressure changes quicker (Fig. 14). Similarly, fracture pressure changes slower with a small L value (Fig. 15). The difference in pressure change consequently leads to a difference in mechanical behavior (Fig. 16).

Sensitivity analysis of fracture permeability

The hydraulic transport is highly affected by permeability. In this section, the permeability sensitivity is explored by setting the fracture permeability as $k^{Fw} = 5*10^{-19}m^2, 5*10^{-18}m^2, 5*10^{-17}m^2$ while keeping the pore permeability as $k^{Mw} = 5*10^{-20}m^2$ to represent the permeability difference at different magnitudes. Other parameters remain the same as those listed in Table 1.

The fracture water pressure under different permeabilities is shown in Fig. 17, from which it is clear that the fracture water pressure drops much quicker with a higher permeability. Because the water exchange rate between the fracture and matrix pore depends on the pressure difference, hence, the exchange rate under high fracture permeability is quicker (Fig. 18), which further promotes the matrix pore water pressure drop (Fig. 19).

The pressure change trend under different fracture permeability is similar to that in section 6.3, but the porosity change under different fracture permeability is quite different, as shown in Fig. 20. When $k^{Mw} = 5*10^{-19}m^2$, the fracture porosity drops most on the right boundary, but when $k^{Mw} = 5*10^{-18}m^2$, or $k^{Mw} = 5*10^{-17}m^2$, the maximum porosity is not at the right boundary but at a point closed to the right boundary. According to equation (66), the change in fracture porosity $\Delta\upsilon^{Fw}$ comes from three parts: 1. the change of strain $\zeta^{Fw}\Delta\varepsilon_{ii}$; 2. The change of pore pressure $B\Delta p^{Mw}$; 3. The change of fracture pressure $Z\Delta p^{Fw}$. The contribution of the three parts under different permeabilities is presented in Fig. 21. The consolidation (strain change) and fracture pressure drop would decrease the fracture porosity while the matrix pressure change trends to increase the fracture porosity, leading to the overall decrease of fracture porosity. It can be found that the main difference among the three permeabilities is the fracture pressure contribution part: under all permeabilities, the strain and pore pressure changes slow and their contribution to the fracture porosity are similar. However, when permeability is higher, the fracture pressure drops quickly, leading to a quick and significant decrease of fracture porosity; when permeability is lower, fracture pressure drops slowly and fracture porosity changes slowly. The combined influence of the strain, matrix pressure and fracture pressure results in the dramatic trend in Fig. 20. Owing to the permeability difference, the matrix porosity also changes in a dramatic trend, as presented in Fig. 22 and Fig. 23.

Conclusion

This paper derives the constitutive equations for double porosity formation under a coupled hydro-mechanical situation by using the Mixture Coupling Theory. The cross-coupling relations between stress, strain, porous/fracture water pressure and porous/fracture porosity are obtained, allowing us to explore the Hydro-Mechanical response in a broad way. The final governing equations are formed for the elastic condition, leading to the same equations developed by other approaches.

The constitutive models are solved by the finite element method, and the results show the hydraulic and mechanical deformation, as well as the porosity and permeability change. The sensitivity analysis shows that the smaller fracture spacing greatly increases the exchange rate and facilitates the matrix water pressure change, the fracture permeability sensitivity analysis shows that the greater permeability significantly accelerates the pressure change and affects the porosity change.

Data Availability statement

Some or all data, models, or code that support the findings of this study are available from the corresponding author upon reasonable request.

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