

Modeling Multiphase Multicomponent Porous Flows

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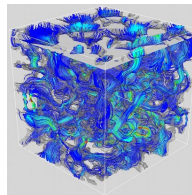
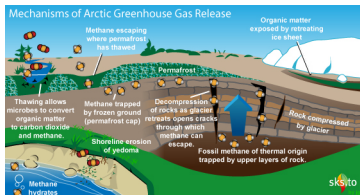
Brian Seguin (Loyola)

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Multicomponent–Multiphase Flow

Geophysical Flows



Application: Release of CH_4 and CO_2 as permafrost melts.

Computational Limitations:

- A scalar equation to represent the balance of mass for each conserved component (species or molecule).
- A scalar equation to represent the macroscopic balance of energy if the system is not isothermal.

Momentum & energy balances, chemistry, etc. are all “modeled”.

Balance of Mass

Multiphase Flow

Macroscopic Model:

- There exist N_c **Components** which are conserved.
- The components combine to form N_p immiscible **Phases**

Component Densities: $\Omega \subset \mathbb{R}^d$

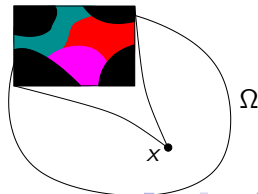
- m_c = mass of component c **per unit volume** of Ω
- $M_{c\pi}$ = mass of component c in phase π **per unit volume** of Ω

$$m_c = \sum_{\pi=1}^{N_p} M_{c\pi} \quad \text{write} \quad \mathbf{m} = M\mathbf{1}$$

Notation:

- $\mathbf{m} = (m_1, \dots, m_c, \dots, m_{N_c})$
- $\mathbf{1} = (1, 1, \dots, 1)$

Phase Densities: $\rho = M^T \mathbf{1}$



Macroscopic Model:

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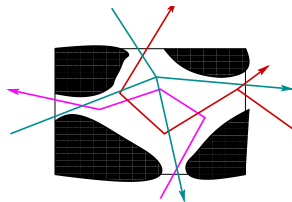
Balances of Mass: $\partial_t m_c + \text{div} \left(\sum_{\pi=1}^{N_p} M_{c\pi} \mathbf{v}_\pi + \mathbf{h}_c \right) = 0.$

Constraint: $\mathbf{m} = M\mathbf{1}$

Phase Velocities: $\{\mathbf{v}_1, \dots, \mathbf{v}_{N_p}\}$

Mass Averages: $\mathbf{v}_\pi = \frac{\int_{V_\pi} \rho \mathbf{v}}{\int_V \rho}$

Mass Diffusion: $\{\mathbf{h}_1, \dots, \mathbf{h}_{N_c}\}$



Balance of Mass

Multiphase Flow

Macroscopic Model:

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Balances of Mass:
$$\partial_t m_c + \operatorname{div} \left(\sum_{\pi=1}^{N_p} M_{c\pi} \mathbf{v}_\pi + \mathbf{h}_c \right) = 0.$$

Postulate: At the pore scale, components form **Immiscible, Homogeneous** phases in **Thermodynamic Equilibrium**.

(transport time scale \gg time to equilibrate)





- **Ensemble Free Energy:** (rigid, chemically inert medium)

$$\Psi(\mathbf{s}, M) = \sum_{\pi=1}^{N_p} \Psi_{\pi}(s_{\pi}, \{M_{c\pi}\}_{c=1}^{N_c}, \theta) + \Upsilon(\mathbf{s}, \theta)$$

- **Saturations:** s_{π} volume of phase π per unit volume of Ω
- **Interfacial Energy:** $\Upsilon(\mathbf{s})$ (surface tension/wetting energy)
- **Homogeneity:**

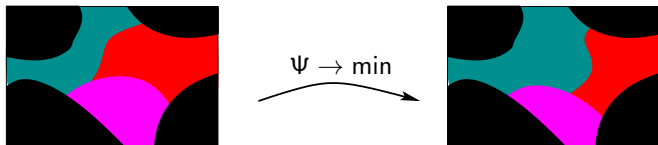
$$\lambda \Psi_{\pi}(\mathcal{V}_{\pi}, \{\mathcal{M}_{c\pi}\}_{c=1}^{N_c}) = \Psi_{\pi}(\lambda \mathcal{V}_{\pi}, \{\lambda \mathcal{M}_{c\pi}\}_{c=1}^{N_c}), \quad \lambda \geq 0$$

- **Ideal Gas:**

$$\Psi(\mathcal{V}, \mathcal{M}; \theta) = k\theta \mathcal{M} \left(c + \ln \left(\frac{\mathcal{M}}{\mathcal{V}} \right) - \ln((const)\theta^c) \right).$$

Classical Thermodynamics

Canonical Ensemble (Isothermal System)



- **Ensemble Free Energy:** (rigid, chemically inert medium)

$$\Psi(\mathbf{s}, M) = \sum_{\pi=1}^{N_p} \Psi_{\pi}(s_{\pi}, \{M_{c\pi}\}_{c=1}^{N_c}, \theta) + \Upsilon(\mathbf{s}, \theta)$$

- **Equilibrium:** Fix (ϕ, \mathbf{m}) , then Ψ is *minimized* subject to:

$$\mathbf{s} \cdot \mathbf{1} = \phi, \quad \text{and} \quad \mathbf{m} = M\mathbf{1}.$$

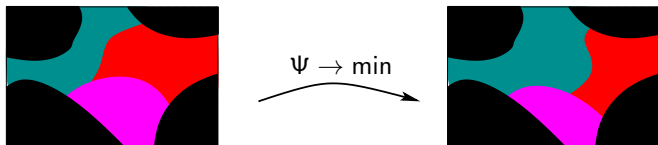
Porosity: $\phi = 1 - s_0$.

Macroscopic Free Energy:

$$\psi(\mathbf{m}) = \inf_{(\mathbf{s}, M)} \{ \Psi(\mathbf{s}, M) \mid \mathbf{s} \cdot \mathbf{1} = \phi \text{ and } M\mathbf{1} = \mathbf{m} \}$$

Classical Thermodynamics

Canonical Ensemble (Isothermal System)



- **Ensemble Free Energy:** (rigid, chemically inert medium)

$$\Psi(\mathbf{s}, M) = \sum_{\pi=1}^{N_p} \Psi_{\pi}(s_{\pi}, \{M_{c\pi}\}_{c=1}^{N_c}, \theta) + \Upsilon(\mathbf{s}, \theta)$$

- **Equilibrium:** Fix (ϕ, \mathbf{m}) , then Ψ is *minimized* subject to:

$$\mathbf{s} \cdot \mathbf{1} = \phi, \quad \text{and} \quad \mathbf{m} = M \mathbf{1}.$$

- **Lagrange Multipliers:**

$$-\frac{\partial \Psi_{\pi}}{\partial s_{\pi}} = p + \frac{\partial \Upsilon}{\partial s_{\pi}} \equiv p_{\pi} \quad \text{and} \quad \frac{\partial \Psi_{\pi}}{\partial M_{c\pi}} = \mu_c, \quad 1 \leq \pi \leq N_p.$$

Multicomponent–Multiphase Flow

Isothermal Problem

Mass Balances: Densities $\mathbf{m} = (m_1, \dots, m_c, \dots, m_{N_c}) \in [0, \infty)^{N_c}$

$$\partial_t m_c + \operatorname{div} \left(\sum_{\pi=1}^{N_p} M_{c\pi} \mathbf{v}_\pi + \mathbf{h}_c \right) = 0.$$

Constitutive Input: Given \mathbf{m} and porosity $\phi \in [0, 1]$

- **Phases:** (flash calculation)

$$(\mathbf{s}, M) = \arg \min_{(\mathbf{s}, M)} \left\{ \Psi(\mathbf{s}, M) \mid \mathbf{s} \cdot \mathbf{1} = \phi \text{ and } M \mathbf{1} = \mathbf{m} \right\}$$

- **Fluxes:** Darcy and Fick Laws ($\rho_\pi \equiv \sum_{c=1}^{N_c} M_{c\pi}$)

$$\mathbf{v}_\pi = -K_\pi (s_\pi \nabla p_\pi - \rho_\pi \mathbf{g}) \quad \text{and} \quad \mathbf{h}_c = -K_c \nabla \mu_c.$$

- **Energy Law:** ...

Darcy Laws

Balance of Momentum/Force Balance

Classical Darcy Law:

$$\mathbf{v}_\pi = -K_\pi(\mathbf{s}) \left(s_\pi \nabla p_\pi - \rho_\pi \mathbf{g} \right) \quad \text{where} \quad \rho_\pi = \sum_{c=1}^{N_c} M_{c\pi}$$

Homogeneity: $\Psi_\pi(s_\pi, \{M_{c\pi}\}_{c=1}^{N_c})$ is homogeneous

- Euler's Identity: $\Psi_\pi = -s_\pi p_\pi + \sum_{c=1}^{N_c} M_{c\pi} \mu_c$
- Gibbs–Duhem Identity: $-s_\pi \nabla p_\pi + \sum_{c=1}^{N_c} M_{c\pi} \nabla \mu_c = 0$

$$\text{Darcy Law: } \mathbf{v}_\pi = -K_\pi(\mathbf{s}) \sum_{c=1}^{N_c} M_{c\pi} \left(\nabla \mu_c - \mathbf{g} \right)$$

Multicomponent–Multiphase Flow

Isothermal Problem

Weak Statement: (zero flux b.c)

$$\begin{aligned} \int_{\Omega} (\mathbf{m}_t, \hat{\boldsymbol{\mu}}) + \sum_{\pi=1}^{N_p} \sum_{c,c'=1}^{N_c} (M_{c\pi} \nabla \mu_c, M_{c'\pi} \nabla \hat{\mu}_{c'})_{K_\pi} + \sum_{c=1}^{N_c} (\nabla \mu_c, \nabla \hat{\mu}_{c'})_{K_c} \\ = \int_{\Omega} \sum_{\pi=1}^{N_p} \sum_{c,c'=1}^{N_c} (M_{c\pi} \mathbf{g}, M_{c'\pi} \nabla \hat{\mu}_{c'})_{K_\pi} \end{aligned}$$

Energy Law: $\partial\psi/\partial m_c = \mu_c \dots$

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \psi(\mathbf{m}) + \int_{\Omega} \sum_{\pi=1}^{N_p} \left| \sum_{c=1}^{N_c} M_{c\pi} \nabla \mu_c \right|_{K_\pi}^2 + \sum_{c=1}^{N_c} |\nabla \mu_c|_{K_c}^2 \\ = \int_{\Omega} \sum_{\pi=1}^{N_p} \sum_{c,c'=1}^{N_c} (M_{c\pi} \mathbf{g}, M_{c'\pi} \nabla \mu_{c'})_{K_\pi} \end{aligned}$$

Multicomponent–Multiphase Flow

Isothermal Problem – Numerics

Balance Law: $\partial_t m_c - \operatorname{div}(\sum_{\pi=1}^{N_p} M_{c\pi} \mathbf{v}_\pi) = 0$

Euler Approximation: $m_c^n - m_c^{n-1} - \tau \operatorname{div}(\sum_{\pi=1}^{N_p} M_{c\pi}^{n-1} \mathbf{v}_\pi) = 0$

Variational Problem:

$$I(\boldsymbol{\mu}) = \int_{\Omega} \left(\psi^*(\boldsymbol{\mu}) - \boldsymbol{\mu} \cdot \mathbf{m}^{n-1} + \frac{\tau}{2} \sum_{\pi=1}^{N_p} \left| \sum_{c=1}^{N_c} M_{c\pi}^{n-1} (\nabla \mu_c - \mathbf{g}) \right|_{K^{n-1}}^2 \right)$$

Constitutive Relation: $\boldsymbol{\mu} \in \partial\psi(\mathbf{m}) \Leftrightarrow \mathbf{m} \in \partial\psi^*(\boldsymbol{\mu})$.

Problem: Only $\psi(\mathbf{m})$ is computable, ψ^* is not available.

Saddle Point Problem:

$$L(\mathbf{m}, \boldsymbol{\mu}) = \int_{\Omega} \left(-\psi(\mathbf{m}) + \boldsymbol{\mu} \cdot (\mathbf{m} - \mathbf{m}^{n-1}) + \frac{\tau}{2} \sum_{\pi=1}^{N_p} \left| \sum_{c=1}^{N_c} M_{c\pi}^{n-1} (\nabla \mu_c - \mathbf{g}) \right|_{K^{n-1}}^2 \right)$$

Multicomponent–Multiphase Flow

Non–Isothermal Problem

Balance of Energy¹:

$$\partial_t e + \operatorname{div} \left(\sum_{\pi=1}^{N_p} (e_\pi + s_\pi p_\pi) \mathbf{v}_\pi + \sum_{c=1}^{N_c} \mu_c \mathbf{h}_c + \mathbf{q} \right) = r + \sum_{\pi=1}^{N_p} \rho_\pi \mathbf{g} \cdot \mathbf{v}_\pi$$

- e Internal energy per unit volume of Ω .
- $\{e_\pi\}_{\pi=1}^{N_p}$ internal energy of phase π per unit volume.
- \mathbf{q} heat flux.
- r heat supply (radiation) per unit volume.

Fourier/Darcy/Fick Laws:

$$\mathbf{q} = -K_\theta \nabla \theta, \quad K_\pi \mathbf{v}_\pi = -(s_\pi \nabla p_\pi - \rho_\pi \mathbf{g}), \quad \mathbf{h}_c = -K_c \nabla \mu_c.$$

¹Farid F Smaiï, A thermodynamic formulation for multiphase compositional flows in porous media.



- Ensemble Entropy:

$$S(\mathbf{e}, \mathbf{s}, M) = S_0(e_0) + \sum_{\pi=1}^{N_p} S_{\pi}(e_{\pi}, s_{\pi}, \{M_{c\pi}\}_{c=1}^{N_c})$$

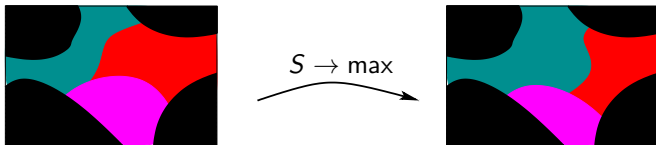
- **Medium:** e_0 internal energy of medium per unit volume of Ω .
- **Concavity:** $S_{\pi}(\cdot, \cdot, \cdot)$ is concave.
- **Homogeneity:**

$$\lambda S_{\pi}(\mathcal{E}_{\pi}, \mathcal{V}_{\pi}, \{\mathcal{M}_{c\pi}\}_{c=1}^{N_c}) = S_{\pi}(\lambda \mathcal{E}_{\pi}, \lambda \mathcal{V}_{\pi}, \{\lambda \mathcal{M}_{c\pi}\}_{c=1}^{N_c})$$

- **Ideal Gas:** $S(\mathcal{E}, \mathcal{V}, \mathcal{M}) = k \mathcal{M} \ln \left[(\text{const}) \frac{\mathcal{V}}{\mathcal{M}} \left(\frac{\mathcal{E}}{ck \mathcal{M}} \right)^c \right]$

Classical Thermodynamics

Microcanonical Ensemble (Non-Isothermal Problem)



- Ensemble Entropy:

$$S(\mathbf{e}, \mathbf{s}, M) = S_0(e_0) + \sum_{\pi=1}^{N_p} S_{\pi}(e_{\pi}, s_{\pi}, \{M_{c\pi}\}_{c=1}^{N_c})$$

- Equilibrium: Fix (e, ϕ, \mathbf{m}) , then S is maximized subject to:

$$e = e_0 + \mathbf{e} \cdot \mathbf{1} + \Upsilon(\mathbf{s}), \quad \phi = \mathbf{s} \cdot \mathbf{1}, \quad \mathbf{m} = M\mathbf{1}.$$

- Lagrange Multipliers:

$$\theta \frac{\partial S_{\pi}}{\partial e_{\pi}} = 1 \quad \theta \frac{\partial S_{\pi}}{\partial s_{\pi}} = p + \frac{\partial \Upsilon}{\partial s_{\pi}} \equiv p_{\pi}, \quad \theta \frac{\partial S_{\pi}}{\partial M_{c\pi}} = \mu_c.$$

Multicomponent–Multiphase Flow

Non–Isothermal Problem

Dissipation Relation: $\eta_t = \frac{1}{\theta}(e_t - \mathbf{m}_t \cdot \boldsymbol{\mu})$ where

$$\eta(\mathbf{e}, \mathbf{m}) = \max \{ S(\mathbf{e}, \mathbf{s}, M) \mid e = e_0 + \mathbf{e} \cdot \mathbf{1} + \Upsilon(\mathbf{s}), \phi = \mathbf{s} \cdot \mathbf{1}, \mathbf{m} = M \mathbf{1} \}$$

$$S(\mathbf{e}, \mathbf{s}, M) = S_0(e_0) + \sum_{\pi=1}^{N_p} S_{\pi}(e_{\pi}, s_{\pi}, \{M_{c\pi}\}_{c=1}^{N_c})$$

Homogeneity: $S_{\pi}(e_{\pi}, s_{\pi}, \{M_{c\pi}\}_{c=1}^{N_c})$ is homogeneous.

- Euler's Representation: $\theta \eta_{\pi} = e_{\pi} + s_{\pi} p_{\pi} - \sum_{c=1}^{N_c} M_{c\pi} \mu_c$
- Gibbs–Duhem Relation: $\eta_{\pi} \nabla \theta - s_{\pi} \nabla p_{\pi} + \sum_{c=1}^{N_c} M_{c\pi} \nabla \mu_c = 0$.

Multicomponent–Multiphase Flow

Non–Isothermal Problem

Dissipation Relation: $\eta_t = \frac{1}{\theta}(e_t - \mathbf{m}_t \cdot \boldsymbol{\mu})$ where

$$\eta(\mathbf{e}, \mathbf{m}) = \max \{ S(\mathbf{e}, \mathbf{s}, M) \mid e = e_0 + \mathbf{e} \cdot \mathbf{1} + \Upsilon(\mathbf{s}), \phi = \mathbf{s} \cdot \mathbf{1}, \mathbf{m} = M \mathbf{1} \}$$

Weak Statement: Set $\beta = 1/\theta \dots$

$$(\mathbf{m}_t, \beta \hat{\boldsymbol{\mu}}) - \sum_{\pi=1}^{N_p} \sum_{c=1}^{N_c} (M_{c\pi} \mathbf{v}_\pi, \beta \nabla \hat{\mu}_c + \hat{\mu}_c \nabla \beta) - \sum_{c=1}^{N_c} (\mathbf{h}_c, \beta \nabla \hat{\mu}_c + \hat{\mu}_c \nabla \beta) = 0.$$

$$\begin{aligned} (\mathbf{e}_t, \hat{\beta}) - \left(\sum_{\pi=1}^{N_p} (\eta_\pi / \beta + \sum_{c=1}^{N_c} M_{c\pi} \mu_c) \mathbf{v}_\pi + \sum_{c=1}^{N_c} \mu_c \mathbf{h}_c + \mathbf{q}, \nabla \hat{\beta} \right) \\ + \sum_{\pi=1}^{N_p} \left((\eta_\pi / \beta^2) \nabla \beta - \sum_{c=1}^{N_c} M_{c\pi} \nabla \mu_c, \mathbf{v}_\pi \hat{\beta} \right) = \left(r + \sum_{\pi=1}^{N_p} |\mathbf{v}_\pi|_{K_\pi}^2, \hat{\beta} \right). \end{aligned}$$

Multicomponent–Multiphase Flow

Non–Isothermal Problem

Dissipation Relation: $\eta_t = \frac{1}{\theta}(e_t - \mathbf{m}_t \cdot \boldsymbol{\mu})$ where

$$\eta(\mathbf{e}, \mathbf{m}) = \max \{ S(\mathbf{e}, \mathbf{s}, M) \mid e = e_0 + \mathbf{e} \cdot \mathbf{1} + \Upsilon(\mathbf{s}), \phi = \mathbf{s} \cdot \mathbf{1}, \mathbf{m} = M \mathbf{1} \}$$

Dissipation Relation: Set $(\hat{\boldsymbol{\mu}}, \hat{\beta}) = (\boldsymbol{\mu}, \beta) \dots$

$$(\mathbf{m}_t, \beta \boldsymbol{\mu}) - \sum_{\pi=1}^{N_p} \sum_{c=1}^{N_c} (M_{c\pi} \mathbf{v}_\pi, \beta \nabla \mu_c + \mu_c \nabla \beta) - \sum_{c=1}^{N_c} (\mathbf{h}_c, \beta \nabla \mu_c + \mu_c \nabla \beta) = 0.$$

$$\begin{aligned} (e_t, \beta) - & \left(\sum_{\pi=1}^{N_p} (\eta_\pi / \beta + \sum_{c=1}^{N_c} M_{c\pi} \mu_c) \mathbf{v}_\pi + \sum_{c=1}^{N_c} \mu_c \mathbf{h}_c + \mathbf{q}, \nabla \beta \right) \\ & + \sum_{\pi=1}^{N_p} \left((\eta_\pi / \beta^2) \nabla \beta - \sum_{c=1}^{N_c} M_{c\pi} \nabla \mu_c, \mathbf{v}_\pi \beta \right) = \left(r + \sum_{\pi=1}^{N_p} |\mathbf{v}_\pi|_{K_\pi}^2, \beta \right). \end{aligned}$$

Multicomponent–Multiphase Flow

Non–Isothermal Problem

Dissipation Relation: $\eta_t = \frac{1}{\theta}(e_t - \mathbf{m}_t \cdot \boldsymbol{\mu})$ where

$$\eta(\mathbf{e}, \mathbf{m}) = \max \{ S(\mathbf{e}, \mathbf{s}, M) \mid e = e_0 + \mathbf{e} \cdot \mathbf{1} + \Upsilon(\mathbf{s}), \phi = \mathbf{s} \cdot \mathbf{1}, \mathbf{m} = M \mathbf{1} \}$$

Dissipation Relation: Set $(\hat{\boldsymbol{\mu}}, \hat{\beta}) = (\boldsymbol{\mu}, \beta) \dots$

$$-\frac{d}{dt} \int_{\Omega} \eta + \int_{\Omega} \left\{ |\nabla \ln(\beta)|_{K_{\theta}}^2 + \beta \left(\sum_{\pi=1}^{N_p} |\mathbf{v}_{\pi}|_{K_{\pi}}^2 + \sum_{c=1}^{N_c} |\nabla \mu_c|_{K_c}^2 \right) \right\} = \int_{\Omega} -\beta r.$$

Fourier/Darcy/Fick Laws:

$$\mathbf{q} = -K_{\theta} \nabla \theta = (1/\beta)^2 K_{\theta} \nabla \beta, \quad K_{\pi} \mathbf{v}_{\pi} = -(s_{\pi} \nabla p_{\pi} - \rho_{\pi} \mathbf{g}), \quad \mathbf{h}_c = -K_c \nabla \mu_c.$$

Classical Poroelasticity

Isothermal & Linear

Classical Single Phase Poroelasticity:

$$\begin{aligned}\frac{\partial}{\partial t} \rho_{ref} (\alpha p + a \operatorname{div}(\mathbf{u})) - \operatorname{div} (K(\nabla p - \rho_{ref} \mathbf{g})) &= 0, \\ -\operatorname{div} (\mathbb{C}(\nabla \mathbf{u}) - a p \mathbf{I}) &= \mathbf{f}.\end{aligned}$$

- Fluid pressure p
- Macroscopic displacement \mathbf{u} .
- Elasticity tensor, e.g. $\mathbb{C}(\nabla \mathbf{u}) = 2\mu D(\mathbf{u}) + \lambda D(\mathbf{u})$.
- Fluid compressibility α , $\rho/\rho_{ref} = \alpha(p - p_{ref})$
- Biot constant a (\sim bulk modulus of medium).

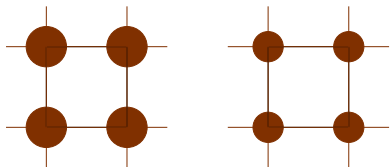
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Medium Kinematics²: p pore pressure, s_0 solid volume



$$\delta p > 0, \nabla \mathbf{u} = 0, \delta s_0 < 0$$



$$\delta p > 0, \delta s_0 = \nabla \mathbf{u} : \mathbf{A} < 0$$

²Sanchez Palencia, Non-Homogeneous Media and Vibration Theory (Springer)

Multiphase Linear Poroelasticity

Isothermal & Inertialess

Balances of Mass: $\partial_t m_c + \operatorname{div} \left(\sum_{\pi=1}^{N_p} M_{c\pi} (\mathbf{u}_t + \mathbf{v}_\pi) + \mathbf{h}_c \right) = 0,$

Elastic Medium: $-\operatorname{div}(T) = \mathbf{f}$ with $T = \frac{\partial \psi}{\partial \nabla \mathbf{u}}$

Ensemble Free Energy:

$$\Psi(\mathbf{s}, M, \nabla \mathbf{u}) = \Psi_0(s_0, \nabla \mathbf{u}) + \sum_{\pi=1}^{N_p} \Psi_\pi(s_\pi, \{M_{c\pi}\}_{c=1}^{N_c}) + \Upsilon(\mathbf{s}).$$

Equilibrium:

$$\psi(\mathbf{m}, \nabla \mathbf{u}) = \inf \{ \Psi(\mathbf{s}, M, \nabla \mathbf{u}) \mid \mathbf{s}_0 + \mathbf{s} \cdot \mathbf{1} = 1 + \mathbf{A} : \nabla \mathbf{u}, M \mathbf{1} = \mathbf{m} \}$$

Lagrange Multipliers: $\frac{\partial \psi}{\partial m_c} = \mu_c$ and $\frac{\partial \psi}{\partial \nabla \mathbf{u}} = \frac{\partial \Psi_0}{\partial \nabla \mathbf{u}} - p \mathbf{A}$

$$-p = \frac{\partial \Psi_0}{\partial s_0} = \frac{\partial \Psi_\pi}{\partial s_\pi} + \frac{\partial \Upsilon}{\partial s_\pi} \quad \text{and} \quad \mu_c = \frac{\partial \Psi_\pi}{\partial M_{c\pi}}, \quad 1 \leq \pi \leq N_p.$$

Multiphase Linear Poroelasticity

Isothermal & Inertialess

$$\text{Balances of Mass: } \partial_t m_c + \operatorname{div} \left(\sum_{\pi=1}^{N_p} M_{c\pi} (\mathbf{u}_t + \mathbf{v}_\pi) + \mathbf{h}_c \right) = 0,$$

$$\text{Elastic Medium: } -\operatorname{div}(\mathbf{T}) = \mathbf{f} \text{ with } \mathbf{T} = \frac{\partial \psi}{\partial \nabla \mathbf{u}}$$

Ensemble Free Energy:

$$\Psi(\mathbf{s}, M, \nabla \mathbf{u}) = \Psi_0(s_0, \nabla \mathbf{u}) + \sum_{\pi=1}^{N_p} \Psi_\pi(s_\pi, \{M_{c\pi}\}_{c=1}^{N_c}) + \Upsilon(\mathbf{s}).$$

Linear Poroelasticity: Biot constant and tensor (a, A) ,

$$\Psi_0(s_0, \nabla \mathbf{u}) = \frac{1}{2} \mathbb{C}(\nabla \mathbf{u}) : (\nabla \mathbf{u}) + \frac{1}{2a} (A : \nabla \mathbf{u} + (s_0 - \phi))^2$$

then

- $\frac{\partial \Psi_0}{\partial \nabla s_0} = \frac{1}{a} (A : \nabla \mathbf{u} + (s_0 - \phi)) = -p$
- $\frac{\partial \Psi_0}{\partial \nabla \mathbf{u}} = \mathbb{C}(\nabla \mathbf{u}) + \frac{1}{a} (A : \nabla \mathbf{u} + (s_0 - \phi)) A = \mathbb{C}(\nabla \mathbf{u}) - p A.$

Multiphase Linear Poroelasticity

Isothermal & Inertialess

Balances of Mass: $\partial_t m_c + \operatorname{div} \left(\sum_{\pi=1}^{N_p} M_{c\pi} \mathbf{v}_\pi + \mathbf{h}_c \right) = 0,$

Elastic Medium: $-\operatorname{div}(T) = \mathbf{f}$ with $T = \frac{\partial \psi}{\partial \nabla \mathbf{u}} = \frac{\partial \Psi_0}{\partial \nabla \mathbf{u}} - p A$

Equilibrium:

$$\psi(\mathbf{m}, \nabla \mathbf{u}) = \inf \left\{ \Psi(\mathbf{s}, M, \nabla \mathbf{u}) \mid s_0 + \mathbf{s} \cdot \mathbf{1} = 1 + A : \nabla \mathbf{u}, M \mathbf{1} = \mathbf{m} \right\}$$

Dissipation Relation: $\partial_t \psi = \mathbf{m}_t \cdot \boldsymbol{\mu} + T : \nabla \mathbf{u}_t, \dots$

$$\frac{d}{dt} \int_{\Omega} \psi + \int_{\Omega} \sum_{\pi} \left| \sum_c M_{c\pi} (\nabla \mu_c - \mathbf{g}) \right|_{K_\pi}^2 + \sum_{c=1}^{N_c} |\nabla \mu_c|_{K_c}^2 = \int_{\Omega} \mathbf{f} \cdot \mathbf{u}_t.$$

Multiphase Linear Poroelasticity

Isothermal & Inertialess

Balances of Mass: $\partial_t m_c + \operatorname{div} \left(\sum_{\pi=1}^{N_p} M_{c\pi} \mathbf{v}_\pi + \mathbf{h}_c \right) = 0,$

Elastic Medium: $-\operatorname{div}(T) = \mathbf{f}$ with $T = \frac{\partial \psi}{\partial \nabla \mathbf{u}} = \frac{\partial \Psi_0}{\partial \nabla \mathbf{u}} - p A$

Equilibrium:

$$\psi(\mathbf{m}, \nabla \mathbf{u}) = \inf \left\{ \Psi(\mathbf{s}, M, \nabla \mathbf{u}) \mid s_0 + \mathbf{s} \cdot \mathbf{1} = 1 + A : \nabla \mathbf{u}, M \mathbf{1} = \mathbf{m} \right\}$$

Dissipation Relation: $\partial_t \psi = \mathbf{m}_t \cdot \boldsymbol{\mu} + T : \nabla \mathbf{u}_t, \dots$

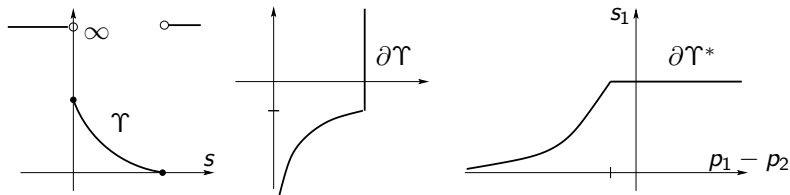
Weak Statement: $p = \dots$

$$\int_{\Omega} (\mathbf{m}_t, \hat{\boldsymbol{\mu}}) + \sum_{\pi=1}^{N_p} \sum_{c,c'=1}^{N_c} (M_{c\pi} \nabla \mu_c, M_{c'\pi} (\nabla \hat{\mu}_{c'} - \mathbf{g}))_{K_\pi} + \sum_{c=1}^{N_c} (\nabla \mu_c, \nabla \hat{\mu}_{c'})_{K_c} = 0$$

$$\left(\frac{\partial \Psi_0}{\partial \nabla \mathbf{u}} - p A, \nabla \mathbf{v} \right) = (\mathbf{f}, \mathbf{v})$$

Two Incompressible Immiscible Fluids

Numerical Example



Balances of Mass: $s_\pi^n - \tau \operatorname{div}(k_\pi^{n-1}(\nabla p_\pi^n - \mathbf{b}_\pi^{n-1})) = s_\pi^{n-1}$

Interfacial Energy: $\Upsilon(s_1 - s_2) = \Upsilon(2s_1 - \phi)$

$$\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} \in p \begin{pmatrix} 1 \\ 1 \end{pmatrix} + (1/2)\partial\Upsilon(s_1 - s_2) \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

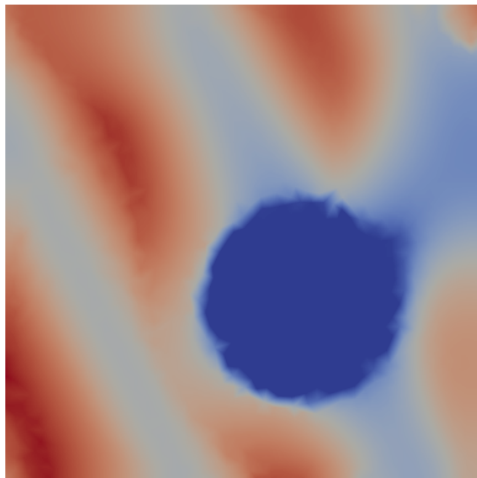
$$\begin{pmatrix} s_1 \\ s_2 \end{pmatrix} = \phi \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \partial\Upsilon^*(p_1 - p_2) \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Energy Estimate:

$$\frac{d}{dt} \int_\Omega \Upsilon(s_1 - s_2) + \sum_{\pi=1}^2 \int_\Omega |\nabla p_\pi|^2_{k_\pi} = \sum_{\pi=1}^2 \int_\Omega (\mathbf{b}_\pi, \nabla p_\pi)_{k_\pi}$$

Two Incompressible Immiscible Fluids

T. J. Murphy



Delaunay Mesh
Domain $[-1, 1]^2$
Time $t \in [0, 5]$
1592 Vertices
3061 Triangles
512 Time Steps
3184 Variables
25600 Nesterov
1854 Newton
iterations

Thank You