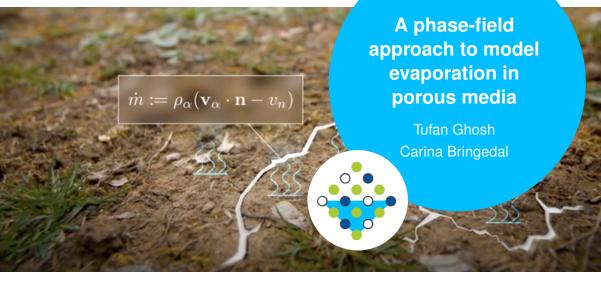


University of Stuttgart

Institute for Modelling Hydraulic and Environmental Systems (IWS)





InterPore 2022, 1 June 2022

Introduction

Motivation

- Evaporation and drying in porous media occur in many environmental and industrial systems
- Moving fluid-fluid interface at the pore-scale

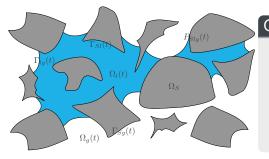




Introduction

Motivation

- Evaporation and drying in porous media occur in many environmental and industrial systems
- Moving fluid-fluid interface at the pore-scale



Objectives

- Formulate a mathematical model of the relevant processes at the pore scale, including a better description of the evolving liquid-gas interface
- Derive effective models valid at the REV scale through upscaling the pore-scale processes







- Advantage: determines the location of the moving interface





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- Challenge: location not known a-priori, depends on the model unknowns





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- Information: this velocity is directly linked to the mass transfer across the interface





- Advantage: determines the location of the moving interface
- Challenge: location not known a-priori, depends on the model unknowns
- Question: how does the normal velocity of the interface v_n behave?
- Information: this velocity is directly linked to the mass transfer across the interface
- Requirement: some kinematic condition coupling the normal velocity to an evaporation rate



Mass conservation -

$$\partial_t \rho_\alpha + \nabla \cdot (\rho_\alpha \mathbf{v}_\alpha) = 0 \qquad \qquad \text{in } \Omega_\alpha(t), \ \alpha = l, g \qquad (1)$$

$$(\rho_l \mathbf{v}_l - \rho_g \mathbf{v}_g) \cdot \mathbf{n} = v_n (\rho_l - \rho_g) \qquad \qquad \text{on } \Gamma_{lg}(t) \qquad (2)$$

$$\partial_t \left(\rho_g \chi_g^{\nu} \right) + \nabla \cdot \left(\rho_g \chi_g^{\nu} \mathbf{v}_g \right) = \nabla \cdot \left(\mathcal{D}_g^{\nu} \rho_g \nabla \chi_g^{\nu} \right) \qquad \text{in } \Omega_g(t) \tag{3}$$

$$\left(\rho_{l}\mathbf{v}_{l}-\left(\rho_{g}\chi_{g}^{v}\mathbf{v}_{g}-\mathrm{D}_{g}^{v}\rho_{g}\nabla\chi_{g}^{v}\right)\right)\cdot\mathbf{n}=v_{n}\left(\rho_{l}-\rho_{g}\chi_{g}^{v}\right)\qquad\text{on }\Gamma_{lg}(t)$$
(4)





Mass conservation -

$$\partial_t \rho_\alpha + \nabla \cdot (\rho_\alpha \mathbf{v}_\alpha) = 0 \qquad \qquad \text{in } \Omega_\alpha(t), \ \alpha = l, g \qquad (1)$$

$$(\rho_l \mathbf{v}_l - \rho_g \mathbf{v}_g) \cdot \mathbf{n} = v_n (\rho_l - \rho_g) \qquad \qquad \text{on } \Gamma_{lg}(t) \qquad (2)$$

$$\partial_t \left(\rho_g \chi_g^{\nu} \right) + \nabla \cdot \left(\rho_g \chi_g^{\nu} \mathbf{v}_g \right) = \nabla \cdot \left(\mathcal{D}_g^{\nu} \rho_g \nabla \chi_g^{\nu} \right) \qquad \qquad \text{in } \Omega_g(t) \tag{3}$$

$$\left(\rho_{l}\mathbf{v}_{l}-\left(\rho_{g}\chi_{g}^{\nu}\mathbf{v}_{g}-\mathrm{D}_{g}^{\nu}\rho_{g}\nabla\chi_{g}^{\nu}\right)\right)\cdot\mathbf{n}=\nu_{n}\left(\rho_{l}-\rho_{g}\chi_{g}^{\nu}\right)\qquad\text{on }\Gamma_{lg}(t)$$
(4)

Momentum balance -

$$\partial_t \rho_\alpha + \nabla \cdot (\rho_\alpha \mathbf{v}_\alpha \otimes \mathbf{v}_\alpha) = -\nabla p_\alpha + \nabla \cdot \mathcal{T}_\alpha + \rho \mathbf{g} \qquad \text{in } \Omega_\alpha(t), \ \alpha = l, g \qquad (5)$$

$$(-(p_l - p_g)\mathbf{I} + (\mathcal{T}_l - \mathcal{T}_g)) \cdot \mathbf{n} = \dot{m}(\mathbf{v}_l - \mathbf{v}_g) - \sigma \kappa \mathbf{n} \qquad \text{on } \Gamma_{lg}(t) \qquad (6)$$

$$\mathbf{v}_{l} \cdot \mathbf{t}_{i} = \mathbf{v}_{g} \cdot \mathbf{t}_{i} \qquad \qquad \text{on } \Gamma_{lg}(t) \qquad (7)$$

where, $\mathcal{T}_{\alpha} := \mu_{\alpha} \left(\nabla \mathbf{v}_{\alpha} + \nabla \mathbf{v}_{\alpha}^{T} \right) + \xi_{\alpha} (\nabla \cdot \mathbf{v}_{\alpha}) \mathbf{I}, \ \dot{m} := \rho_{\alpha} (\mathbf{v}_{\alpha} \cdot \mathbf{n} - v_{n}), \ \sigma$ - surface tension, $\kappa = \nabla_{\Gamma} \cdot \mathbf{n}$ - curvature





Energy balance -

$$\partial_t \left(\rho_\alpha \mathbf{u}_\alpha \right) + \nabla \cdot \left(\rho_\alpha \mathbf{h}_\alpha \mathbf{v}_\alpha \right) = \nabla \cdot \left(\mathbf{k}_\alpha \nabla \mathbf{T}_\alpha \right) + \mathbf{v}_\alpha \cdot \nabla p_\alpha + \mathcal{T}_\alpha : \nabla \mathbf{v}_\alpha \qquad \text{in } \Omega_\alpha(t), \ \alpha = l, g \qquad (8)$$

$$(\mathbf{k}_{g}\nabla \mathbf{T}_{g} - \mathbf{k}_{l}\nabla \mathbf{T}_{l}) \cdot \mathbf{n} = \dot{m}(\mathbf{h}_{g} - \mathbf{h}_{l}) = \dot{m}\mathcal{L}$$
 on $\Gamma_{lg}(t)$ (9)

$$\Gamma_l = T_g = T^{sat}$$
 on $\Gamma_{lg}(t)$ (10)

where, u_{α} - internal energy per unit mass of phase α , $h_{\alpha} := u_{\alpha} + p_{\alpha}/\rho_{\alpha}$ - specific enthalpy of phase α , $\mathcal{L} := h_g - h_l$ - latent heat of evaporation

$$\partial_t \left(\rho_S C_{\rho,S} \mathbf{T}_S \right) = \nabla \cdot \left(\mathbf{k}_S \nabla \mathbf{T}_S \right) \qquad \qquad \text{in } \Omega_S \qquad (11)$$

$$k_{S} \nabla T_{S} \cdot \mathbf{n}_{S} = k_{\alpha} \nabla T_{\alpha} \cdot \mathbf{n}_{S} \qquad \text{on } \Gamma_{S\alpha}(t) \qquad (12)$$

$$T_S = T_\alpha$$
 on $\Gamma_{S\alpha}(t)$ (13)





Energy balance -

$$\partial_t \left(\rho_\alpha \mathbf{u}_\alpha \right) + \nabla \cdot \left(\rho_\alpha \mathbf{h}_\alpha \mathbf{v}_\alpha \right) = \nabla \cdot \left(\mathbf{k}_\alpha \nabla \mathbf{T}_\alpha \right) + \mathbf{v}_\alpha \cdot \nabla p_\alpha + \mathcal{T}_\alpha : \nabla \mathbf{v}_\alpha \qquad \text{in } \Omega_\alpha(t), \ \alpha = l, g \quad (8)$$

$$(k_g \nabla T_g - k_l \nabla T_l) \cdot \mathbf{n} = \dot{m} (h_g - h_l) = \dot{m} \mathcal{L}$$
 on $\Gamma_{lg}(t)$ (9)

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$$\partial_t \left(\rho_S C_{\rho,S} \mathbf{T}_S \right) = \nabla \cdot \left(\mathbf{k}_S \nabla \mathbf{T}_S \right) \qquad \text{in } \Omega_S \tag{11}$$

$$k_{\mathcal{S}} \nabla T_{\mathcal{S}} \cdot \mathbf{n}_{\mathcal{S}} = k_{\alpha} \nabla T_{\alpha} \cdot \mathbf{n}_{\mathcal{S}} \qquad \text{on } \Gamma_{\mathcal{S}\alpha}(t) \qquad (12)$$

$$T_{\mathcal{S}} = T_{\alpha}$$
 on $\Gamma_{\mathcal{S}\alpha}(t)$ (13)

Reaction/Evaporation rate -

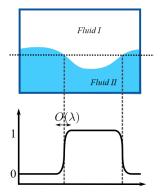
$$\frac{(\rho_l + \rho_g)}{2} \left(v_n - \mathbf{v}_g \cdot \mathbf{n} \right) = -f(\chi_g^v) = -R \left\{ \left(\frac{\chi_g^v}{\chi_{sat}^v} \right)^2 - 1 \right\}$$
(14)

where, f is the resulting evaporation rate, and R is a reaction constant of dimension kg m⁻² s⁻¹





Phase-field Formulation



- $\phi = 1$ (Fluid I), $\phi = 0$ (Fluid II)
- Approximate sharp interface by a smooth phase field ϕ

- Moving interface replaced by a thin, diffuse layer
- All equations solved in a fixed domain

Redeker, M., Rohde, C., Pop., I.S., Upscaling of a tri-phase phase-field model for precipitation in porous media, *IMA J Appl Math*, 81, 898–939, 2016.

Bringedal, C., Von Wolff, L., Pop, I.S., Phase field modeling of precipitation and dissolution processes in porous media: upscaling and numerical experiments, *Multiscale Model. Simul.*, 18(2), 1076–1112, 2020.





Diffuse Interface Model : Our Take

Phase-field equation -

$$\rho\left\{\partial_t \phi + \nabla \cdot (\phi \mathbf{v})\right\} = \frac{\gamma}{\nu} \left\{\nabla^2 \phi - \lambda^{-2} P'(\phi)\right\} - \sqrt{2} \lambda^{-1} \phi(1-\phi) f(\chi_g^{\nu}) \qquad \text{in } \Omega_F \qquad (15)$$

where, $P(\phi) = \phi^2 (1 - \phi)^2$, $\rho = \phi \rho_l + (1 - \phi) \rho_g$, **v** - velocity of the mixture, γ and ν are parameters having dimensions kg s⁻² and m s⁻¹

$$\nabla \phi \cdot \mathbf{n} = 0 \qquad \qquad \text{on } \Gamma_{\mathcal{S}} \tag{16}$$

Mass conservation equation -

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$$
 in Ω_F (17)

$$\partial_t \left(\phi \rho_l + (1 - \phi) \rho_g \chi_g^\nu \right) + \nabla \cdot \left\{ \left(\phi \rho_l + (1 - \phi) \rho_g \chi_g^\nu \right) \mathbf{v} \right\} = \nabla \cdot \left(\mathcal{D}_g^\nu \rho_g (1 - \phi) \nabla \chi_g^\nu \right) \quad \text{in } \Omega_F \quad (18)$$

$$D_g^{\nu} \rho_g (1-\phi) \nabla \chi_g^{\nu} \cdot \mathbf{n} = 0 \qquad \text{on } \Gamma_S \qquad (19)$$





Diffuse Interface Model : Our Take

Momentum balance equation -

$$\partial_t \left(\rho \mathbf{v} \right) + \nabla \cdot \left(\rho \mathbf{v} \otimes \mathbf{v} \right) = -\nabla \rho + \nabla \cdot \mathcal{T} - \nabla \cdot \left(\lambda \sigma \nabla \phi \otimes \nabla \phi \right) + \rho \mathbf{g} \qquad \text{in } \Omega_F \qquad (20)$$

where, *p* - pressure of the mixture and $T = \phi T_l + (1 - \phi)T_g$

$$\mathbf{v} = \mathbf{0}$$
 on Γ_S (21)

Energy balance equation -

 $\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{h} \mathbf{v}) = \nabla \cdot (\mathbf{k} \nabla \mathbf{T}) + \mathbf{v} \cdot \nabla \mathbf{p} + \mathcal{T} : \nabla \mathbf{v} + \mathbf{v} \cdot \{\nabla \cdot (\lambda \sigma \nabla \phi \otimes \nabla \phi)\} \quad \text{in } \Omega_F \quad (22)$

where, ${\rm u}, {\rm h}, {\rm k}$ and ${\rm T}$ are the internal energy, specific enthalpy, heat conductivity and Temperature of the mixture, respectively

$$k\nabla T \cdot \mathbf{n} = k_{\mathcal{S}} \nabla T_{\mathcal{S}} \cdot \mathbf{n} \qquad \text{on } \Gamma_{\mathcal{S}}$$
(23)

$$T = T_S$$
 on Γ_S (24)





Decreasing Energy

The energy associated with the above phase-field model is given by

$$E = \int_{\Omega_F} \left(\frac{1}{2} \rho \mathbf{v}^2 + \gamma \lambda^{-1} P(\phi) + \frac{1}{2} \gamma \lambda | \nabla \phi |^2 + \rho \mathbf{u} + \rho F(\rho, \phi) \right) d\mathbf{x}$$
(25)

Here the density energy $\rho F(\rho, \phi)$ is defined as follows

$$\partial_{\phi}(\rho F(\rho, \phi)) = \sqrt{2}\nu \phi(1-\phi)f(\chi_{g}^{\nu})$$
(26)

Then one can compute

$$\frac{d}{dt}E(t) = \int_{\Omega_F} \left(\mathbf{v} \cdot \rho \mathbf{g} - \eta \nabla \cdot (\phi \mathbf{v}) - \frac{\eta^2}{\rho \lambda \nu} - \partial_\rho \left(\rho F(\rho, \phi) \right) \nabla \cdot (\rho \mathbf{v}) \right) d\mathbf{x}$$
(27)

where, $\eta = \gamma \lambda^{-1} P'(\phi) - \gamma \lambda \nabla^2 \phi + \sqrt{2} \nu \phi (1 - \phi) f(\chi_g^v)$.

 \Rightarrow Decreasing energy for zero velocities, or low enough divergence.

Ghosh, T., Bringedal, C., A phase-field approach to model evaporation in porous media: Upscaling from pore to Darcy scale, arXiv preprint, 2021. https://arxiv.org/abs/2112.13104





Sharp Interface Limit

- Phase field/diffuse interface model can be seen as an approximation of the sharp interface model
- Introduce the dimensionless parameter $\zeta=\lambda/L$ related to thickness of the diffuse interface region
- Investigate the behavior of the solution as $\zeta \rightarrow 0$: We recover the sharp interface formulation!



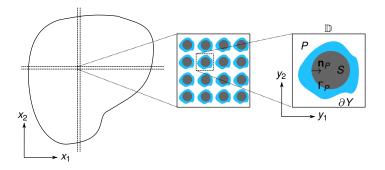


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- Introduce the dimensionless parameter $\zeta=\lambda/L$ related to thickness of the diffuse interface region
- Investigate the behavior of the solution as $\zeta \rightarrow 0$: We recover the sharp interface formulation!
- Matched asymptotic expansion: away from the diffuse interface (outer expansion), close to it (inner expansion) and applying matching condition at the transition region
- Outer expansion: gives the governing equations in the corresponding phases Outer Expansion
- Inner expansion: provides the interface conditions between the two phases Inner Expansion







- Scale separation: $\varepsilon = \frac{l}{L} << 1$ and $\mathbf{y} = \varepsilon^{-1} \mathbf{x}$
- Write the unknowns as a series expansion in terms of the scale separation arepsilon
- Diffusion dominated regime, *i.e.* $Pe = O(\varepsilon)$





Upscaled equations: Summary

$$\partial_t \overline{\rho}_0 + \varepsilon \nabla_{\mathbf{x}} \cdot (\overline{\rho_0 \mathbf{v}_0}) = \mathcal{O}(\varepsilon) \qquad \qquad \text{in } \mathbb{D} \qquad (28)$$

$$\partial_t \left(\overline{(\rho \chi_g^{\nu})_0} \right) + \varepsilon \nabla_{\mathbf{x}} \cdot \left\{ \overline{(\rho \chi_g^{\nu})_0 \mathbf{v}_0} \right\} = \nabla_{\mathbf{x}} \cdot \left(\mathcal{D} \nabla_{\mathbf{x}} \chi_{g0}^{\nu} \right) + \mathcal{O}(\varepsilon) \qquad \text{in } \mathbb{D}$$
(29)

$$\overline{\mathbf{v}}_0 = -\mathcal{K} \nabla_{\mathbf{x}} p_0 - \mathcal{G} \qquad \qquad \text{in } \mathbb{D} \qquad (30)$$

$$\partial_t \left(\overline{\rho_0 \mathbf{u}_0} \right) + \partial_t \left(\rho_S C_{\rho,S} \mathbf{T}_{S0} \right) + \varepsilon \nabla_{\mathbf{x}} \cdot \left(\overline{\rho_0 \mathbf{h}_0 \mathbf{v}_0} \right) = \nabla_{\mathbf{x}} \cdot \left(\mathcal{A} \nabla_{\mathbf{x}} \mathbf{T}_0 \right) + \mathcal{O}(\varepsilon) \qquad \text{in } \mathbb{D} \qquad (31)$$

The phase field $\phi_0(t, \mathbf{x}, \mathbf{y})$ is updated locally in each pore by solving

$$\rho_0\left\{\partial_t \phi_0 + \nabla_{\mathbf{y}} \cdot (\phi_0 \mathbf{v}_0)\right\} = \frac{\gamma}{\nu} \left\{\nabla_{\mathbf{y}}^2 \phi_0 - \lambda^{-2} P'(\phi_0)\right\} - \frac{\sqrt{2}}{\lambda} \phi_0(1 - \phi_0) f(\chi_{g0}^{\nu}) \qquad \text{in } P$$

$$\nabla_{\mathbf{y}}\phi_0 \cdot \mathbf{n}_P = 0 \qquad \qquad \text{on } \Gamma_P \qquad (32)$$

Periodicity in **y** across
$$\partial Y$$





• The effective diffusion matrix $\mathcal{D}(t, \mathbf{x})$:

$$\boldsymbol{d}_{ij}(t,\mathbf{x}) = \int_{P} \mathrm{D}_{g}^{v} \rho_{g0}(1-\phi_{0}) \left(\delta_{ij}+\partial_{y_{i}}\kappa^{j}\right) d\mathbf{y}, \quad \text{with } i,j \in \{1,2,\cdots,d\}$$
(33)

where

$$abla_{\mathbf{y}} \cdot \left\{ \mathrm{D}_{g}^{\mathbf{v}}
ho_{g0} (1 - \phi_0) (\boldsymbol{e}_j + \nabla_{\mathbf{y}} \kappa^j) \right\} = \mathbf{0} \qquad \qquad \mathrm{in} \ \boldsymbol{P}$$

$$D_g^{\nu} \rho_{g0} (1 - \phi_0) (\boldsymbol{e}_j + \nabla_{\mathbf{y}} \kappa^j) \cdot \mathbf{n}_P = 0 \qquad \text{on } \Gamma_P$$
(34)

Periodicity in **y** across ∂Y

$$\partial_t \left(\overline{(\rho \chi_g^{\nu})_0} \right) + \varepsilon \nabla_{\mathbf{x}} \cdot \left\{ \overline{(\rho \chi_g^{\nu})_0 \mathbf{v}_0} \right\} = \nabla_{\mathbf{x}} \cdot \left(\mathcal{D} \nabla_{\mathbf{x}} \chi_{g0}^{\nu} \right) + \mathcal{O}(\varepsilon)$$





• The effective "permeability" matrix $\mathcal{K}(t, \mathbf{x})$:

$$\boldsymbol{k}_{ij}(\boldsymbol{t}, \mathbf{x}) = \int_{P} w_{i}^{j} d\mathbf{y}, \quad \text{with } i, j \in \{1, 2, \cdots, d\}$$
(35)

where

$$\begin{aligned} \left(\mathbf{e}_{j} + \nabla_{\mathbf{y}} \Pi^{j} \right) + \nabla_{\mathbf{y}} \cdot \left\{ \mu_{0} \left(\nabla_{\mathbf{y}} \mathbf{w}^{j} + \nabla_{\mathbf{y}} \mathbf{w}^{j^{T}} \right) \right\} + \nabla_{\mathbf{y}} \cdot \left\{ \xi_{0} \left(\nabla_{\mathbf{y}} \cdot \mathbf{w}^{j} \right) \mathbf{I} \right\} &= 0 \qquad \text{in } P \\ \nabla_{\mathbf{y}} \cdot \left(\rho_{0} \mathbf{w}^{j} \right) &= 0 \qquad \qquad \text{in } P \\ \mathbf{w}^{j} &= \mathbf{0} \qquad \qquad \text{on } \Gamma_{P} \end{aligned}$$
(36)

Periodicity in y

across ∂Y

 $\overline{\mathbf{v}}_0 = -\boldsymbol{\mathcal{K}} \nabla_{\mathbf{x}} \boldsymbol{\mathcal{p}}_0 - \boldsymbol{\mathcal{G}}$





• The effective gravity vector $\mathcal{G}(t, \mathbf{x})$:

$$g_i(t, \mathbf{x}) = \int_P w_i^0 d\mathbf{y}, \quad \text{with } i \in \{1, 2, \cdots, d\}$$
(37)

where

$$\nabla_{\mathbf{y}} \Pi^{0} = \nabla_{\mathbf{y}} \cdot \left\{ \mu_{0} \left(\nabla_{\mathbf{y}} \mathbf{w}^{0} + \nabla_{\mathbf{y}} \mathbf{w}^{0^{T}} \right) + \xi_{0} \left(\nabla_{\mathbf{y}} \cdot \mathbf{w}^{0} \right) \mathbf{I} \right\} - \nabla_{\mathbf{y}} \cdot \left(\lambda \sigma \nabla_{\mathbf{y}} \phi_{0} \otimes \nabla_{\mathbf{y}} \phi_{0} \right) + \rho_{0} \mathbf{g} \quad \text{in } P$$

$$\nabla_{\mathbf{y}} \cdot \left(\rho_0 \mathbf{w}^0\right) = \partial_t \rho_0 \qquad \qquad \text{in } \boldsymbol{P}$$

$$\mathbf{w}^0 = \mathbf{0} \qquad \qquad \text{on } \Gamma_P \tag{38}$$

$$\overline{\mathbf{v}}_0 = -\mathcal{K} \nabla_{\mathbf{x}} \boldsymbol{\rho}_0 - \boldsymbol{\mathcal{G}}$$





• The effective heat conductivity matrix $A(t, \mathbf{x})$:

$$\mathbf{a}_{ij}(t,\mathbf{x}) = \int_{P} \left\{ \mathbf{k}_{0} \left(\delta_{ij} + \partial_{y_{i}} \psi^{j} \right) + \mathbf{k}_{S} \left(\delta_{ij} + \partial_{y_{i}} \eta^{j} \right) \right\} d\mathbf{y}, \quad \text{with } i, j \in \{1, 2, \cdots, d\}$$
(39)

where

$$abla_{\mathbf{y}} \cdot \left\{ \mathrm{k}_{\mathbf{0}} \left(\boldsymbol{e}_{j} +
abla_{\mathbf{y}} \psi^{j} \right) \right\} = \mathbf{0}$$
 in \boldsymbol{P}

$$abla_{\mathbf{y}} \cdot \left\{ \mathrm{k}_{\mathcal{S}} \left(\boldsymbol{e}_{j} +
abla_{\mathbf{y}} \eta^{j} \right) \right\} = \mathbf{0}$$
 in \boldsymbol{S}

$$\psi^j = \eta^j$$
 on Γ_P

$$k_{0} \left(\boldsymbol{e}_{j} + \nabla_{\mathbf{y}} \psi^{j}\right) \cdot \mathbf{n}_{P} + k_{S} \left(\boldsymbol{e}_{j} + \nabla_{\mathbf{y}} \eta^{j}\right) \cdot \mathbf{n}_{P} = 0 \qquad \text{on } \Gamma_{P}$$

Periodicity in y

across ∂Y

 $\partial_t \left(\overline{\rho_0 \mathbf{u}_0} \right) + \partial_t \left(\rho_S \mathcal{C}_{\rho,S} \mathbf{T}_{S0} \right) + \varepsilon \nabla_{\mathbf{x}} \cdot \left(\overline{\rho_0 \mathbf{h}_0 \mathbf{V}_0} \right) = \nabla_{\mathbf{x}} \cdot \left(\mathcal{A} \nabla_{\mathbf{x}} \mathbf{T}_0 \right) + \mathcal{O}(\varepsilon)$



(40)



Summary

- Derived a new phase field model to describe evaporation on the pore scale
- Proposed model follows a decreasing free energy only for the diffusion dominated case
- Sharp interface limit of the phase field formulation recovers the sharp interface formulation (i.e., governing equations and boundary conditions)
- Derived an upscaled (REV-scale) model taking into account the pore-scale information

Ghosh, T., Bringedal, C., A phase-field approach to model evaporation in porous media: Upscaling from pore to Darcy scale, arXiv preprint, 2021. https://arxiv.org/abs/2112.13104







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Thank you!



Tufan Ghosh tufan.ghosh@iws.uni-stuttgart.de +49 711 686 60136 Institute for Modelling Hydraulic and Environmental Systems



Outer Expansion : Leading Order

- Phase field equation: $P'(\phi_0^{out}) = 0 \implies \phi_0^{out} = 0, \ 1/2, \ 1.$
- Governing equations in Ω^l₀(t):

$$\partial_{t}\rho_{l,0}^{out} + \nabla \cdot \left(\rho_{l,0}^{out} \mathbf{v}_{l,0}^{out}\right) = \mathbf{0}$$
$$\partial_{t} \left(\rho_{l,0}^{out} \mathbf{v}_{l,0}^{out}\right) + \nabla \cdot \left(\rho_{l,0}^{out} \mathbf{v}_{l,0}^{out} \otimes \mathbf{v}_{l,0}^{out}\right) = -\nabla p_{l,0}^{out} + \nabla \cdot \mathcal{T}_{l,0}^{out} + \rho_{l,0}^{out} \mathbf{g}$$
$$\partial_{t} \left(\rho_{l,0}^{out} \mathbf{u}_{l,0}^{out}\right) + \nabla \cdot \left(\rho_{l,0}^{out} \mathbf{h}_{l,0}^{out} \mathbf{v}_{l,0}^{out}\right) = \nabla \cdot \left(\mathbf{k}_{l} \nabla \mathbf{T}_{l,0}^{out}\right) + \mathbf{v}_{l,0}^{out} \cdot \nabla p_{l,0}^{out} + \mathcal{T}_{l,0}^{out} : \nabla \mathbf{v}_{l,0}^{out}$$

Governing equations in Ω^g₀(t):

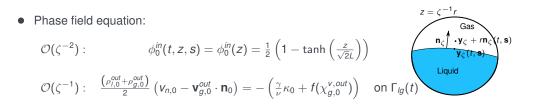
$$\partial_{t}\rho_{g,0}^{out} + \nabla \cdot \left(\rho_{g,0}^{out} \mathbf{v}_{g,0}^{out}\right) = \mathbf{0}, \qquad \partial_{t} \left(\rho_{g,0}^{out} \chi_{g,0}^{v,out}\right) + \nabla \cdot \left(\rho_{g,0}^{out} \chi_{g,0}^{v,out} \mathbf{v}_{v,0}^{out}\right) = \nabla \cdot \left(\mathbf{D}_{g}^{v} \rho_{g,0}^{out} \nabla \chi_{g,0}^{v,out}\right)$$
$$\partial_{t} \left(\rho_{g,0}^{out} \mathbf{v}_{g,0}^{out}\right) + \nabla \cdot \left(\rho_{g,0}^{out} \mathbf{v}_{g,0}^{out} \otimes \mathbf{v}_{g,0}^{out}\right) = -\nabla \rho_{g,0}^{out} + \nabla \cdot \mathcal{T}_{g,0}^{out} + \rho_{g,0}^{out} \mathbf{g}$$
$$\partial_{t} \left(\rho_{g,0}^{out} \mathbf{u}_{g,0}^{out}\right) + \nabla \cdot \left(\rho_{g,0}^{out} \mathbf{v}_{g,0}^{out}\right) = \nabla \cdot \left(\mathbf{k}_{g} \nabla \mathbf{T}_{g,0}^{out}\right) + \mathbf{v}_{g,0}^{out} \cdot \nabla \rho_{g,0}^{out} + \mathcal{T}_{g,0}^{out} : \nabla \mathbf{v}_{g,0}^{out}$$

Back - Sharp-interface Limit





Inner Expansion



Mass conservation equations:

$$\mathcal{O}(\zeta^{-1}): \qquad \mathbf{v}_{n,0} \left(\rho_{g,0}^{out} - \rho_{l,0}^{out} \right) = \left(\rho_{g,0}^{out} \mathbf{v}_{g,0}^{out} - \rho_{l,0}^{out} \mathbf{v}_{l,0}^{out} \right) \cdot \mathbf{n}_{0} \qquad \text{on } \Gamma_{lg}(t)$$

$$\mathcal{O}(\zeta^{-2}): \quad \mathbf{v}_{n,0} \left(\rho_{g,0}^{out} \chi_{r,0}^{v,out} - \rho_{l,0}^{out} \right) = \left(\left(\rho_{g,0}^{out} \chi_{r,0}^{v,out} \mathbf{v}_{g,0}^{out} - \mathcal{D}_{g,0}^{v} \rho_{0,0}^{out} \nabla \chi_{r,0}^{v,out} \right) - \rho_{l,0}^{out} \mathbf{v}_{l,0}^{out} \right) \cdot \mathbf{n}_{0} \qquad \text{on } \Gamma_{lg}(t)$$

$$\mathcal{D}(\zeta^{-2}): \quad \mathbf{v}_{n,0} \left(\rho_{g,0}^{out} \chi_{g,0}^{\mathbf{v},out} - \rho_{l,0}^{out} \right) = \left(\left(\rho_{g,0}^{out} \chi_{g,0}^{\mathbf{v},out} \mathbf{v}_{g,0}^{out} - \mathrm{D}_{g}^{\mathbf{v}} \rho_{g,0}^{out} \nabla \chi_{g,0}^{\mathbf{v},out} \right) - \rho_{l,0}^{out} \mathbf{v}_{l,0}^{out} \right) \cdot \mathbf{n}_{0} \quad \text{on } \Gamma_{lg}(t)$$





Inner Expansion

• Momentum balance equation:

$$\mathcal{O}(\zeta^{-2}): \qquad v_{g,0}^{out} \cdot \mathbf{t}_0 = v_{l,0}^{out} \cdot \mathbf{t}_0 \qquad \qquad \text{on } \Gamma_{lg}(t)$$

 $\mathcal{O}(\zeta^{-1})$: Provides normal velocity condition on $\Gamma_{lg}(t)$

• Energy balance equation:

 $\mathcal{O}(\zeta^{-2}): \quad \mathbf{T}_{g,0}^{out} = \mathbf{T}_{l,0}^{out} \qquad \qquad \text{on } \Gamma_{lg}(t)$ $\mathcal{O}(\zeta^{-1}): \quad \left(\mathbf{k}_g \nabla \mathbf{T}_{g,0}^{out} - \mathbf{k}_l \nabla \mathbf{T}_{l,0}^{out}\right) \cdot \mathbf{n}_0 = \dot{m}_0 \left(\mathbf{u}_{g,0}^{out} - \mathbf{u}_{l,0}^{out}\right) = \dot{m}_0 \mathcal{L} \qquad \qquad \text{on } \Gamma_{lg}(t)$

Back - Sharp-interface Limit



