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How Turbulence and Interface Properties Affect Porous-Medium / Free Flow Exchange Processes

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## Introduction

# Challenges – Evaporation from a Porous Medium



# Porous Medium

- REV concept
- multiphase Darcy's law
- two fluid phases (gas, liquid)
- two components (air, water)
- compositional, non-isothermal
- local thermodynamic equilibrium
- $p_{\rm g}$ ,  $S_{\rm I}$ , T or  $p_{\rm g}$ ,  $X_{\rm g}^{\rm w}$ , T



# Porous Medium Equations

mass balance

$$\sum_{\alpha \in \{\mathbf{I}, \mathbf{g}\}} \left\{ \phi \frac{(\partial \varrho_{\alpha} S_{\alpha})}{\partial t} + \nabla \cdot (\varrho_{\alpha} \mathbf{v}_{\alpha}) - q_{\alpha} \right\} = 0$$
storage

momentum balance (Darcy)

$$\frac{k_{\mathsf{r},\alpha}}{\nu_{\alpha}\varrho_{\alpha}}\mathsf{K}\left(\nabla p_{\alpha}-\varrho_{\alpha}\mathbf{g}\right)+\mathsf{v}_{\alpha}=\mathsf{0}$$
pressure gravity

• component mass balance  $\sum_{\alpha \in \{\mathsf{I},\mathsf{g}\}} \left\{ \phi \frac{\partial \left( \varrho_{\alpha} S_{\alpha} X_{\alpha}^{\kappa} \right)}{\partial t} + \nabla \cdot \left( \varrho_{\alpha} X_{\alpha}^{\kappa} \mathbf{v}_{\alpha} \right) - \nabla \cdot \left( D_{\alpha,\mathsf{pm}}^{\kappa} \varrho_{\alpha,\mathsf{mol}} M^{\kappa} \nabla x_{\alpha}^{\kappa,\mathsf{if}} \right) - q_{\alpha}^{\kappa} \right\} = 0$ storage advection diffusion source

energy balance

$$\sum_{\alpha \in \{\mathsf{I},\mathsf{g}\}} \left\{ \phi \frac{\partial \left(\varrho_{\alpha} S_{\alpha} u_{\alpha}\right)}{\partial t} + \nabla \cdot \left(\varrho_{\alpha} h_{\alpha} \mathbf{v}_{\alpha}\right) \right\} + (1 - \phi) \frac{\left(\partial \varrho_{\mathsf{s}} c_{\mathsf{s}} T\right)}{\partial t} - \nabla \cdot \left(\lambda_{\mathsf{pm}} \nabla T\right) - q^{T} = 0$$
storage (solid) conduction source

# Free Flow

- laminar / turbulent (RANS)
- single phase (gas)
- two components (air / water)
- compositional, non-isothermal
- Ma < 0.3
- $p_{\rm g}$ ,  $\mathbf{v}_{\rm g}$ ,  $X_{\rm g}^{\rm w}$ , T



# Free Flow Equations

mass balance

$$\frac{\partial \varrho_{g}}{\partial t} + \nabla \cdot (\varrho_{g} \bar{\mathbf{v}}_{g}) = 0$$
  
• momentum balance (RANS)

$$\frac{\partial \left(\varrho_{g} \bar{\mathbf{v}}_{g}\right)}{\partial t} + \nabla \cdot \left(\varrho_{g} \bar{\mathbf{v}}_{g} \bar{\mathbf{v}}_{g}^{\mathsf{T}}\right) - \nabla \cdot \left(\left[\varrho_{g} \nu_{g} + \varrho_{g} \nu_{g,t}\right] \nabla \left(\bar{\mathbf{v}}_{g} + \bar{\mathbf{v}}_{g}^{\mathsf{T}}\right)\right) + \nabla \bar{p}_{g} - \varrho_{g} \mathbf{g} = 0$$
inertia viscous eddy viscosity pressure gravity

component mass balance

$$\frac{\partial \left(\varrho_{g} X_{g}^{\kappa}\right)}{\partial t} + \nabla \cdot \left(\varrho_{g} \bar{X}_{g}^{\kappa} \bar{\mathbf{v}}_{g}\right) - \nabla \cdot \left(\begin{bmatrix} D_{g}^{\kappa} + \frac{D_{g,t}^{\kappa}}{g,t} \end{bmatrix} \varrho_{g,mol} M^{\kappa} \nabla \bar{x}_{g}^{\kappa}\right) - q_{g}^{\kappa} = 0$$
advection
diffusion
eddy diffusion
source

energy balance

$$\frac{\partial \left(\varrho_{g} \bar{u}_{g}\right)}{\partial t} + \nabla \cdot \left(\varrho_{g} \bar{h}_{g} \bar{\mathbf{v}}_{g}\right) - \sum_{\kappa \in \{a,w\}} \left\{ \nabla \cdot \left(\bar{h}_{g}^{\kappa} \bar{j}_{g,\text{ff},\text{t},\text{diff}}^{\kappa}\right) \right\} - \nabla \cdot \left( \left[\lambda_{g} + \lambda_{g,\text{t}}\right] \nabla \bar{T} \right) - q_{g}^{T} = 0$$

$$(\text{eddy-)diffusion} \quad \text{conduction} \quad \text{eddy conduction source}$$

Gordon Research Seminar, 31 July 2016, Girona

# Model Turbulence



# Coupling

- after [Mosthaf et al. 2011, Fetzer et al. 2016]
- local thermodynamic equilibrium
- continuity of fluxes
- continuity of primary variables



# **Coupling Discretization**



# **Coupling Equations**

• mass 
$$[(\varrho_g \overline{\mathbf{v}}_g) \cdot \mathbf{n}]^{ff} = -[(\varrho_g \mathbf{v}_g + \varrho_I \mathbf{v}_I) \cdot \mathbf{n}]^{pm}$$

tangential momentum (only free flow)

$$\left[ \overline{\mathbf{v}_{t,g}^{if}} - \frac{\sqrt{K}}{\alpha_{BJ}} \frac{\overline{\mathbf{v}_{t,g}^{ff}} - \overline{\mathbf{v}_{t,g}^{if}}}{\frac{1}{2}\Delta y} \right]^{ff} = 0$$



normal momentum (only free flow)

$$\begin{bmatrix} \left( \left\{ \varrho_{g} \bar{\mathbf{v}}_{g} \bar{\mathbf{v}}_{g}^{\mathsf{T}} - \bar{\boldsymbol{\tau}}_{g,t} + \bar{p}_{g} \mathbf{I} \right\} \mathbf{n} \right) \cdot \mathbf{n} \end{bmatrix}^{\text{ff}} = \begin{bmatrix} \boldsymbol{p}_{g}^{\text{if}} \end{bmatrix}^{\text{pm}}$$
$$\begin{bmatrix} \varrho_{g} v_{n,g}^{\text{if}} \end{bmatrix}^{\text{ff}} = - \begin{bmatrix} -\varrho_{g} \frac{k_{r,g} K}{\mu_{g}} \frac{\boldsymbol{p}_{g}^{\text{if}} - \boldsymbol{p}_{g}^{\text{pm}}}{\frac{1}{2} \Delta y} n_{y} - \varrho_{I} \frac{k_{r,I} K}{\mu_{I}} \frac{\boldsymbol{p}_{I}^{\text{if}} - \boldsymbol{p}_{I}^{\text{pm}}}{\frac{1}{2} \Delta y} n_{y} \end{bmatrix}^{\text{pm}}$$

# **Coupling Equations 2**

component mass

$$\begin{bmatrix} \left( \varrho_{g} \bar{X}_{g}^{\kappa} \bar{\mathbf{v}}_{g} - \left( D_{g}^{\kappa} + D_{g,t}^{\kappa} \right) \varrho_{g,mol} M^{\kappa} \nabla x_{g}^{\kappa,if} \right) \cdot \mathbf{n} \end{bmatrix}^{\text{ff}} \\ = - \begin{bmatrix} \left( \varrho_{g} X_{g}^{\kappa} \mathbf{v}_{g} - \mathbf{j}_{g,pm,diff}^{\kappa} + \varrho_{l} \mathbf{v}_{l} X_{l}^{\kappa} - \mathbf{j}_{l,pm,diff}^{\kappa} \right) \cdot \mathbf{n} \end{bmatrix}^{\text{pm}}$$



#### energy

$$\begin{bmatrix} \left( \varrho_{g} \bar{h}_{g} \bar{\mathbf{v}}_{g} - \bar{h}_{g}^{a} \bar{\mathbf{j}}_{g,ff,t,diff}^{a} - \bar{h}_{g}^{w} \bar{\mathbf{j}}_{g,ff,t,diff}^{w} - \lambda_{g,t} \nabla \bar{\mathcal{T}}^{if} \right) \cdot \mathbf{n} \end{bmatrix}^{ff} \\ = - \left[ \left( \varrho_{g} h_{g} \mathbf{v}_{g} + \varrho_{l} h_{l} \mathbf{v}_{l} - \lambda_{pm} \nabla \mathcal{T} \right) \cdot \mathbf{n} \right]^{pm}$$

# Implementation and Setup

- MAC / cell-centered FV
- fully implicit
- monolithic
- numerical simulator





## **Turbulence Modeling**











#### **Beavers-Joseph Coefficient**













## Obstacles with H=10mm





Obstacles





# **Summary and Outlook**

#### Summary

- coupling of free flow (MAC) to porous-medium flow (CCFV)
- turbulent models of different complexity
- influence of interface properties

#### Outlook

- turbulent / barometric pumping
- Forchheimer extension to Darcy's law
- local thermodynamic non-equilibrium
- pore network model at the interface

### Thank you for your attention!

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- [Fetzer et al. 2016] Effect of Turbulence and Roughness on Coupled Porous-Medium/Free Flow Exchange Processes
   Transport in Porous Media, 2016
- [Grüninger, Fetzer, Flemisch, Helmig (in preparation)] Coupling DuMuX and DUNE-PDELab to investigate evaporation at the interface between Darcy and Navier-Stokes flow
- [Mosthaf et al. 2011] A coupling concept for two-phase compositional porous-medium and singlephase compositional free flow Water Resources Research, 2011, 47, W10522