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Multiphase flow in highly permeable porous media

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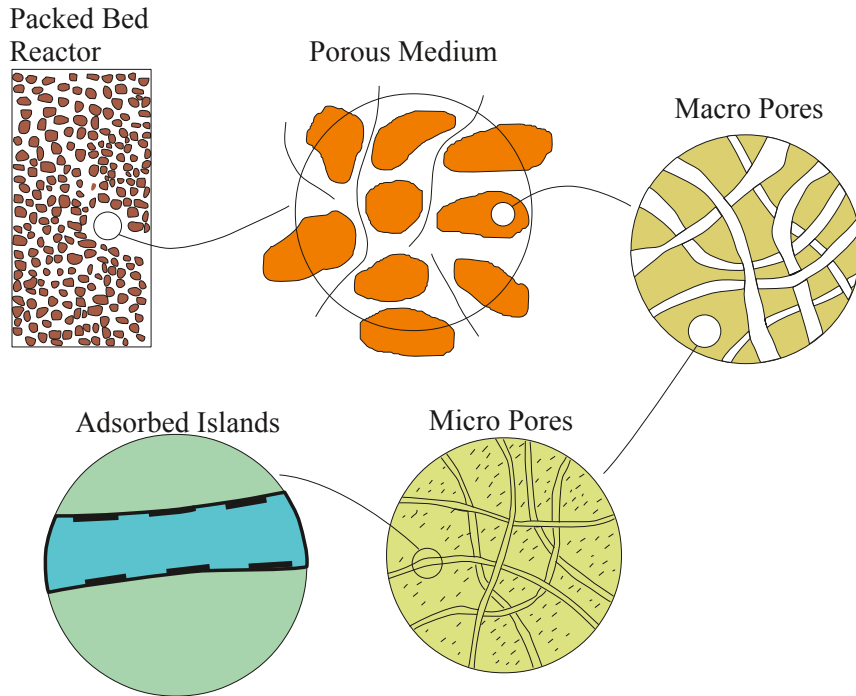
Outline (emphasis on some *theoretical aspects*)

- Introduction: background, multiple-scale, averaging
- One-Phase Flows
 - Phenomenology: Departure from Darcy's law, Weak inertia regimes, Strong Inertia regimes, Transitions, Turbulence (pore-scale or macro-scale?)
 - Macro-scale models?
- Two-Phase Flows:
 - theoretical framework and specificity for HPPM
 - several models for dynamic flows:
 - Models with phase interaction
 - Dynamic PNM
 - Phase splitting: application to structured porous media
- Conclusions



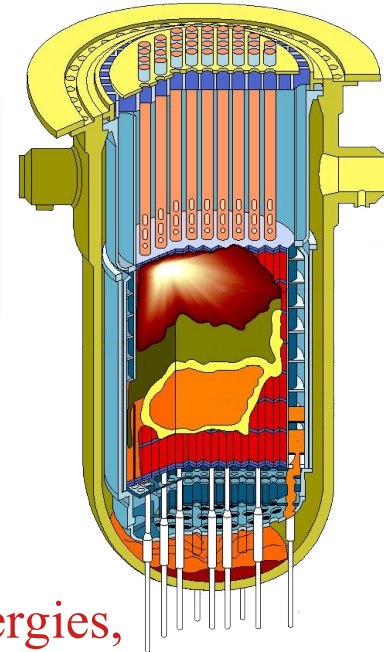
Examples of HPPM:

Structured and Packed bed reactors, nuclear safety, fractured media, karsts, ...



$$Re = \frac{\rho_r U_r \sqrt{k}}{\mu_r} > 1$$

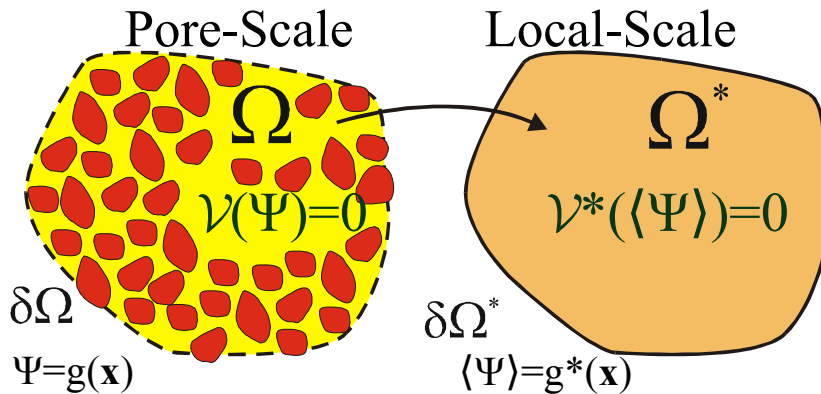
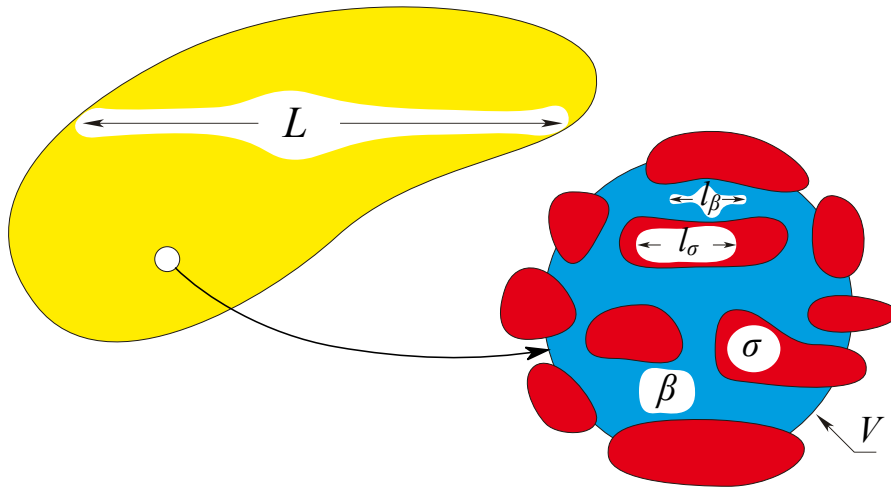
as well as important Ca and Bo numbers



Financial support from Air Liquide, IFPen, IRSN, TotalEnergies,



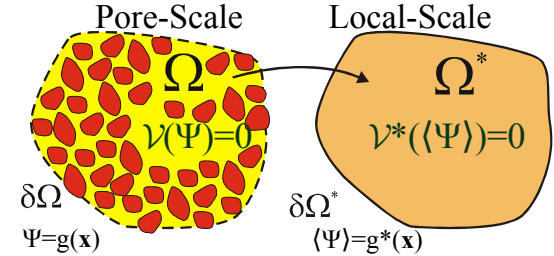
Upscaling?



- Separation of scales:
 - $l_\beta, l_\sigma \ll L$ *or not!*
- If seeking a macro-scale theory?
 - Smoothing “operator” → macro-scale equations and BCs?
 - Link between micro- and macro-scale?
 - Effective properties?
- Different techniques
- Different types of models: 1-Eq, mixed models, N-Eqs., etc...



Upscaling: different point of views



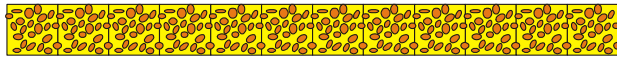
- **Heuristic: Darcy's law (1856)!**
- **Upscaling with *closure*: homogenization theory (Sanchez-Palencia, Bensoussans et al.,...), volume averaging (Whitaker, ... and variants),**

$$p_\beta = \langle p_\beta \rangle^\beta + \tilde{p}_\beta \quad \tilde{p}_\beta \stackrel{?}{=} f \left(\langle p_\beta \rangle^\beta, \nabla \langle p_\beta \rangle^\beta, \dots \right)$$

- **Stochastic theories (Matheron, Dagan, Gelhar, ...), ...**
- **Mixture theories: volume averaging + irreversible thermodynamics (Marle, Hassanizadeh and Gray, Bowen, ...)**
- **Other point of views....: dual-phase-lagging heat conduction (Wang et al., 2008; Vadasz, 2005...); mixed models; fractional derivatives (Néel,...); CTRW; ...**



Different Model Types



DNS



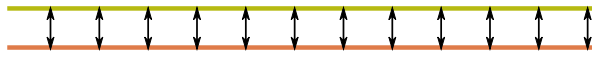
meso-scale Network model



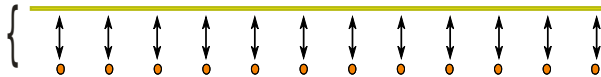
1-eq local equilibrium



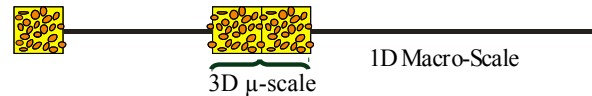
1-eq non-eq: convolution,
asympt. 2-eq, frac. deriv.,
wave eq., CTRW,...



2-equation, N-equation (multi-
rate, ...)



Mixed or Hybrid models



Mixed or Hybrid models
for fronts, entrance regions



Mixed or Hybrid Network
model (PNM+pore-scale VOF)



Mixed or Hybrid Network
model (PNM+Darcy-scale)

HPPM: a class of largely
open problems



This talk: suggestion of
possible routes



One-Phase Flow as an example of highly non-linear problem

- **Pore-scale equation** $\nabla \cdot \mathbf{v}_\beta = 0$

$$\rho_\beta \frac{\partial \mathbf{v}_\beta}{\partial t} + \rho_\beta \mathbf{v}_\beta \cdot \nabla \mathbf{v}_\beta = -\nabla p_\beta + \rho_\beta \mathbf{g} + \mu_\beta \nabla^2 \mathbf{v}_\beta \quad \text{B.C.1 } \mathbf{v}_\beta = 0 \quad \text{at } A_{\beta\sigma}$$

$$\text{Re} = \frac{\rho_\beta U_r \ell_\beta}{\mu_\beta}; p_\beta^c = \frac{p_\beta \ell_\beta}{\mu_\beta U_r}; \text{Fr} = \frac{U_r}{\sqrt{\ell_\beta g}} \Rightarrow \text{Re} \left(\frac{\partial \mathbf{v}'_l}{\partial t'} + \mathbf{v}'_l \cdot \nabla' \mathbf{v}'_l \right) = -\nabla' p_l^c + \frac{\text{Re}}{\text{Fr}^2} \frac{\mathbf{g}}{g} + \nabla'^2 \mathbf{v}'_l$$

- **Pore-Scale regimes as a function of Re**

- **Creeping (Re → 0): leads to Darcy's law**

- **Laminar**

- **Turbulent**

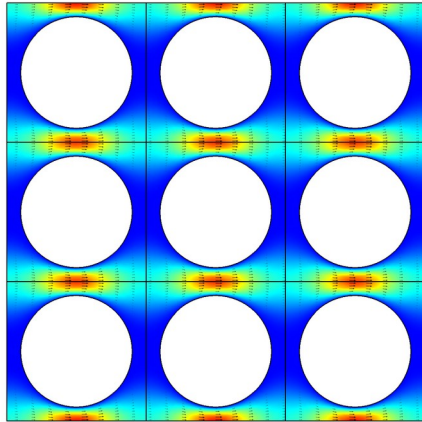


Various regimes and transitions, impact of subcritical and supercritical instabilities → which macro-scale model?



The linear (Stokes) problem

Re~0

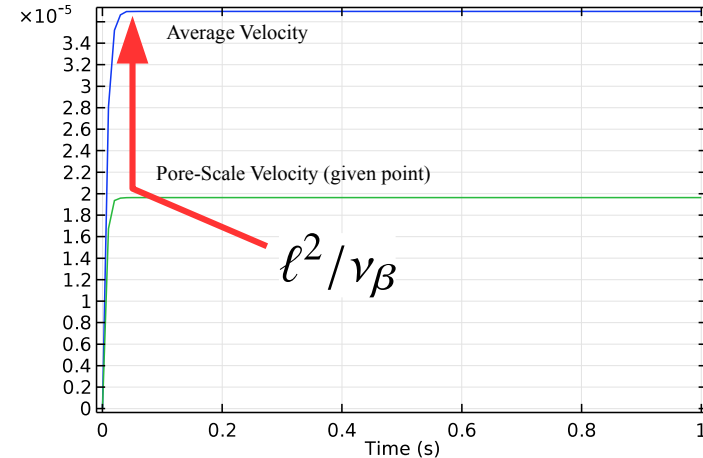


$$0 = -\nabla \tilde{p}_\beta - \mathbf{h} + \mu_\beta \nabla^2 \mathbf{v}_\beta$$

$$\mathbf{h} = \nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g}$$

$$p_\beta = \langle p_\beta \rangle^\beta + \tilde{p}_\beta$$

$$\mathbf{v}_\beta = \langle \mathbf{v}_\beta \rangle^\beta + \tilde{\mathbf{v}}_\beta$$



Localized problem → nearly constant averaged velocity and gradient of intrinsic pressure over UC/REV (if far from boundaries)

Quasi-steady flow, Brinkman terms discarded

$$0 = -\varepsilon_\beta \nabla \langle p_\beta \rangle^\beta + \varepsilon_\beta \rho_\beta \mathbf{g} + \mu_\beta \nabla^2 \langle \mathbf{v}_\beta \rangle^\beta - \mu_\beta \nabla \varepsilon_\beta \cdot \nabla \langle \mathbf{v}_\beta \rangle^\beta$$

$$+ \frac{1}{\nu} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\tilde{p}_\beta \mathbf{I} + \mu_\beta \nabla \tilde{\mathbf{v}}_\beta) dA$$

\swarrow $O\left(\frac{\langle v_\beta \rangle^\beta}{\ell^2}\right)$ \swarrow $O\left(\frac{\langle v_\beta \rangle^\beta}{L^2}\right)$



Closure and Macro-Scale Equation (Darcy regime)

thanks to linearity:

$$\begin{aligned}\tilde{p}_\beta &= \mu_\beta \mathbf{b} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \dots \\ \tilde{\mathbf{v}} &= \mathbf{B} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \dots\end{aligned}$$

$$\begin{aligned}\nabla \cdot \mathbf{B} &= 0 \\ -\nabla \mathbf{b} + \nabla^2 \mathbf{B} &= \varepsilon_\beta^{-1} \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\mathbf{I} \mathbf{b} + \nabla \mathbf{B}) dA\end{aligned}$$

$$\mathbf{B} = -\mathbf{I} \quad \text{at } A_{\beta\sigma}, \quad \langle \mathbf{b} \rangle^\beta = 0$$

$$\mathbf{b}(\mathbf{r} + \ell_i) = \mathbf{b}(\mathbf{r}) \quad \mathbf{B}(\mathbf{r} + \ell_i) = \mathbf{B}(\mathbf{r})$$

$$\langle \mathbf{v}_\beta \rangle = -\frac{1}{\mu_\beta} \mathbf{K} \cdot \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right)$$

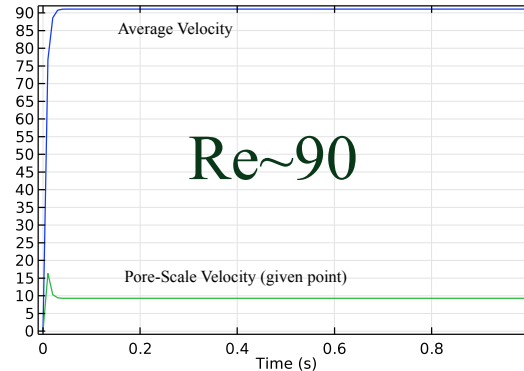
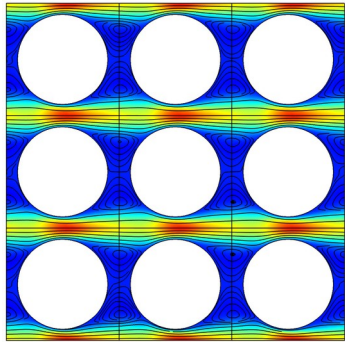
$$\mathbf{K}^{-1} = -\varepsilon_\beta^{-2} \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\mathbf{I} \mathbf{b} + \nabla \mathbf{B}) dA$$

\mathbf{K} intrinsic permeability

See Sanchez-Palencia (homogenization), Whitaker, ...



Laminar Inertial



$$\rho_\beta \frac{\partial \mathbf{v}_\beta}{\partial t} + \rho_\beta \mathbf{v}_\beta \cdot \nabla \mathbf{v}_\beta = -\nabla \tilde{p}_\beta - \mathbf{h} + \mu_\beta \nabla^2 \mathbf{v}_\beta$$

Still localized flow pattern?

If yes, non-linear relationship between average velocity and pressure drop!

~~$$\begin{aligned} \tilde{p}_\beta &= \mu_\beta \mathbf{b} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \dots \\ \tilde{\mathbf{v}} &= \mathbf{B} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \dots \end{aligned}$$~~

\Rightarrow

$$\langle \mathbf{v}_\beta \rangle = -\frac{1}{\mu_\beta} \mathbf{K}_{app} \cdot \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right)$$

where f , \mathbf{P} (rotation matrix) depend on

$$\mathbf{K}_{app} = \frac{1}{1+f} \mathbf{P} \cdot \mathbf{K}$$

$$\left(\left\| \nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right\|, \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right) / \left\| \nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right\| \right)$$



Models for all Non Darcy regimes

Re definition? Still a heated debate!

- **Heuristic: Forchheimer, Ergun, ...**

- **Upscaling? If localized flow!**

generalized Forchheimer eq.

$$0 = -\nabla \langle p_\beta \rangle^\beta + \rho_\beta \mathbf{g} - \mu_\beta \mathbf{K}_{app}^{-1} \cdot \langle \mathbf{v}_\beta \rangle \quad \Rightarrow \quad 0 = -\nabla \langle p_\beta \rangle^\beta + \rho_\beta \mathbf{g} - \mu_\beta \mathbf{K}^{-1} \cdot \langle \mathbf{v}_\beta \rangle - \mathbf{F}(\langle \mathbf{v}_\beta \rangle) \cdot \langle \mathbf{v}_\beta \rangle$$

(variants: modified Navier-Stokes equations)

- **How to check for localization? DNS, stability analysis...**

- **Bifurcations depends on Re and number of UC (Aagnaou et al., 2016)...and topology! → REV size = $f(\langle \mathbf{v}_\beta \rangle^\beta)$**

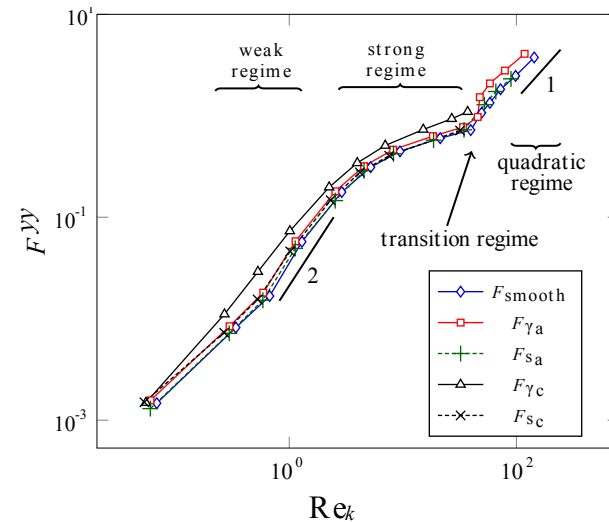
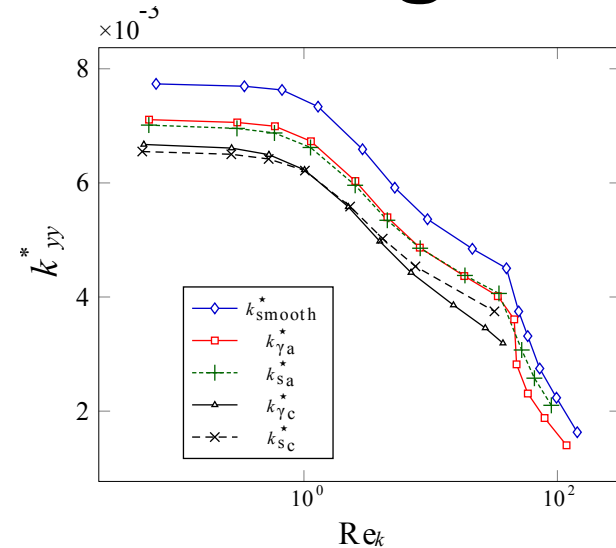
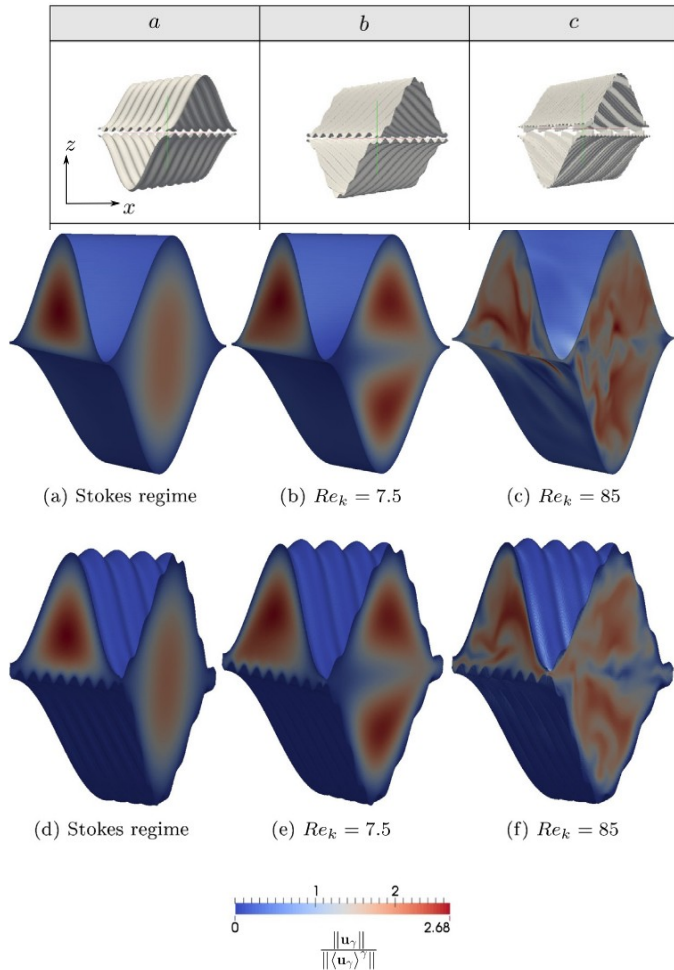
- **Localized turbulence (nearly periodic over N-UC) up to large Re numbers (Jin et al., 2015) need spatial & time average $\overline{\langle \mathbf{v}_\beta \rangle}$**

- **Not necessarily true in entrance regions (D'Hueppe et al., ...) → macro-scale turbulence models?**



Example for Structured Packings

Pasquier et al., 2017



Summary of Models for Non Darcy regimes ($Re > 1$)

- $Re \rightarrow 0$: Darcy, $F=0$, linear closure
- $Re \sim 0$: weak inertia, $F \cdot \langle v_\beta \rangle \sim \langle v_\beta \rangle^3$ (Levy, Mei & Auriault, Firdaouss, Pauthenet et al., ...), perturbation solution with respect to Re , not quantitatively significant most of the time
- $Re > 0$ (before macro-scale turbulence)
 - strong inertia, $F \cdot \langle v_\beta \rangle \sim \langle v_\beta \rangle^2$ (Lasseux et al., 2011;...), mostly if disordered media, but after *transition regimes*
 - anisotropic effect (Pauthenet et al., 2018; Qinjun et al., 2023...), necessary for structured packings, nuclear reactors, ...
- Estimating K_{app} requires heavy computations, building correlations for anisotropic effects may be complex (analytic correlations, machine learning, ...)



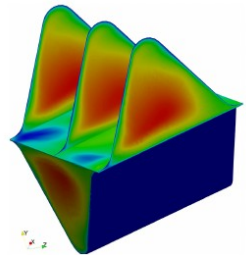
Turbulent flows in porous media ($Re \gg 1$)

see Pedras & De Lemos, Masuoka & Takatsu (1996), Nakayama & Kuwahara (1999), ...

- **Turbulence: time and spatial averaging (book De Lemos, 2006; ...)**
 - Time and spatial averaging commute!
 - Not necessarily the same result if sequential closure because of involved approximations!
 - I. $\mathbf{v}_\beta \rightarrow \langle \mathbf{v}_\beta \rangle \rightarrow \overline{\langle \mathbf{v}_\beta \rangle}$
 - II. $\mathbf{v}_\beta \rightarrow \overline{\mathbf{v}_\beta}$ (RANS, ...) $\rightarrow \langle \overline{\mathbf{v}_\beta} \rangle$
 - Scheme “II” seems preferable: contrary to Antohe & Lage (1997), Getachew et al. (2000), see discussion in Nakayama & Kuwahara (1999), Pedras and de Lemos (2001), etc...
- In general leads to a macro-scale turbulence model
- However: If localized RANS simulation, scheme II leads to a generalized Forchheimer law...

Example: structured packings (Soulaine & Quintard, 2014)

$$K_{yy}^* = \frac{K_0}{1 + \gamma_l \sqrt{Re}} \text{ (laminar)} \quad ; \quad K_{yy}^* = \frac{K_1}{1 + \beta_t Re} \text{ (turbulent)}$$



Two-Phase Flow

● Pore-scale

$$\nabla \cdot \mathbf{v}_\alpha = 0$$

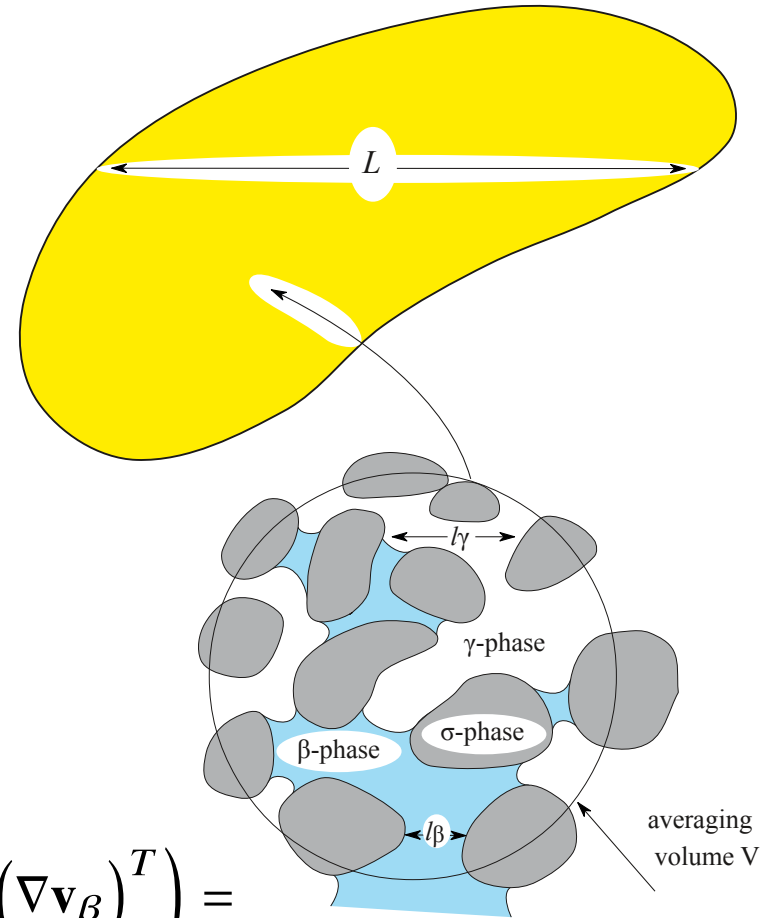
$$\frac{\partial \rho_\alpha \mathbf{v}_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha) = -\nabla p_\alpha + \rho_\alpha \mathbf{g} + \mu_\alpha \nabla^2 \mathbf{v}_\alpha \text{ in } V_\alpha \quad \alpha = \beta, \gamma$$

$$\text{B.C. 1 } \mathbf{v}_\beta = 0 \text{ at } A_{\beta\sigma}(t)$$

$$\text{B.C. 2 } \mathbf{v}_\gamma = 0 \text{ at } A_{\gamma\sigma}(t)$$

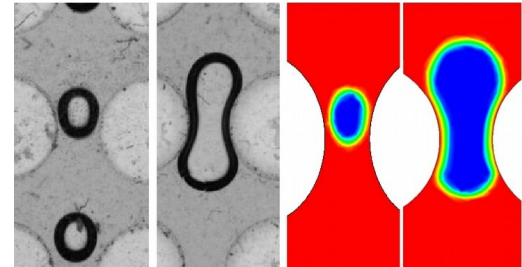
$$\text{B.C. 3 } \mathbf{v}_\beta = \mathbf{v}_\gamma \text{ at } A_{\beta\gamma}(t)$$

$$\begin{aligned} \text{B.C. 4} \quad & -\mathbf{n}_{\beta\gamma} p_\beta + \mu_\beta \mathbf{n}_{\beta\gamma} \cdot \left(\nabla \mathbf{v}_\beta + (\nabla \mathbf{v}_\beta)^T \right) = \\ & -\mathbf{n}_{\beta\gamma} p_\gamma + \mu_\gamma \mathbf{n}_{\beta\gamma} \cdot \left(\nabla \mathbf{v}_\gamma + (\nabla \mathbf{v}_\gamma)^T \right) + 2\sigma H_{\beta\gamma} \mathbf{n}_{\beta\gamma} \text{ at } A_{\beta\gamma}(t) \end{aligned}$$

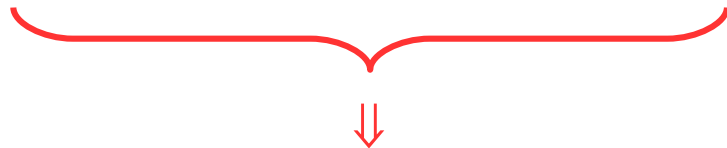


Phenomenology for HPPM: potentially unsteady flows

- Front position is in general time dependent!
- Specific features: Haines jumps, snap-off, ...
- Boiling, turbulence, ...

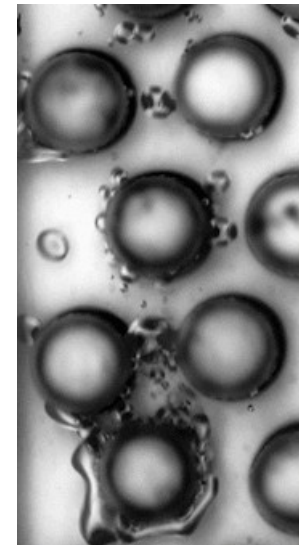


Horgue et al.



- **Common practice: quasi-static approximation...** $\langle \phi \rangle$ and not $\overline{\langle \phi \rangle}$

Justification: Ergodicity (not validated)?



See paper
Gourbil et al.

Sapin et al., 2016



Upscaling: quasi-static theory

Whitaker, 1986; Auriault, 1987; Lasseux et al., 1996; ...

- $A_{\beta\gamma}(t) \rightarrow$ known steady-state position
- Momentum eqs $\rightarrow \sim 2$ flow problems
- Interaction between phases: Case of B.C. 4

$$\mathbf{n}_{\beta\gamma} (P_\gamma|_{\mathbf{x}} - P_\beta|_{\mathbf{x}}) + \mathbf{n}_{\beta\gamma} \mathbf{y} \cdot \left((\nabla P_\gamma|_{\mathbf{x}} - \rho_\gamma \mathbf{g}) - (\nabla P_\beta|_{\mathbf{x}} - \rho_\beta \mathbf{g}) \right) + \mathbf{n}_{\beta\gamma} \mathbf{y} \cdot (\rho_\gamma - \rho_\beta) \mathbf{g} + \dots = -\mathbf{n}_{\beta\gamma} (\tilde{p}_\gamma - \tilde{p}_\beta) + \mu_\gamma \mathbf{n}_{\beta\gamma} \cdot (\nabla \mathbf{v}_\gamma + (\nabla \mathbf{v}_\gamma)^T) - \mu_\beta \mathbf{n}_{\beta\gamma} \cdot (\nabla \mathbf{v}_\beta + (\nabla \mathbf{v}_\beta)^T) + 2\sigma H_{\beta\gamma} \mathbf{n}_{\beta\gamma} \text{ at } A_{\beta\gamma}$$

$$\text{Ca} = \frac{\mu_r U_r}{\sigma}$$

$$\text{Bo} = \frac{|(\rho_\beta - \rho_\gamma) g| r_0^2}{\sigma}$$

+ Re, (We=Re×Ca) numbers

+ *Dynamic* Bond number

} If $\approx 0 \Rightarrow$

$$P_\gamma|_{\mathbf{x}} - P_\beta|_{\mathbf{x}} = 2\sigma H_{\beta\gamma}$$

$H_{\beta\gamma} =$ Constant over REV

i.e., the classical capillary pressure theory!



Macro-Scale Models : Quasi-Static

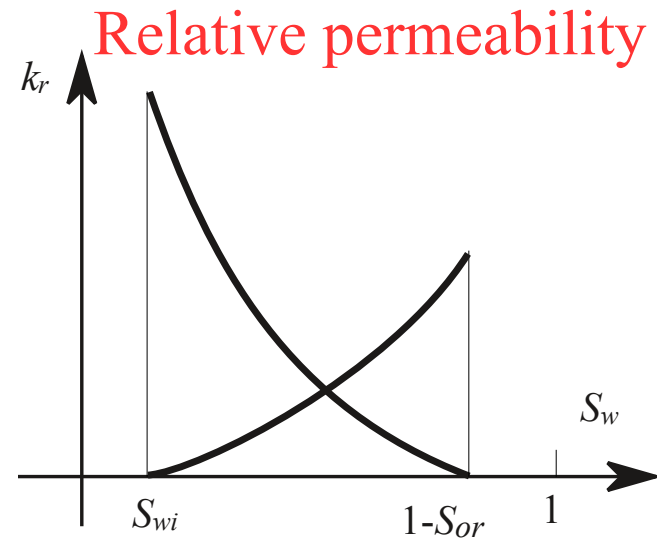
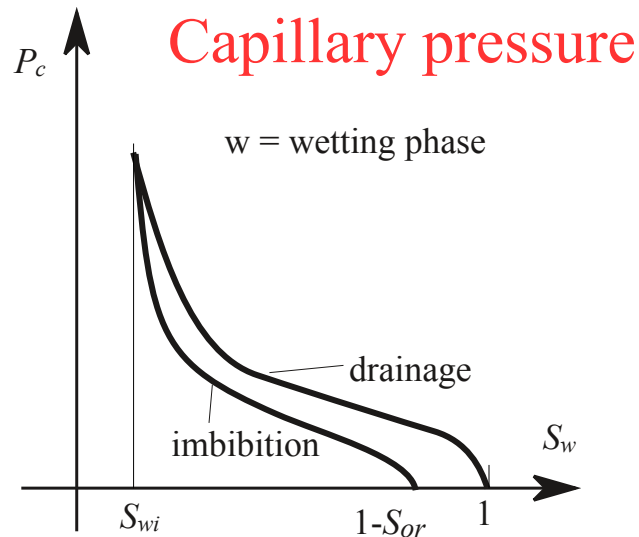
$$\mathbf{V}_\alpha = \langle \mathbf{v}_\alpha \rangle ; P_\alpha = \langle p_\alpha \rangle^\alpha ; \varepsilon_\alpha = \varepsilon S_\alpha \quad \alpha = \beta, \gamma$$

- **Heuristic (Muskat): generalized Darcy's laws**

$$\frac{\partial \varepsilon S_\alpha}{\partial t} + \nabla \cdot \mathbf{V}_\alpha = 0 ; \mathbf{V}_\alpha = -\frac{1}{\mu_\alpha} \mathbf{K}_\alpha \cdot (\nabla P_\alpha - \rho_\alpha \mathbf{g})$$

$$P_\gamma - P_\beta = P_c(S_\beta)$$

$$\mathbf{K}_\gamma = \mathbf{K} k_{r\gamma}(S_\gamma)$$



Macro-Scale Models : Quasi-Static, viscous coupling

- Model with viscous coupling (upscaling with heuristic parts ☺ ,...)

(Ex. : Whitaker, 1986; ...)

no real closure, quasi-static with known interface position, mapping legitimacy?

$$\left\{ \begin{array}{l} \tilde{\mathbf{v}}_\alpha = \mathbf{B}_{\alpha\beta} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \mathbf{B}_{\alpha\gamma} \cdot \langle \mathbf{v}_\gamma \rangle^\gamma \\ \tilde{p}_\alpha = \mu_\alpha \left(\mathbf{b}_\alpha \cdot \langle \mathbf{v}_\beta \rangle^\beta + \mathbf{b}_{\alpha\gamma} \cdot \langle \mathbf{v}_\gamma \rangle^\gamma \right) \end{array} \right. \quad \alpha = \beta, \gamma$$

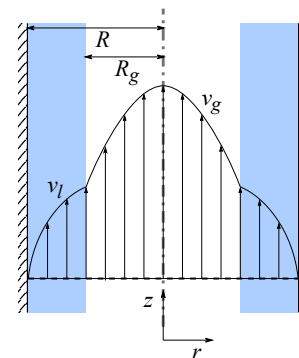
$$\mathbf{V}_\alpha = -\frac{1}{\mu_\alpha} \mathbf{K}_\alpha \cdot (\nabla P_\alpha - \rho_\alpha \mathbf{g}) + \mathbf{K}_{\alpha\kappa} \cdot \mathbf{V}_\kappa \quad \alpha, \kappa = \beta, \gamma \quad \alpha \neq \kappa$$

Phase interaction ↗

Ex. : Two-Phase Poiseuille Flow (often used for identification)

$$K_{ll} \approx K \alpha^2 \quad K_{lg} \approx \frac{\mu_g}{\mu_l} \frac{(1-\alpha)^2}{\alpha} \quad \frac{\mu_g}{\mu_l} \rightarrow 0$$

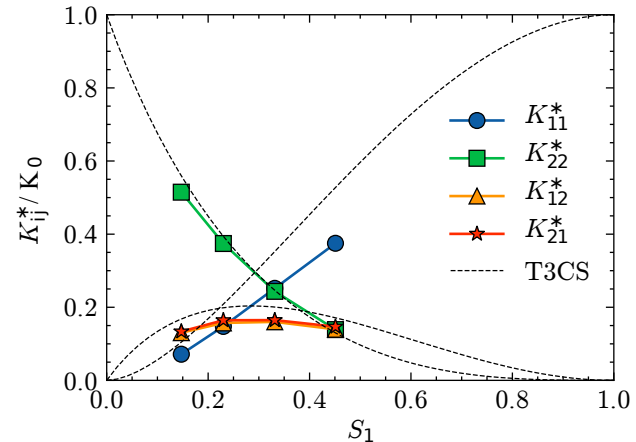
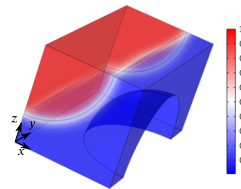
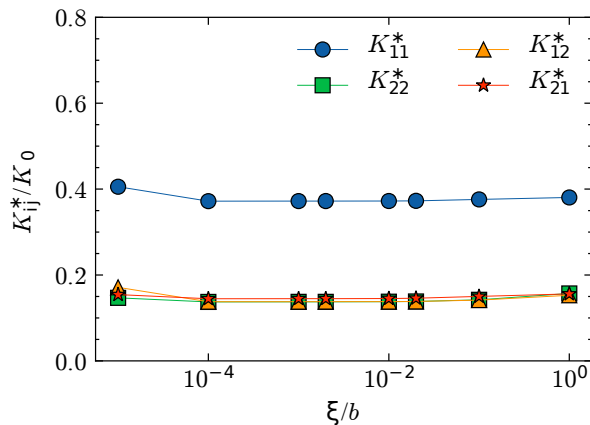
$$K_{gg} \approx K \alpha^2 \quad K_{gl} \approx \frac{\alpha}{1-\alpha} \quad \alpha = S_\gamma$$



Estimation of coupling terms: from DNS, or possibly experiments

- **FoP: Identification through the Force Perturbation technique (Li et al., 2005; Cochenec et al., 2022)**

$$\begin{pmatrix} \mathbf{V}_1 \\ \mathbf{V}_2 \end{pmatrix} = \begin{pmatrix} \frac{K_{11}^*}{\mu_1} & \frac{K_{21}^*}{\mu_1} \\ \frac{K_{12}^*}{\mu_2} & \frac{K_{22}^*}{\mu_2} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{pmatrix}, \text{ with (1): } \mathbf{b} = \mathbf{b}_1 = \mathbf{b}_2 \text{ and (2): } \mathbf{b}_1 = \mathbf{b}_2 + \xi = \mathbf{b} + \xi$$



- **Discussion about discrepancies with original “closure problems” → proposed correction for BCs in “closure” problems**



Inertia Effects and Phase Coupling in Macro-scale models

- Ergun (Heuristic): no-phase interaction terms

$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta \frac{1}{K k_{r\beta}} \mathbf{V}_\beta - \frac{\rho_\beta}{\eta \eta_\beta} \|\mathbf{V}_\beta\| \mathbf{V}_\beta$$

- Schulenberg and Muler (1987) (Heuristic and )

Similar to theory for fluidized beds

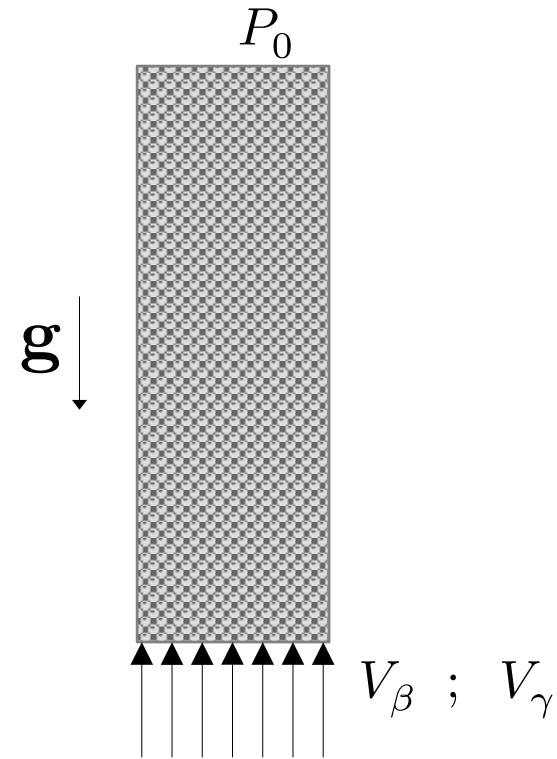
$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta \frac{1}{K k_{r\beta}} \mathbf{V}_\beta - \frac{\rho_\beta}{\eta \eta_\beta} \|\mathbf{V}_\beta\| \mathbf{V}_\beta + \frac{\mathbf{F}_{\beta\gamma}^S}{S_\beta}$$

- Upscaling (Lasseux et al., 2008; ...)

$$\mathbf{V}_\alpha = -\frac{1}{\mu_\alpha} \mathbf{K}_\alpha \cdot (\nabla P_\alpha - \rho_\alpha \mathbf{g}) - \mathbf{F}_{\alpha\alpha} \cdot \mathbf{V}_\alpha \\ + \mathbf{K}_{\alpha\kappa} \cdot \mathbf{V}_\kappa - \mathbf{F}_{\alpha\kappa} \cdot \mathbf{V}_\kappa \quad \alpha, \kappa = \beta, \gamma \quad \alpha \neq \kappa$$



Importance of Cross-Terms, and Non-Linear Effects



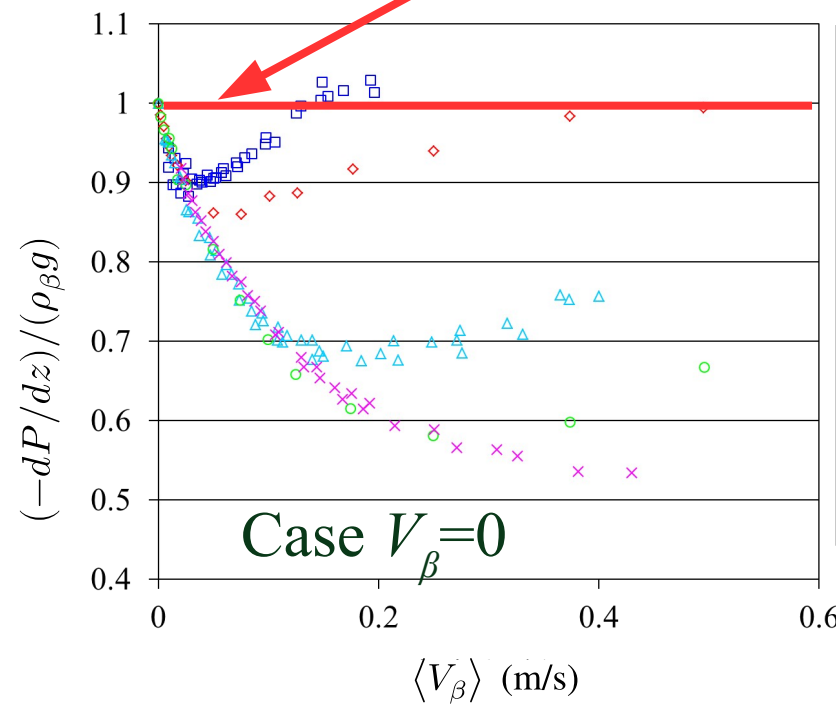
IRSN: context of nuclear reactor
severe accident

See also Taherzadeh & Saidi (2015)



Importance of Cross-Terms, and Non-Linear Effects

Models without cross-terms



$t \rightarrow \infty$

$$\left(\frac{\partial P_\beta}{\partial z} - \rho_\beta \mathbf{g} \cdot \mathbf{e}_z \right) = -\mu_\beta K_\beta^{-1} (1 + F_{\beta\beta}) V_\beta + \mu_\beta K_\beta^{-1} K_{\beta\gamma} (1 - K_{\beta\gamma}^{-1} F_{\beta\gamma}) V_\gamma$$

$$\left(\frac{\partial P_\gamma}{\partial z} - \rho_\gamma \mathbf{g} \cdot \mathbf{e}_z \right) = -\mu_\gamma K_\gamma^{-1} (1 + F_{\gamma\gamma}) V_\gamma + \mu_\gamma K_\gamma^{-1} K_{\gamma\beta} (1 - K_{\gamma\beta}^{-1} F_{\gamma\beta}) V_\beta$$

Case $V_\beta = 0$:

$$\left(\frac{\partial P_\beta}{\partial z} - \rho_\beta \mathbf{g} \cdot \mathbf{e}_z \right) = +\mu_\beta K_\beta^{-1} K_{\beta\gamma} (1 - K_{\beta\gamma}^{-1} F_{\beta\gamma}) V_\gamma$$

from Clavier et al. (2015), Chikhi et al. (2016)

see also Taherzadeh & Saidi (2015) using Tutu et al. experiments



More: Dynamic Models

- impact of $\partial S/\partial t$, V_α , a_ν ...:
 - Quintard & Whitaker (1990, from large-scale heterogeneity effects and multi-zone)
 - Hilfer (1998, multi-zone)
 - Panfilov & Panfilova (2005, meniscus)
 - Hassanizadeh and Gray (Irr. Therm., a_ν as state variable, 1993), also Kalaydjian (1987)...
 - Phase field, Cahn-Hilliard (Cueto-Felgueroso & Juanes, 2009)...



Examples of dynamic equations

- Quintard & Whitaker, 1990

$$\begin{aligned} \mathbf{V}_\beta &= -\frac{1}{\mu_\beta} \mathbf{K}_\beta^* \cdot (\nabla P_\beta - \rho_\beta \mathbf{g}) - \mathbf{u}_\beta \frac{\partial \varepsilon S_\beta}{\partial t} \\ &\quad - \mathbf{U}_\beta \cdot \nabla \frac{\partial \varepsilon S_\beta}{\partial t} - \frac{1}{\mu_\beta} \mathbf{M}_\beta : \nabla \nabla P_\beta \\ &\quad - \frac{1}{\mu_\beta} \Phi_\beta - \frac{1}{\mu_\beta} \mathbf{R}_\beta : \nabla \Phi_\beta \\ p_c &= \mathcal{F} \left(S_\beta, (\rho_\gamma - \rho_\beta) \mathbf{g}, \nabla P_\beta, \frac{\partial \varepsilon S_\beta}{\partial t}, \dots \right) \end{aligned}$$

- Kalaydjian, Hassanizadeh & Gray,

...

$$P_\gamma - P_\beta = p_c - L_1 \frac{\partial \varepsilon S_\beta}{\partial t}$$

- ...see also Petroleum engng literature on pseudo-functions!
- Is it useful for highly permeable media?

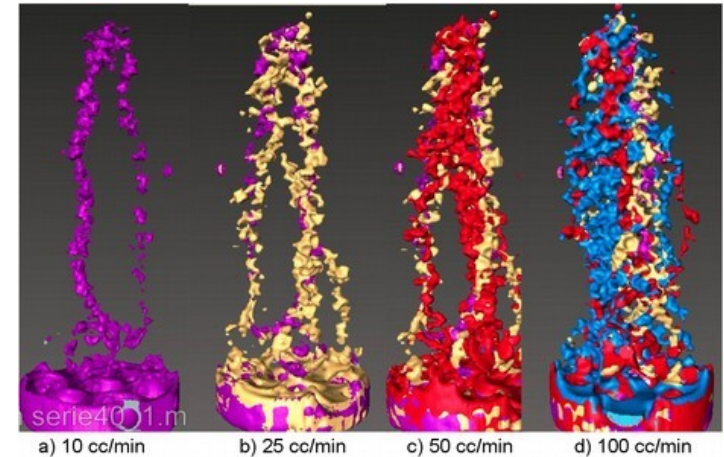


Dynamic Pore Network Models

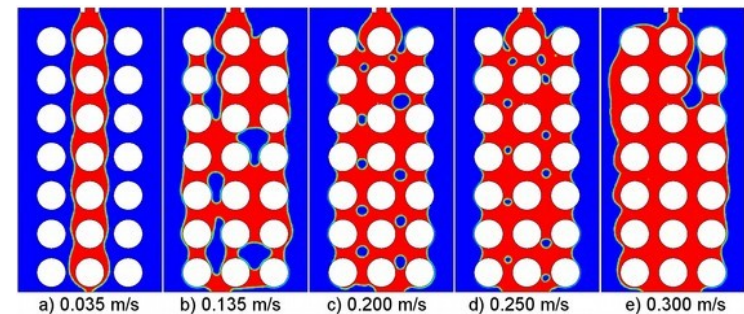
- Network models → a meso-scale representation!
- If low Re , Ca , Bo → percolation theory
- Otherwise: Coupling network model and Dynamic rules (which may come from local VOF simulations in a hybrid formulation)

Melli & Scriven, 1991; Horgue et al., 2013

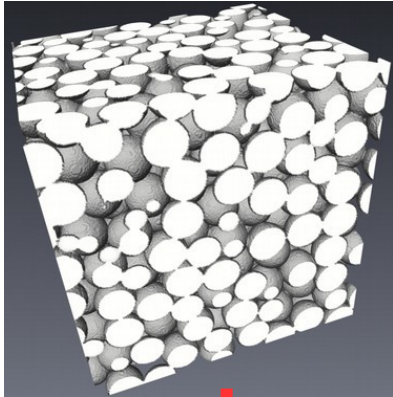
Trickle Bed (X-ray, IFP)



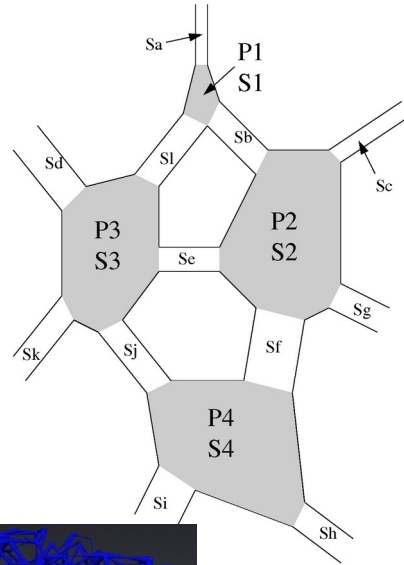
Micromodel experiments + VOF



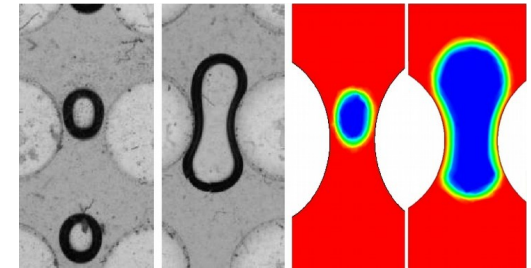
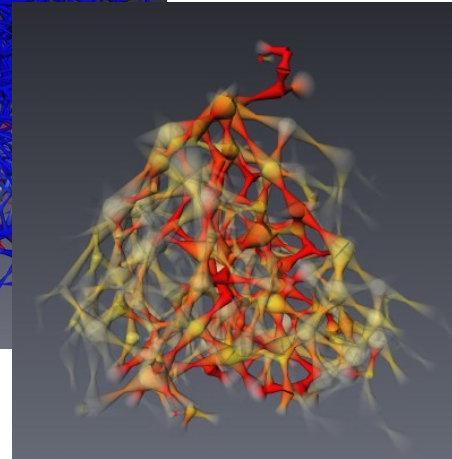
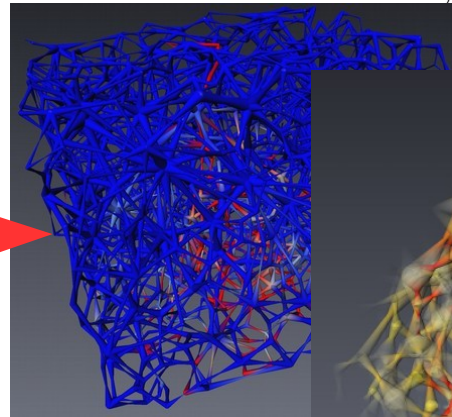
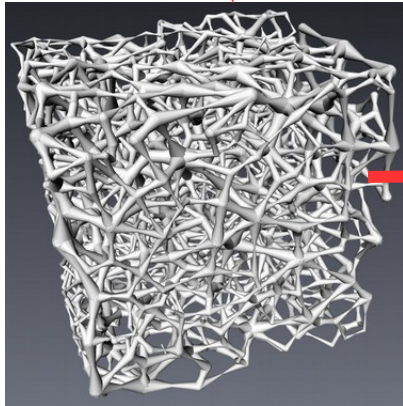
Dynamic Pore Network Models



Horgue
et al.,
2012

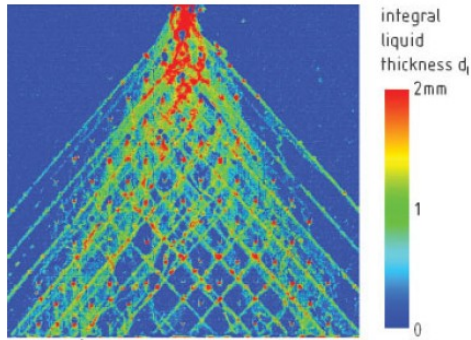


- 1.) Mass and momentum balance for the network links
- 2.) Dynamic rules coming from local VOF simulations (or from experiments) to connect links



Macro-Scale Models with Phase “Splitting”

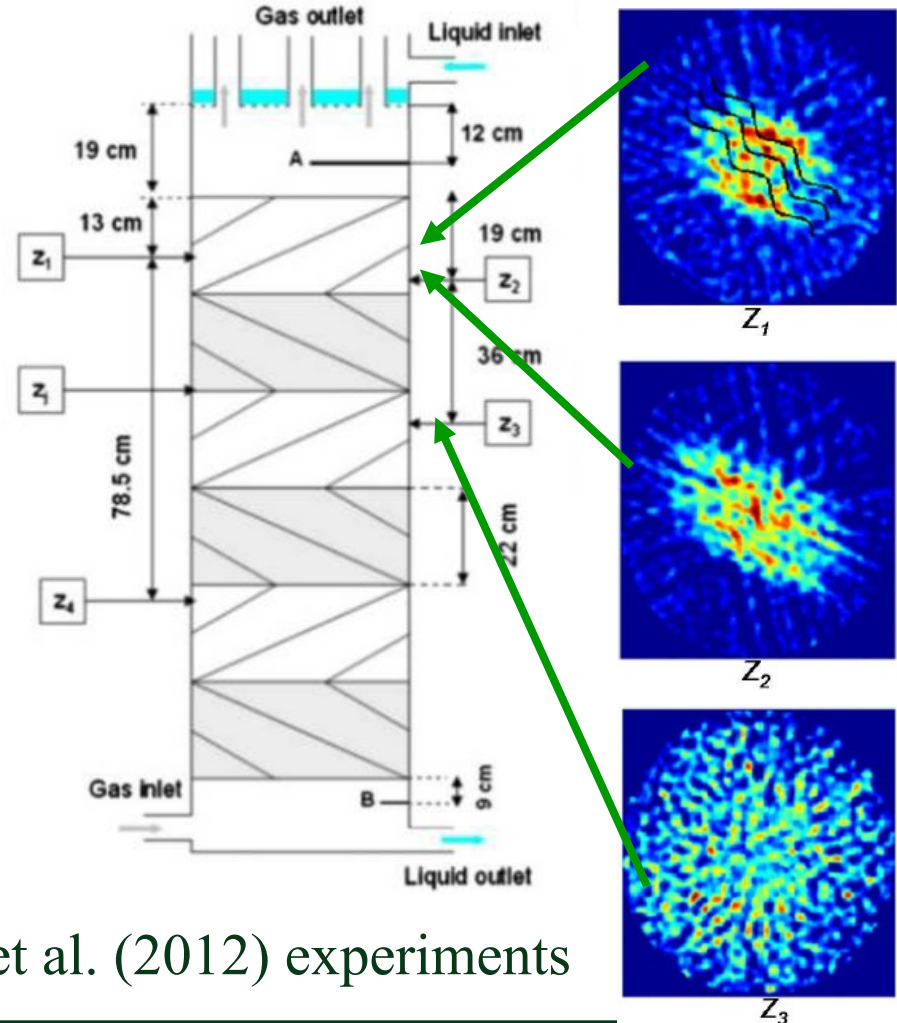
- Example: Flow through Structured Media



$$\dot{V}_l = 100 \text{ l/h, } F\text{-factor} = 0 \text{ Pa}^{\text{0.5}}$$

Mahr and Mewes (2007)

MellaPak (Sulzer Chemtech)

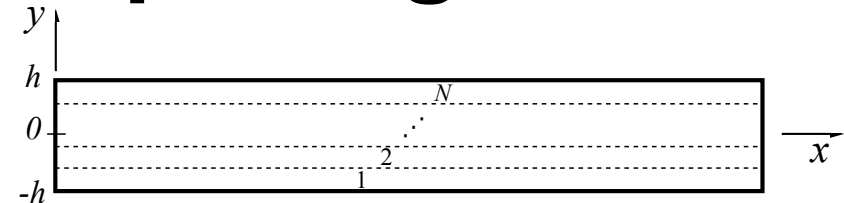


Fourati et al. (2012) experiments

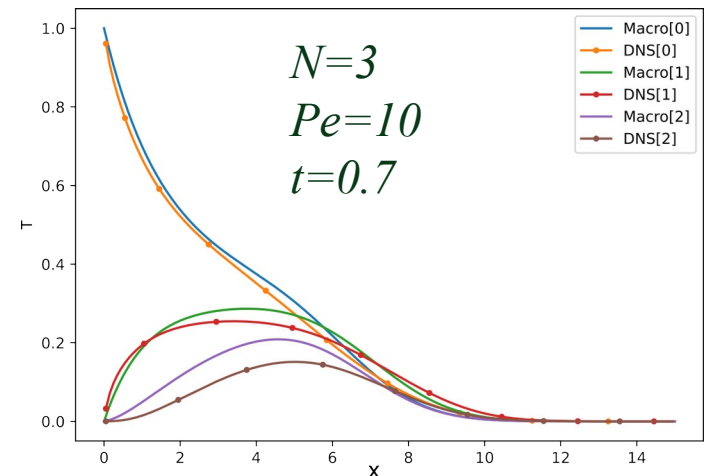
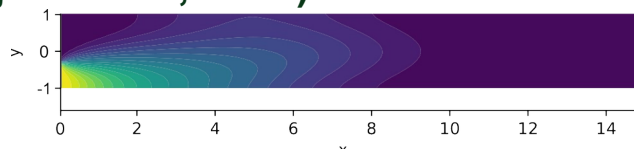


The Fundamental Idea Behind Models with Phase “Splitting”

- Same interest as N-equation models (Davit et al., 2019)
- Example: flow in a tube with spatially distributed BCs and ICs
 - 1 Eq. → complex PDE, need ~ DNS for estimating effective properties for a single set of BCs and ICs
 - Phase splitting: simple closure for large enough t , independent of BCs and ICs
 - Convergence through $N \nearrow$
 - Need to control entropy production (Bellerajoul et al., 2019)



$$\begin{pmatrix} \frac{\partial \phi_1 \mathbb{T}_1}{\partial t} \\ \vdots \\ \frac{\partial \phi_N \mathbb{T}_N}{\partial t} \end{pmatrix} + \begin{pmatrix} \phi_1 U_1 \frac{\partial \mathbb{T}_1}{\partial x} \\ \vdots \\ \phi_N U_N \frac{\partial \mathbb{T}_N}{\partial x} \end{pmatrix} + \text{Pe} [C] \begin{pmatrix} \frac{\partial \mathbb{T}_1}{\partial x} \\ \vdots \\ \frac{\partial \mathbb{T}_N}{\partial x} \end{pmatrix} = [A] \begin{pmatrix} \frac{\partial^2 \mathbb{T}_1}{\partial x^2} \\ \vdots \\ \frac{\partial^2 \mathbb{T}_N}{\partial x^2} \end{pmatrix} - [H] \begin{pmatrix} \mathbb{T}_1 \\ \vdots \\ \mathbb{T}_N \end{pmatrix}$$



Macro-Scale Models with Phase “Splitting” for Structured Packings

- $$\varepsilon \frac{\partial S_\gamma}{\partial t} + \nabla \cdot \mathbf{U}_\gamma = 0,$$

$$\varepsilon \frac{\partial S_{\beta_1}}{\partial t} + \nabla \cdot \mathbf{U}_{\beta_1} = \dot{m},$$

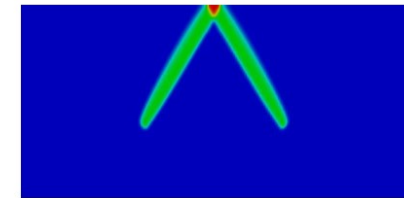
$$\varepsilon \frac{\partial S_{\beta_2}}{\partial t} + \nabla \cdot \mathbf{U}_{\beta_2} = -\dot{m}.$$

+ 3 momentum equations (e.g., generalized Darcy’s laws with cross terms)

- Comparison with Fourati et al. (2012) experiments (Soullaine et al., 2014) → calibration of exchange term on the 1st stack**

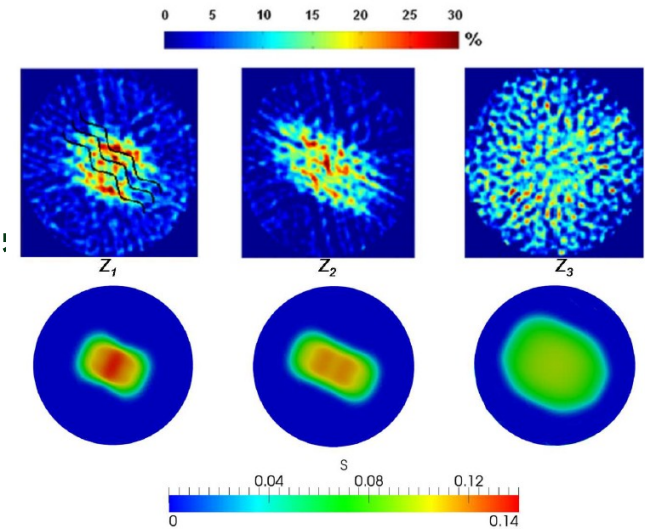
Model with liquid phase splitting:

Case with no-exchange



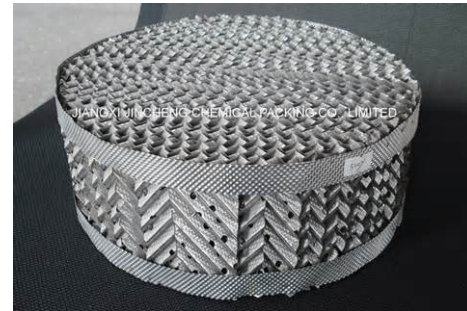
(b) t = 1 s

Case with exchange



Macro-Scale Models with Phase “Splitting”: Open Problems

- Definition of the phase separation (splitting)?
- Estimation of Effective properties?
- Effective Boundary Conditions?
 - Lateral walls
 - Between packs



Is it possible to extend theories on effective BCs (Achdou, Pironneau, Valentin, Mikelic, Aspa, Veran, Introïni, Duval, Guo, Quintard, Pasquier, Davit, ..., or strategies like Ochoa-Tapia, Goyeau, etc...) to 2-phase flows?



Conclusions

- **One-Phase Flows:**
 - Generalized Forchheimer equations → a practical model for laminar inertia regimes or localized turbulence
 - Porous Media Turbulence models?
- **Two-Phase Flows:**
 - Importance of cross-terms, Experimental determination?
 - Extensions to more dynamic flows:
 - Extended generalized Darcy's laws
 - Models with phase splitting
 - Hybrid models
 - Highly transient effects, complex time and space averaging?
- **Coupling with other transport mechanisms (dispersion, heat transfer, ...)?**

