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Transport in Porous Media

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Michel Quintard. Transport in Porous Media. École de recherche en mathématiques pour l'énergie nucléaire, Jul 2018, Roscoff, France. pp.0. hal-03656508

HAL Id: hal-03656508

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Submitted on 2 May 2022

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Quintard, Michel. Transport in Porous Media. (2018) In: École de recherche en mathématiques pour l'énergie nucléaire, 2-6 July 2018 (Roscoff, France). (Unpublished)

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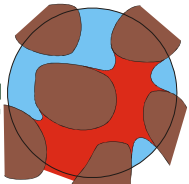
Transport in Porous Media

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Outline

- Introduction
- Multi-scale aspects
- Diffusion/dispersion
- One-Phase flow
- Heat Transfer
- Two-Phase flow
- Coupled transfers: reactive transport, phase change
- Conclusion

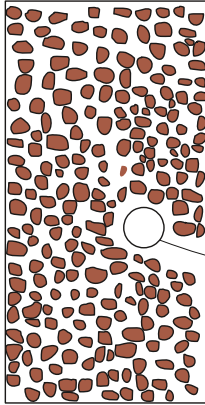


Introduction: multiple-scale analysis

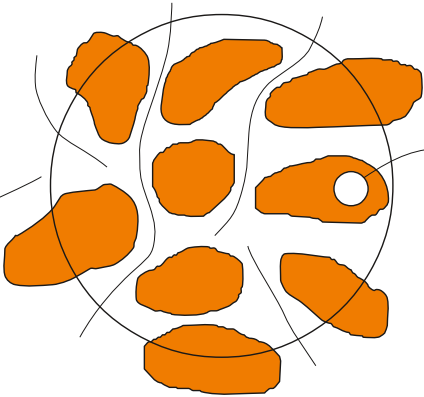


Example: Chal Engng Reactor, Heat Exchanger, ...

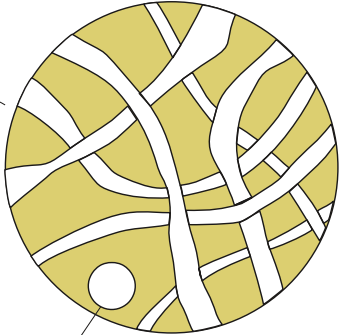
Packed Bed Reactor



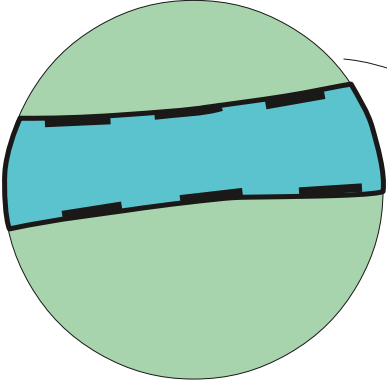
Porous Medium



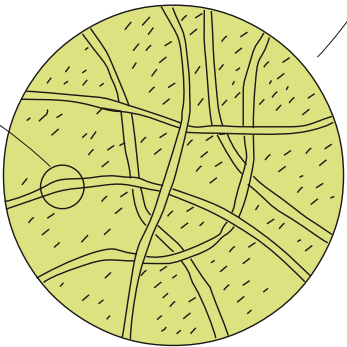
Macro Pores



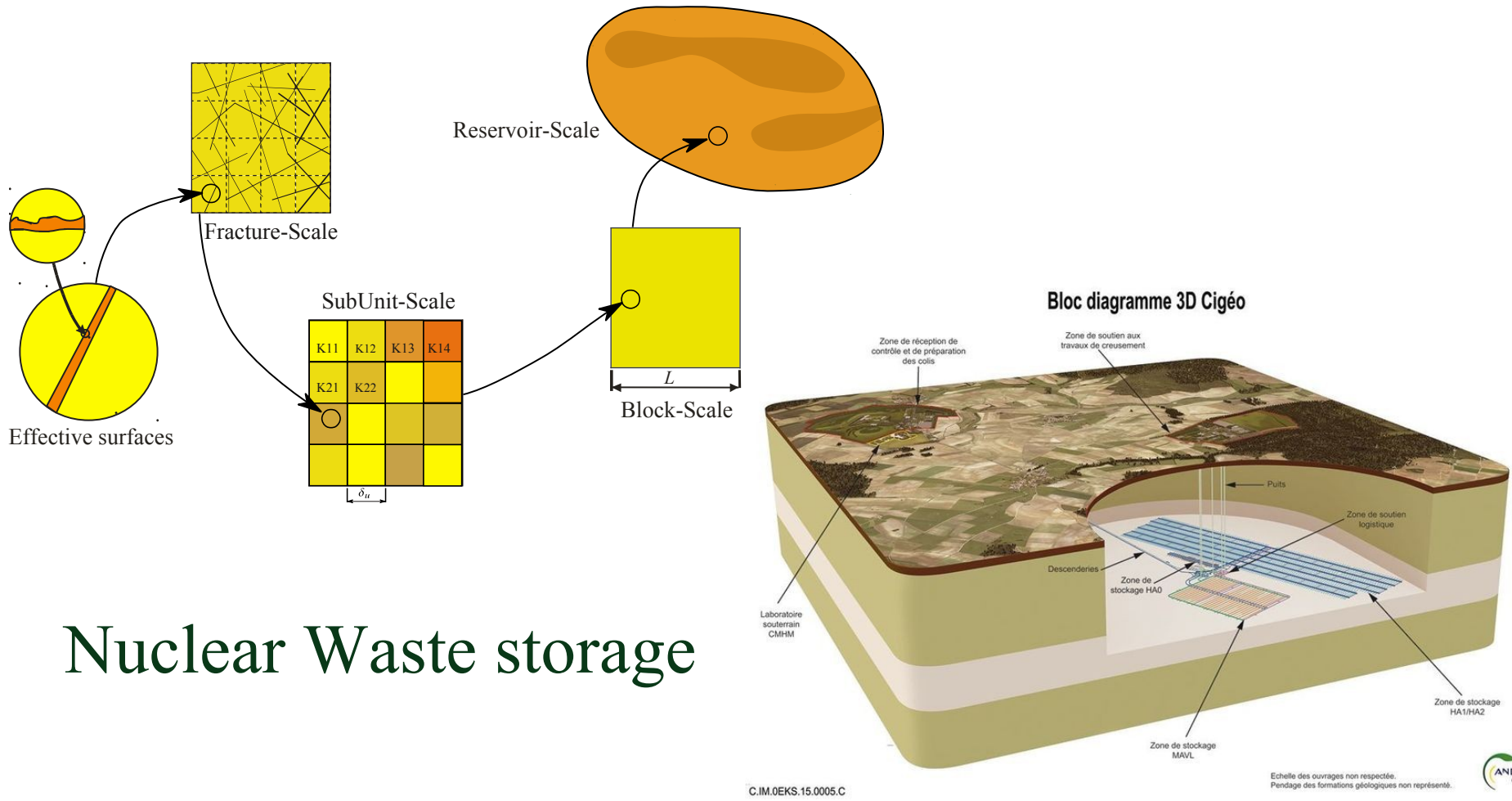
Adsorbed Islands



Micro Pores



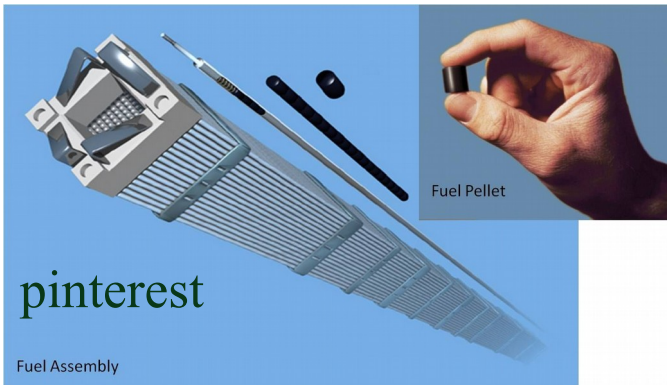
Example: geological formations



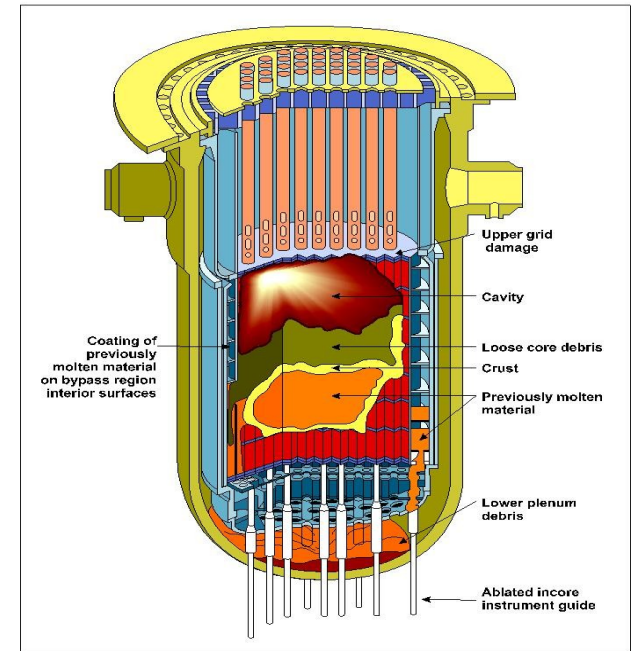
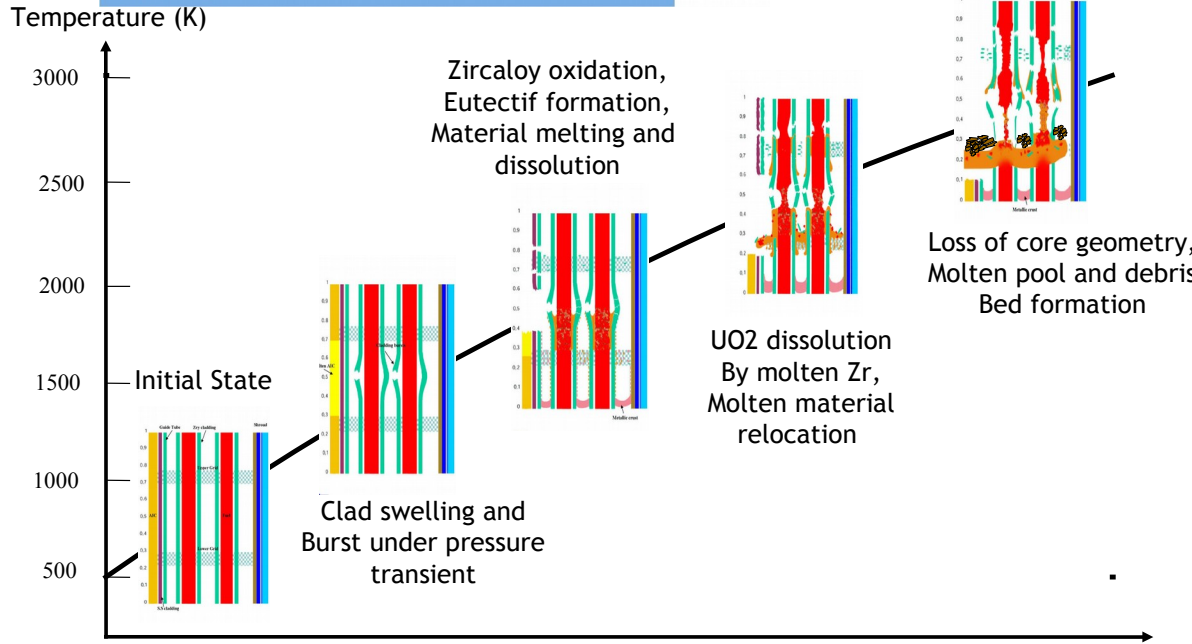
Nuclear Waste storage



Example : Nuclear Reactor



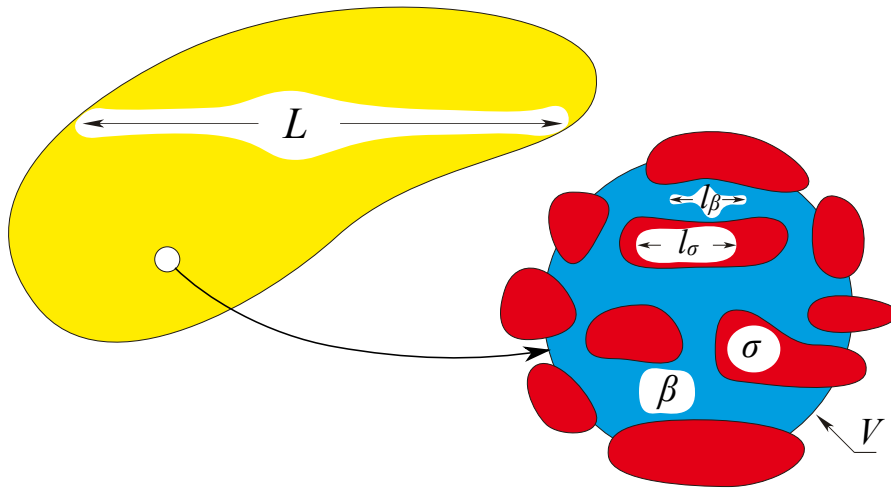
Undamaged reactor....
.... and after severe accident



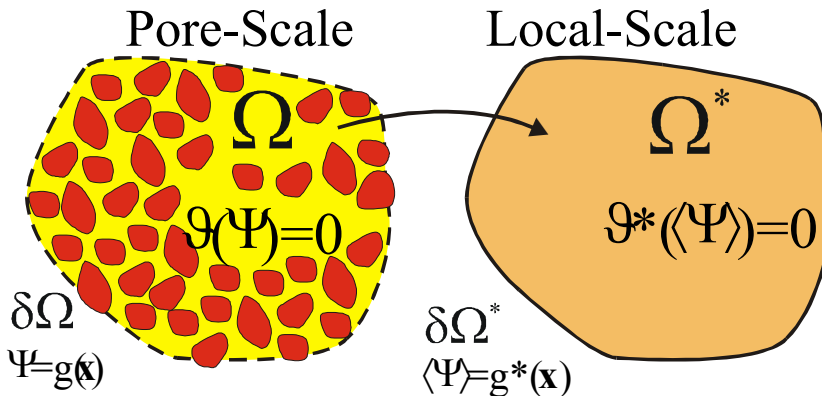
TMI-2 vessel final state



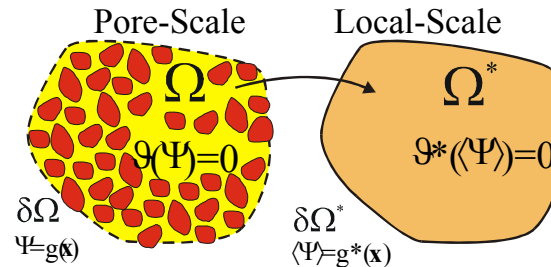
Upscaling



- Separation of scales:
 $l_\beta, l_\sigma \ll L$
- Objectives of a macro-scale theory?
 - Smoothing operator \rightarrow macro-scale equations and BCs
 - Link between micro- and macro-scale
 - Effective properties



Upscaling: different points of view

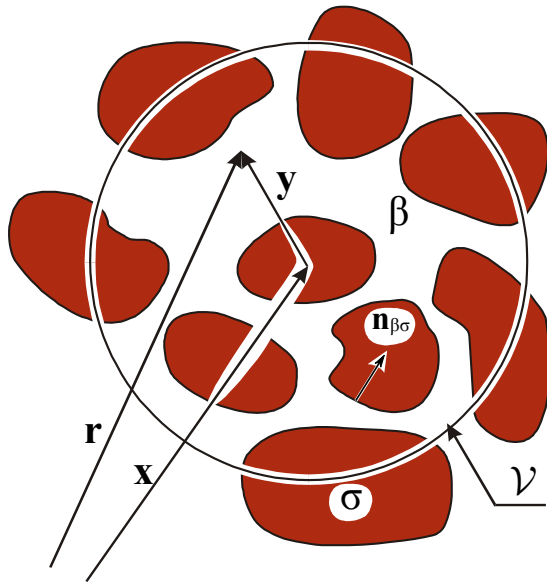


- **Heuristic: Darcy's law (1856)!**
- **Upscaling with *closure*: homogenization theory (Sanchez-Palencia, Bensoussans et al.,...), volume averaging (Whitaker, ... and variants),**

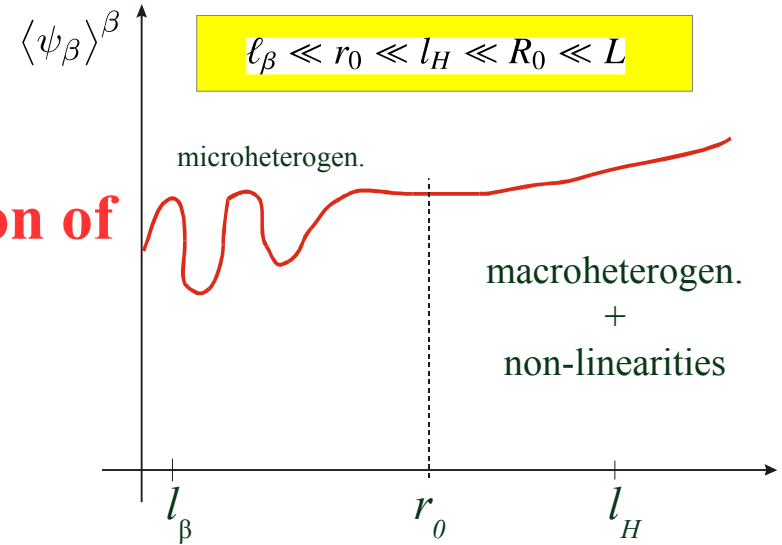
$$p_\beta = P_\beta + \tilde{p}_\beta \quad \tilde{p}_\beta \stackrel{?}{=} f(P_\beta, \nabla P_\beta, \dots)$$
- **Stochastic theories (Matheron, Dagan, Gelhar, ...), ... $P_\beta = E(p_\beta)$**
- **Mixture theories: volume averaging + irreversible thermodynamics (Marle, Hassanizadeh and Gray, Bowen, ...)**
- **Other point of views...: dual-phase-lagging heat conduction (Wang et al., 2008; Vadasz, 2005...); mixed models; fractional derivatives (Néel,...); CTRW; ...**



Macro-scale variables: Example of volume averaging



Need separation of scales!



- β -phase Volume Fraction $\varepsilon_\beta = \langle \gamma_\beta \rangle$
- $\langle \psi_\beta \rangle = \varepsilon_\beta \langle \psi_\beta \rangle^\beta$ Intrinsic phase average

$$\text{Phase indicator: } \gamma_\beta = \begin{cases} 1 & M \in V_\beta \\ 0 & M \notin V_\beta \end{cases}$$

$$\langle \psi_\beta \rangle \Big|_{\mathbf{x}} = m * \psi_\beta \approx \frac{1}{V} \int_{V_\beta} \psi_\beta(\mathbf{x} + \mathbf{y}) dV$$



Phase Indicator, Volume Fraction, Porosity, Saturation

- **Phase Indicator**

$$\gamma_{\beta} = \begin{cases} 1 & M \in V_{\beta} \\ 0 & M \notin V_{\beta} \end{cases}$$

- **Volume Fraction**

$$\varepsilon_{\beta} = \langle \gamma_{\beta} \rangle \quad \sum_{i=1}^{i=N} \varepsilon_i = 1$$

- **Porosity:** $\varepsilon = 1 - \varepsilon_{\sigma}$

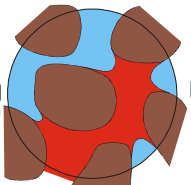
- **Saturation**

$$\varepsilon_{\beta} = \varepsilon S_{\beta} \quad \sum_{i=1}^{i=N} S_i = 1$$

$$S_{\beta} \in [0, 1]$$

- **Intrinsic phase average**

$$\langle \psi_{\beta} \rangle = \varepsilon_{\beta} \langle \psi_{\beta} \rangle^{\beta}$$



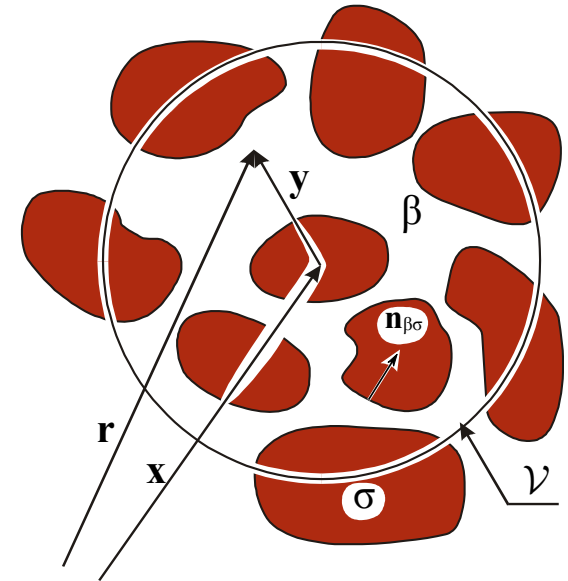
Theorems

$$\langle \nabla \psi_\beta \rangle = \nabla \langle \psi_\beta \rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \psi_\beta dA$$

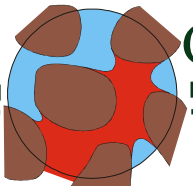
Interfacial Effects
(tortuosity,...)

$$\langle \nabla \cdot \mathbf{A}_\beta \rangle = \nabla \cdot \langle \mathbf{A}_\beta \rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{A}_\beta dA$$

$$\left\langle \frac{\partial \psi_\beta}{\partial t} \right\rangle = \frac{\partial \langle \psi_\beta \rangle}{\partial t} - \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{w}_{\beta\sigma} \psi_\beta dA$$



Phase change,
dissolution, ...



Cf: Quintard & Whitaker (Chem. Eng. Science, 93; TiPM, 94)

Total mass balance (no source/sink)

$$\frac{\partial \rho_\beta}{\partial t} + \nabla \cdot (\rho_\beta \mathbf{v}_\beta) = 0 \quad \text{pore-scale}$$

$$\frac{\partial \langle \rho_\beta \rangle}{\partial t} + \nabla \cdot \langle \rho_\beta \mathbf{v}_\beta \rangle = -\frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \rho_\beta (\mathbf{v}_\beta - \mathbf{w}_{\beta\sigma}) dA$$

macro-scale

- **Macro-scale equation, no phase change :**

$$\mathbf{V}_\beta = \langle \mathbf{v}_\beta \rangle = \varepsilon_\beta \mathbf{U}_\beta$$

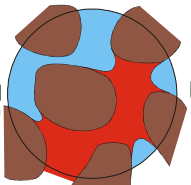
$$\frac{\partial \varepsilon_\beta \rho_\beta}{\partial t} + \nabla \cdot (\rho_\beta \mathbf{V}_\beta) = 0$$

- **Constant density**

$$\frac{\partial \varepsilon_\beta}{\partial t} + \nabla \cdot \mathbf{V}_\beta = 0$$

- **Constant porosity**

$$\nabla \cdot \mathbf{V}_\beta = 0$$



General Structure of a macro-scale transport equation

• Pore-scale

$$\frac{\partial \rho_\beta \omega_\beta}{\partial t} + \nabla \cdot (\rho_\beta \omega_\beta \mathbf{v}_\beta) = \nabla \cdot (\rho_\beta D_\beta \nabla \omega_\beta) - \underbrace{r_\beta(\omega_\beta)}_{\text{homogeneous reaction}}$$

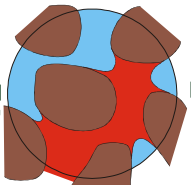
$$\text{B.C. 1} \quad \mathbf{n}_{\beta\sigma} \cdot (\rho_\beta \omega_\beta (\mathbf{v}_\beta - \mathbf{w}_{\beta\sigma}) - \rho_\beta D_\beta \nabla \omega_\beta) = \underbrace{f_\beta(\omega_\beta)}_{\text{heterogeneous reaction}}$$

• Macro-scale

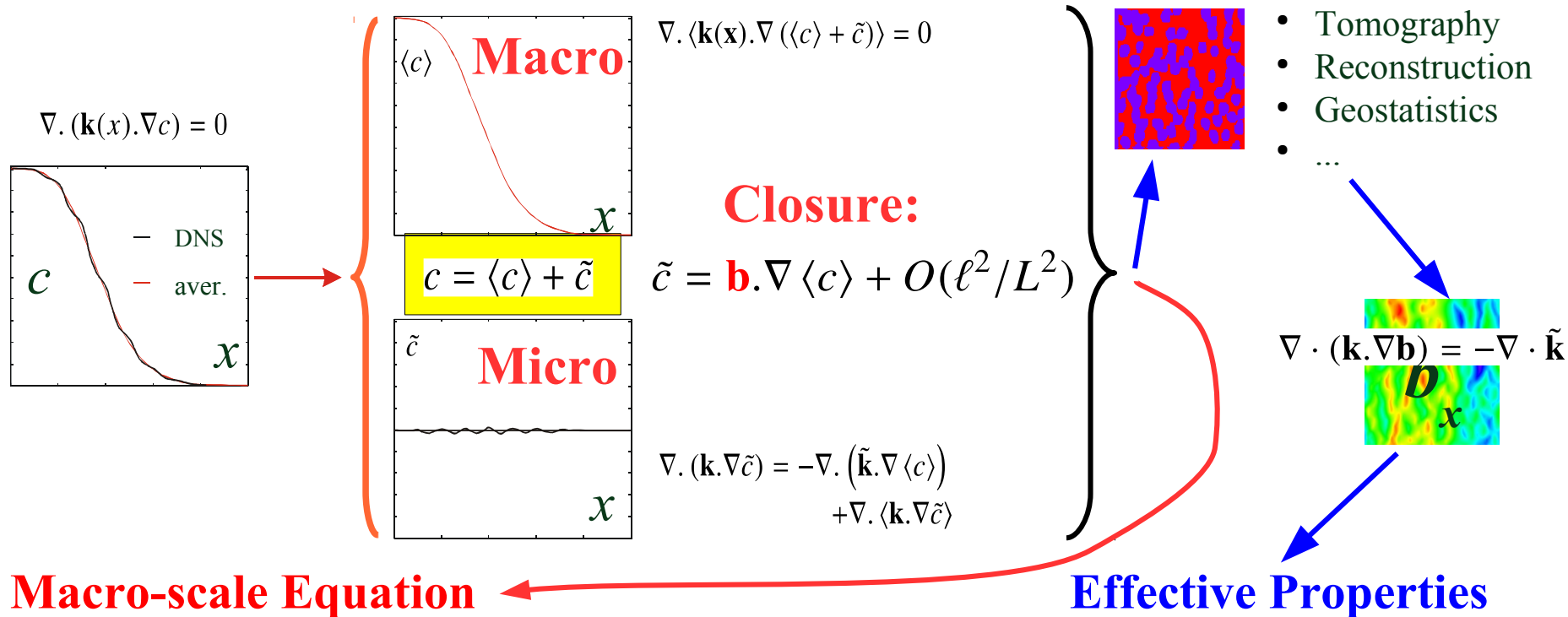
$$\frac{\partial \langle \rho_\beta \omega_\beta \rangle}{\partial t} + \nabla \cdot \langle \rho_\beta \omega_\beta \mathbf{v}_\beta \rangle = \nabla \cdot (\langle \rho_\beta D_\beta \nabla \omega_\beta \rangle) - \langle r_\beta \rangle - K_{\beta\sigma}$$

with

$$K_{\beta\sigma} = \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (\rho_\beta \omega_\beta (\mathbf{v}_\beta - \mathbf{w}_{\beta\sigma}) - \rho_\beta D_\beta \nabla \omega_\beta) dA$$



Upscaling with *closure*: a schematic view for diffusion in a heterogeneous medium



Macro-scale Equation

$$\nabla \cdot (\mathbf{K}_{eff} \cdot \nabla \langle c \rangle) = 0$$

Note: high performance computing \rightarrow up to 2048^3 voxels

Effective Properties

$$\mathbf{K}_{eff} = \langle \mathbf{k} \rangle + \langle \mathbf{k} \cdot \nabla \mathbf{b} \rangle$$



Diffusion: coupled micro-macro eqs

- **Pore-scale problem (tracer case)**

$$c_\beta = \langle c_\beta \rangle^\beta + \tilde{c}_\beta$$

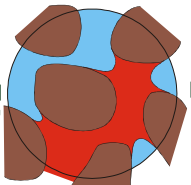
$$\frac{\partial c_\beta}{\partial t} = \nabla \cdot (D_\beta \nabla c_\beta) \rightarrow \cancel{\frac{\partial \tilde{c}_\beta}{\partial t}} = \nabla \cdot (D_\beta \nabla \tilde{c}_\beta) - \underbrace{\nabla \cdot \left(\frac{D_\beta}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{c}_\beta dA \right)}_{\text{non-local effect}}$$

simplification with $\ell_\beta \ll L$

$$\text{B.C.1 } \mathbf{n}_{\beta\sigma} \cdot D_\beta \nabla c_\beta = 0 \rightarrow \text{B.C.1 } \mathbf{n}_{\beta\sigma} \cdot \nabla \tilde{c}_\beta = -\mathbf{n}_{\beta\sigma} \cdot \nabla \langle c_\beta \rangle^\beta \text{ at } A_{\beta\sigma}$$

- **Averaged Equation**

$$\frac{\partial \varepsilon_\beta \langle c_\beta \rangle^\beta}{\partial t} = \nabla \cdot \left(\varepsilon_\beta D_\beta \nabla \langle c_\beta \rangle^\beta + \underbrace{\frac{D_\beta}{V} \int \mathbf{n}_{\beta\sigma} \tilde{c}_\beta dA}_{\text{tortuosity}} \right)$$



Closure and Macro-scale equation

$$\tilde{c}_\beta = \mathbf{b}_\beta \cdot \nabla C_\beta + \dots \quad C_\beta = \langle c_\beta \rangle^\beta$$

- **Local problem over representative UC**

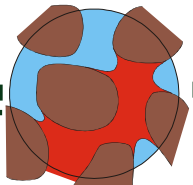
$$0 = \nabla^2 \mathbf{b}_\beta$$

B.C. 1 $\mathbf{n}_{\beta\sigma} \cdot \nabla \mathbf{b}_\beta = -\mathbf{n}_{\beta\sigma}$ at $A_{\beta\sigma}$

$$\mathbf{b}_\beta(\mathbf{r}) = \mathbf{b}_\beta(\mathbf{r} + \mathbf{l}_i)$$

$$\langle \mathbf{b}_\beta \rangle^\beta = 0$$

To be discussed



- **Macro-scale Equation**

$$\frac{\partial \varepsilon_\beta C_\beta}{\partial t} = \nabla \cdot (\varepsilon_\beta \mathbf{D}_\beta^* \cdot \nabla C_\beta)$$

$$\mathbf{J}_\beta^* = -\varepsilon_\beta \mathbf{D}_\beta^* \cdot \nabla C_\beta$$

macro-scale flux density


- **Effective diffusion tensor**

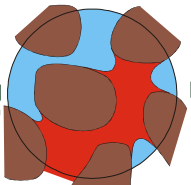
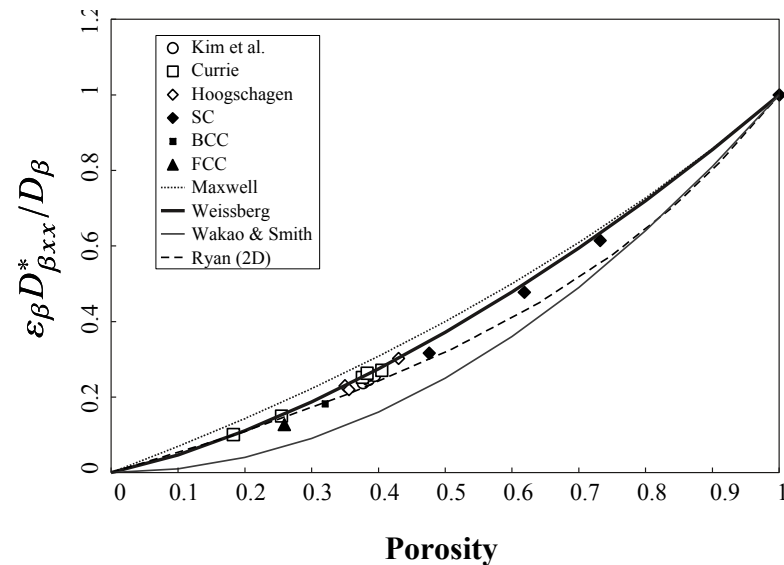
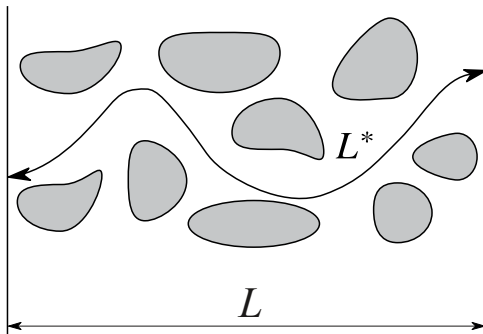
$$\mathbf{D}_\beta^* = D_\beta \left(\mathbf{I} + \frac{1}{\mathcal{V}_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_\beta dA \right)$$

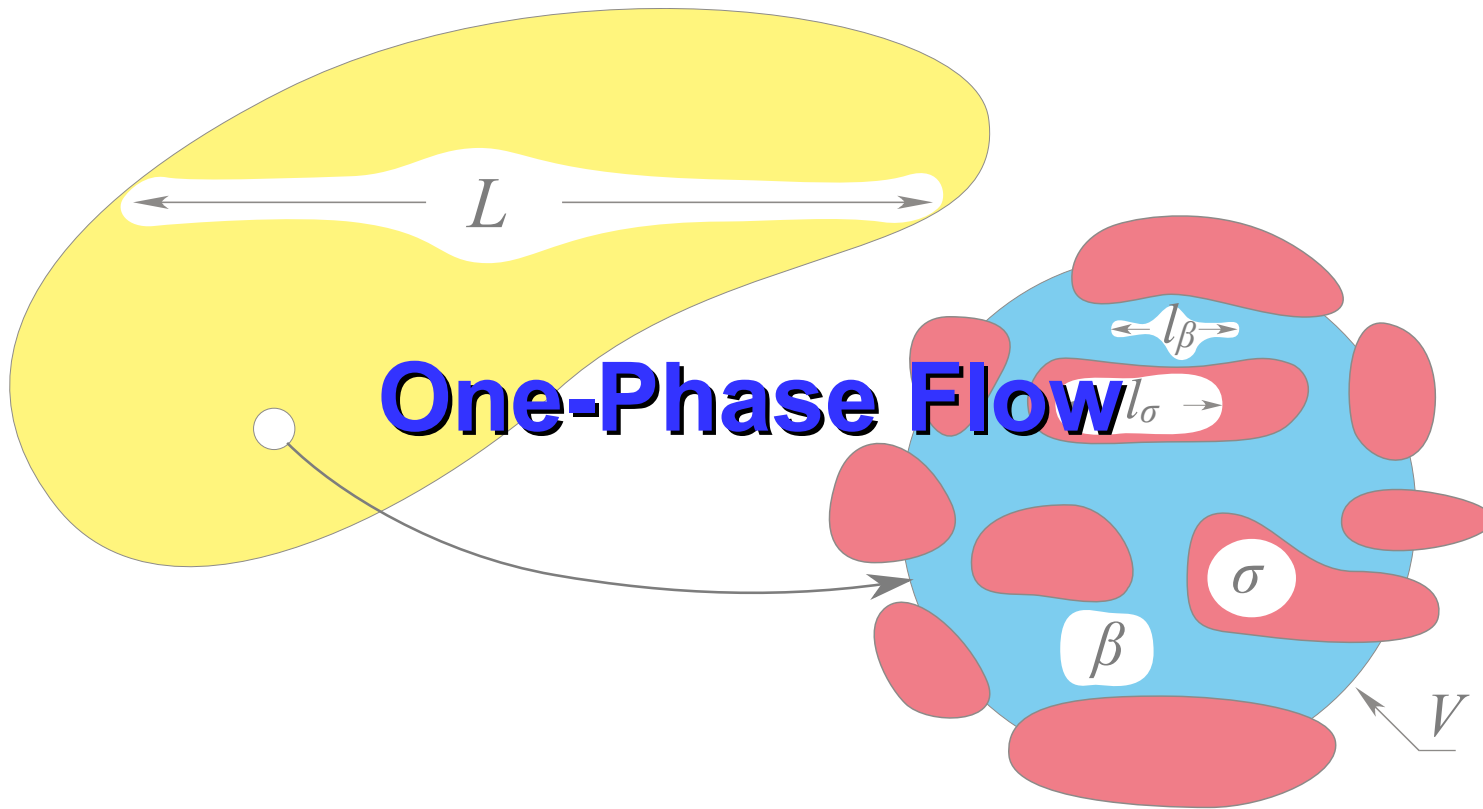
Tortuosity

$$\mathbf{D}_\beta^* = D_\beta \left(\mathbf{I} + \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_\beta dA \right)$$

- Effective diffusion depends on BC at $A_{\beta\sigma}$
- If isotropic : $\mathbf{D}_\beta^* = \frac{D_\beta}{\tau_\beta} \mathbf{I}$ tortuosity: $\tau_\beta \geq 1$
- Not a purely geometrical property

 : $\tau_\beta \neq \frac{L^*}{L}$





One-Phase Flow



One-Phase Flow: Phenomenology

- **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**

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

- **Laminar**

- **Turbulent**



Various regimes and transitions



Upscaling One-Phase Flow

- Averaging**

$$p_\beta = \langle p_\beta \rangle^\beta + \tilde{p}_\beta ; \quad \mathbf{v}_\beta = \langle \mathbf{v}_\beta \rangle^\beta + \tilde{\mathbf{v}}_\beta$$

$$\nabla \cdot \langle \mathbf{v}_\beta \rangle = 0$$

$$\text{B.C.1 } \tilde{\mathbf{v}}_\beta = -\langle \mathbf{v}_\beta \rangle^\beta \quad \text{at } A_{\beta\sigma}$$

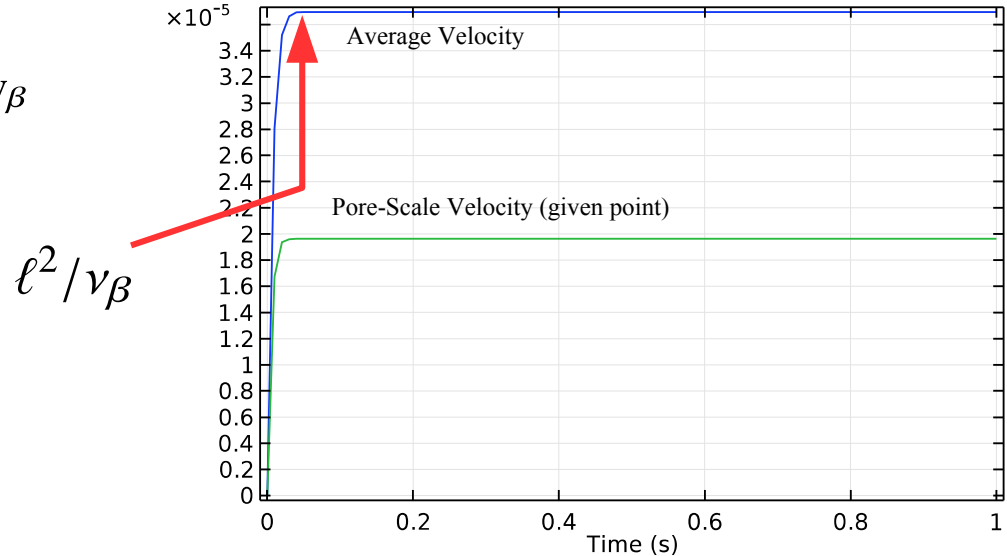
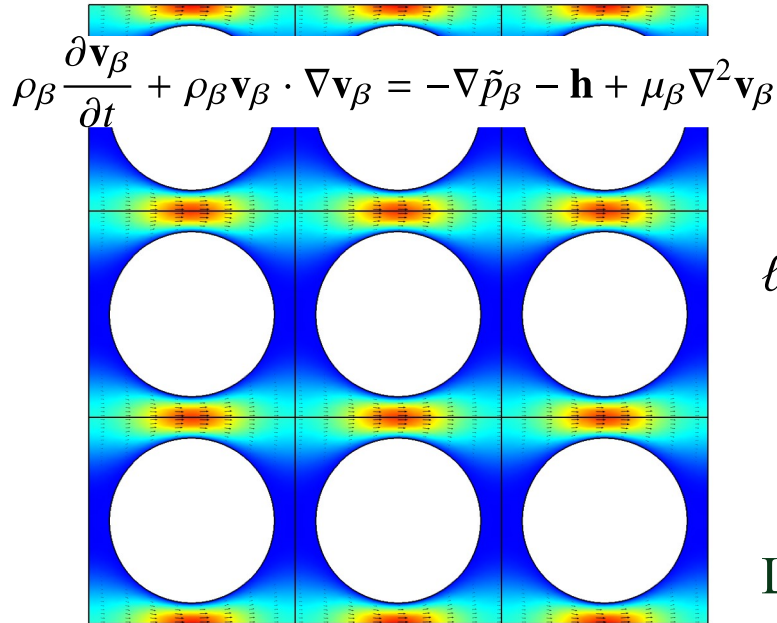
$$\begin{aligned} & \rho_\beta \frac{\partial \langle \mathbf{v}_\beta \rangle}{\partial t} + \rho_\beta \langle \mathbf{v}_\beta \rangle \cdot \nabla \langle \mathbf{v}_\beta \rangle^\beta + \nabla \cdot (\rho_\beta \langle \tilde{\mathbf{v}}_\beta \tilde{\mathbf{v}}_\beta \rangle) = \\ & -\varepsilon_\beta \nabla \langle p_\beta \rangle^\beta + \varepsilon_\beta \rho_\beta \mathbf{g} + \underbrace{\mu_\beta \nabla^2 \langle \mathbf{v}_\beta \rangle - \mu_\beta \nabla \varepsilon_\beta \cdot \nabla \langle \mathbf{v}_\beta \rangle^\beta}_{\text{Brinkman terms}} + \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\tilde{p}_\beta \mathbf{I} + \mu_\beta \nabla \tilde{\mathbf{v}}_\beta) dA \end{aligned}$$

Remark: $\tilde{\mathbf{v}}_\beta \sim \langle \mathbf{v}_\beta \rangle^\beta$



Various Regimes: Creeping

Re~0



Linear relationship between average velocity and pressure drop!

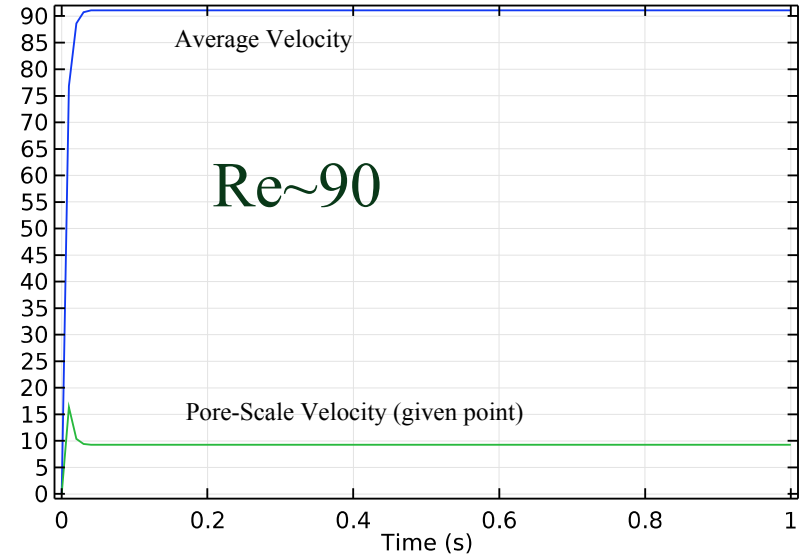
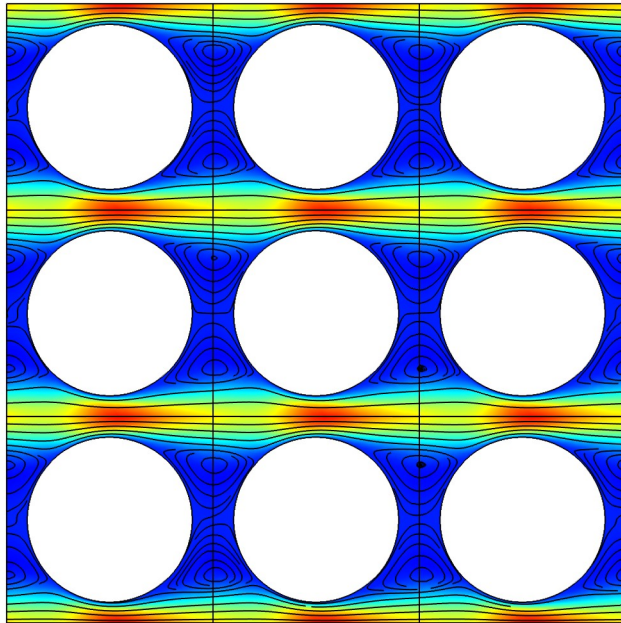
$$0 = -\varepsilon_\beta \nabla \langle p_\beta \rangle^\beta + \varepsilon_\beta \rho_\beta \mathbf{g} + \mu_\beta \nabla^2 \langle \mathbf{v}_\beta \rangle - \mu_\beta \nabla \varepsilon_\beta \nabla \langle \mathbf{v}_\beta \rangle^\beta$$

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

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



Various Regimes: Laminar Inertial



Still

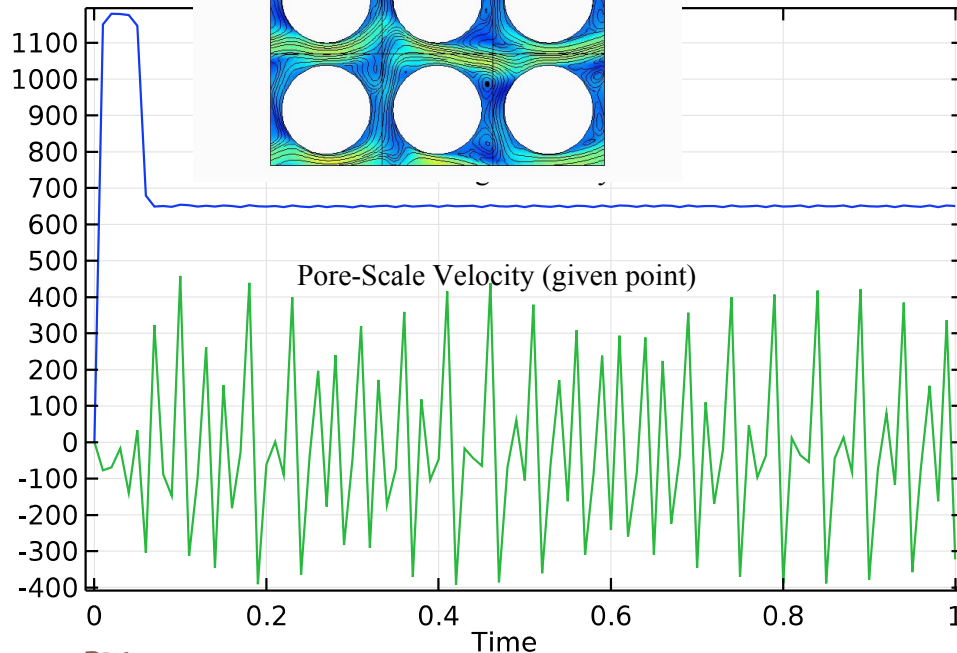
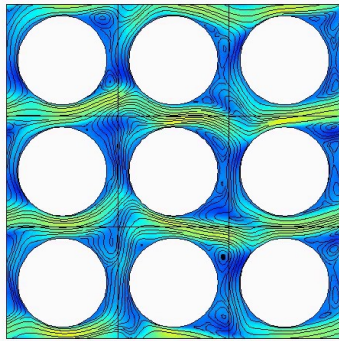
$$0 = -\varepsilon_\beta \nabla \langle p_\beta \rangle^\beta + \varepsilon_\beta \rho_\beta \mathbf{g} + \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\tilde{p}_\beta \mathbf{I} + \mu_\beta \nabla \tilde{\mathbf{v}}_\beta) dA$$

But non-linear relationship between average velocity and pressure drop!



Various Regimes: towards turbulence

- $\langle v \rangle = \text{steady-state}$



- Macro-Scale Turbulence? (see Jin et al., 2015, DNS)

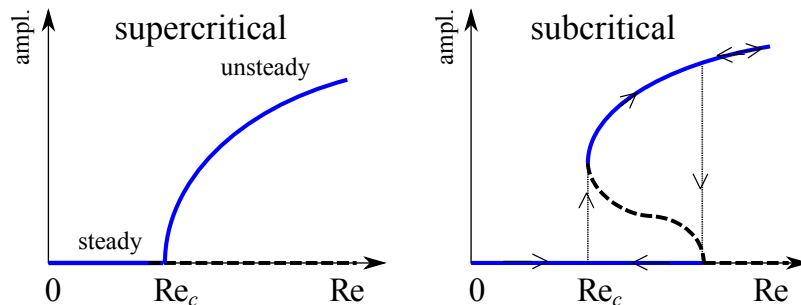
– Localized turbulence (nearly periodic over N -UC) need $\overline{\langle v_{\beta} \rangle}$

– Macro-scale turbulence? Ex.: entrance regions (D'Hueppe et al., ...)



More...

- **NS** → **Various types of bifurcations:**



Ex.: array of cylinders – not same Re_c for flow // or \perp to axis

- **Bifurcations depends on Re and number of UC (Aagnaou et al., 2016)...and topology!** → $REV \text{ size} = f(\langle \mathbf{v}_\beta \rangle^\beta)$
- **Difficult to estimate order of magnitude when fully non-linear** → rely on DNS

• **RESULT:** $(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g})$ and $\langle \mathbf{v}_\beta \rangle$ nearly constant over REV!

and up to localized turbulence one has

$\overline{(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g})}$ and $\overline{\langle \mathbf{v}_\beta \rangle}$ nearly constant over REV!



Closure: Darcy regime (Stokes problem=creeping flow)

Re~0

- PDEs for deviations

$$0 = -\nabla \tilde{p}_\beta + \mu_\beta \nabla^2 \tilde{\mathbf{v}} - \varepsilon_\beta^{-1} \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\tilde{p}_\beta \mathbf{I} + \mu_\beta \nabla \tilde{\mathbf{v}}_\beta) dA$$

$$\nabla \cdot (\tilde{\mathbf{v}}_\beta) = -\nabla \cdot \langle \mathbf{v}_\beta \rangle^\beta \approx 0 \quad \text{B.C. 1} \quad \tilde{\mathbf{v}} = -\langle \mathbf{v}_\beta \rangle^\beta \text{ at } A_{\beta\sigma}$$

- Closure in the linear case (3 elementary solutions for \mathbf{e}_i)

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



Closure and Macro-Scale Equation (Darcy regime)

$$\nabla \cdot \mathbf{B} = 0$$

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

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

$$\mathbf{b}(\mathbf{r} + \mathbf{l}_i) = \mathbf{b}(\mathbf{r})$$

$$\mathbf{B}(\mathbf{r} + \mathbf{l}_i) = \mathbf{B}(\mathbf{r})$$

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

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

\mathbf{K} intrinsic permeability

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



Other version of closure: permeameter-like problems

Note: also suitable for non-linear problems (non-newtonian flows, etc...)

$$\underbrace{\rho_\beta \mathbf{v}_\beta \cdot \nabla \tilde{\mathbf{v}}_\beta}_{=0, \text{ Darcy regime}} = -\nabla \tilde{p}_\beta + \nabla \cdot \left(\mu_\beta \left(\nabla \tilde{\mathbf{v}}_\beta + \nabla \tilde{\mathbf{v}}_\beta^T \right) \right) - \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right)$$

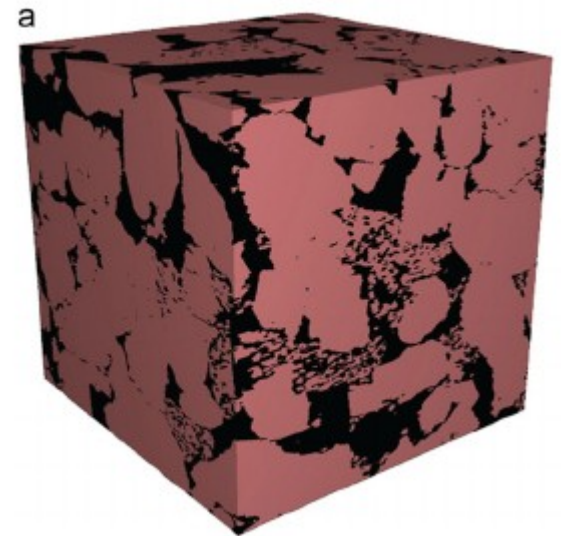
=0, Darcy regime

$$\nabla \cdot (\tilde{\mathbf{v}}_\beta) = 0$$

$$\tilde{\mathbf{v}} = -\langle \mathbf{v}_\beta \rangle^\beta \text{ at } A_{\beta\sigma}$$

BCs (see Guibert et al., 2016)?

- Periodicity conditions: good for anisotropic media, but percolation problem if “periodized” media
- Permeameter (various types: classical, Bamberger, ...)
- Bordering media: fluid or porous layer, ...



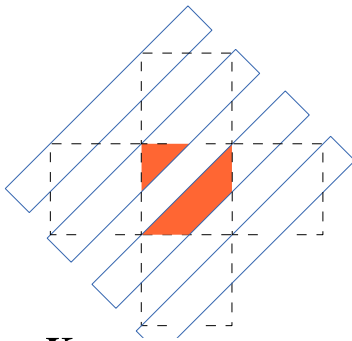
Calculation of the permeability

Case of “diffusion” problem: e.g., permeability, effective diffusion

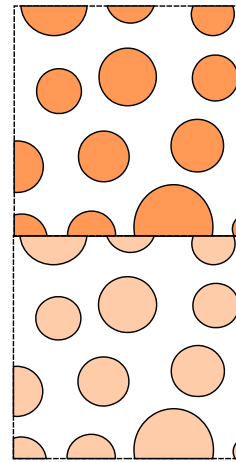
- Periodicity : good for anisotropy
- Making image periodic?

See discussion in Guibert et al., 2015

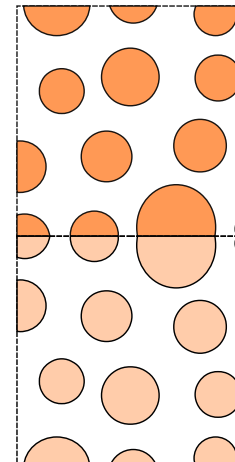
- I: Percolation problem
- II: Loss of anisotropy
- III: potentially various bias



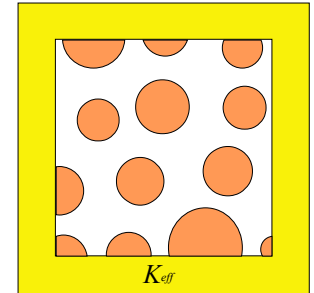
$$\mathbf{K}_{eff} = \varepsilon_{\beta} \mathbf{K}_{\beta} + \varepsilon_{\sigma} \mathbf{K}_{\sigma} + \frac{\varepsilon_{\beta} \varepsilon_{\sigma} (\mathbf{K}_{\beta} - \mathbf{K}_{\sigma}) \cdot \mathbf{i} \cdot (\mathbf{K}_{\sigma} - \mathbf{K}_{\beta})}{\mathbf{i} \cdot (\varepsilon_{\beta} \mathbf{K}_{\sigma} + \varepsilon_{\sigma} \mathbf{K}_{\beta}) \cdot \mathbf{i}}$$



I



II



K_{eff}

- thin layers
- Eff. Medium

III



Calculations over non-periodic images (cont.)

- “permeameters”

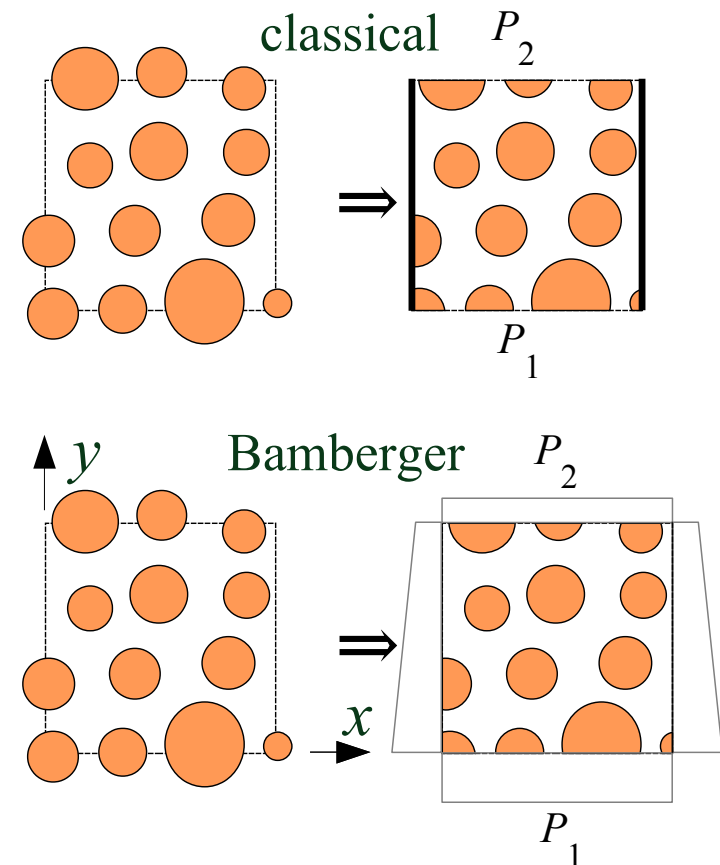
- All methods have bias

- $\langle v_x \rangle^\beta \neq 0$

- $K_{xy} \neq K_{yx}$

Note: minimal bias if large sample and anisotropy along the axis

See discussion in: Manwart et al. 2002; Piller et al. 2009; Guibert et al., 2015; ...



Permeability : $K \sim d_p^2$, 1 Darcy = 10^{-12} m²



Rocks : shale

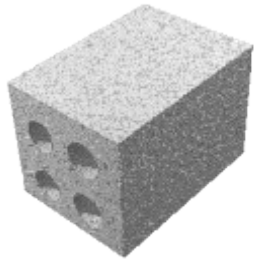
sandstone

Soils: clay

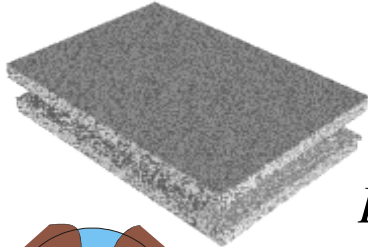
silt

sand

gravel



$$K = \varepsilon \frac{d^2}{32} \text{ capillary}$$



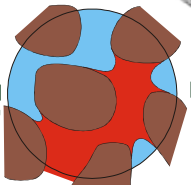
$$K = \varepsilon \frac{b^2}{12} \text{ Hele Shaw}$$

$$a_v = \frac{1}{V} \int_{A_{\beta\sigma}} dA = \frac{A_{\beta\sigma}}{V} : \text{specific area}$$

- **Kozeny-Carman (Carman, 1937)**

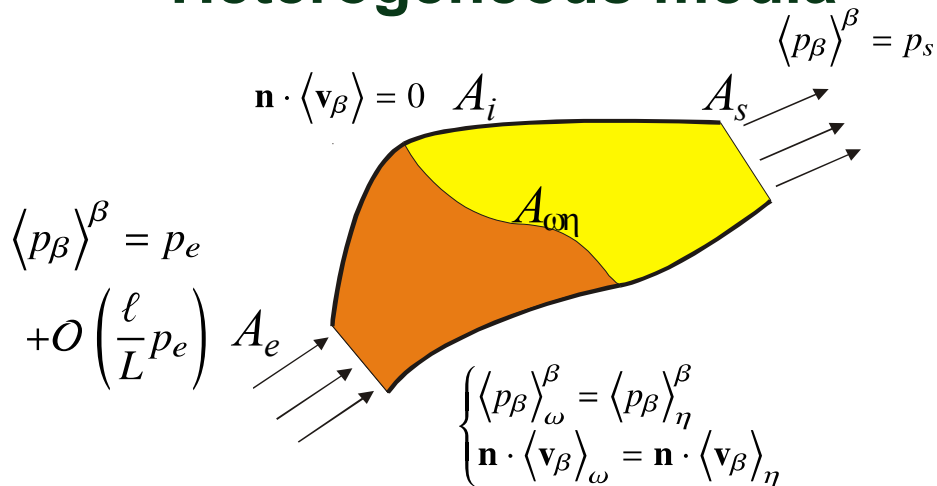
$$K = \frac{\varepsilon^3 d_K^2}{h_K (1 - \varepsilon)^2} \quad a_{vS} = \frac{a_v}{1 - \varepsilon}$$

$$d_K = d_{St} = \frac{6}{a_{vS}} \text{ Sauter diam.}$$

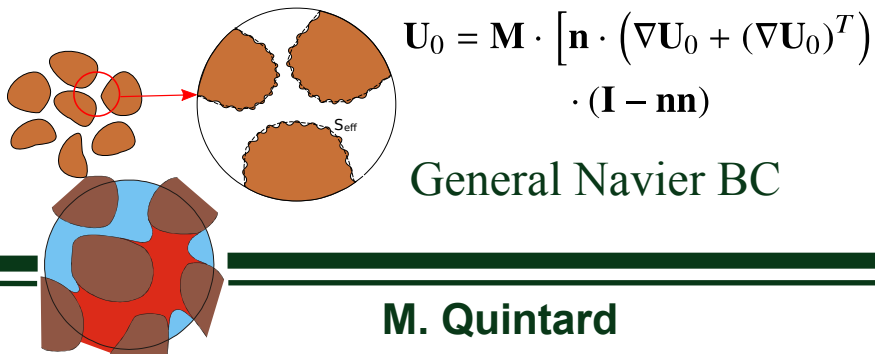


Boundary Conditions

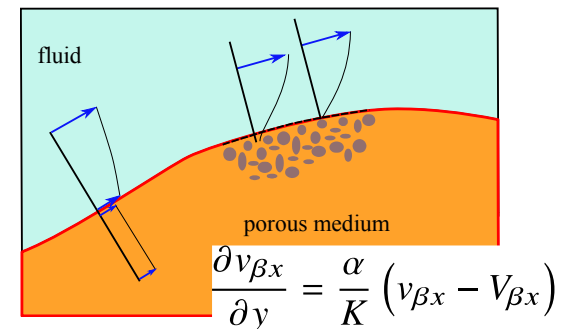
- Heterogeneous media**



- Rough surfaces**



- fluid/porous medium**



$$\mathbf{n} \cdot \mathbf{v}_\beta = \mathbf{n} \cdot \mathbf{V}_\beta \quad ; \quad p_\beta = P_\beta$$

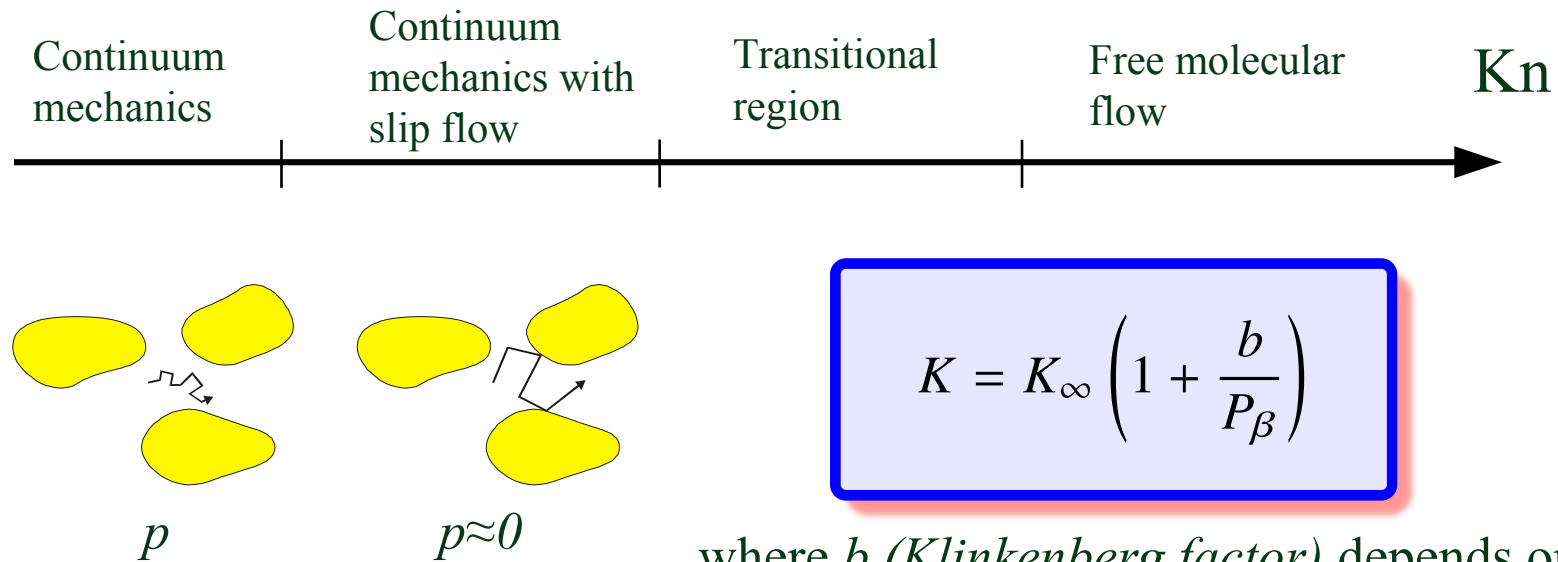
$$\mathbf{n} \cdot \left(-p_\beta \mathbf{I} + \mu_\beta \left(\nabla \mathbf{v}_\beta + (\nabla \mathbf{v}_\beta)^T \right) \right) \cdot (\mathbf{I} - \mathbf{nn}) =$$

$$\left(\alpha \mu_\beta \sqrt{3} / \sqrt{\text{tr}(\mathbf{K})} \right) (\mathbf{v}_\beta - \mathbf{V}_\beta) \cdot (\mathbf{I} - \mathbf{nn})$$

Beavers & Joseph...+ many variants
(Ochoa-Tapia, Le Bars, ...)

$$\mathbf{v}_\beta \cdot (\mathbf{I} - \mathbf{nn}) = 0 \quad ; \quad \text{Da} = \frac{K}{L^2} \rightarrow 0$$

Klinkenberg Effect (1941)

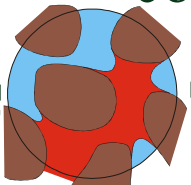


where b (Klinkenberg factor) depends on media.

Example: Sampath and Keighin (1982), N_2

$$b(\text{Pa}) = 0.0955 (K_{\infty}/\varepsilon)^{-0.53}$$

Generalization: See literature on upscaling with slip condition :

$$\mathbf{v}_{\beta} = -\ell_{\beta} (\mathbf{I} - \mathbf{n}_{\beta\sigma} \mathbf{n}_{\beta\sigma}) \cdot (\mathbf{n}_{\beta\sigma} \cdot \mu_{\beta} (\nabla \mathbf{v}_{\beta} + \nabla \mathbf{v}_{\beta}^T))$$


Non Darcy regimes (Re>1)

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

$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta K^{-1} \mathbf{V}_\beta - \rho_\beta \eta^{-1} \|\mathbf{V}_\beta\| \mathbf{V}_\beta \quad \text{with } \mathbf{V}_\beta = \langle \mathbf{v}_\beta \rangle ; P_\beta = \langle p_\beta \rangle^\beta$$

$$K = \frac{\varepsilon^3 d^2}{h_K (1 - \varepsilon)^2} \quad ; \quad \eta = \frac{\varepsilon^3 d}{h_\eta (1 - \varepsilon)}$$

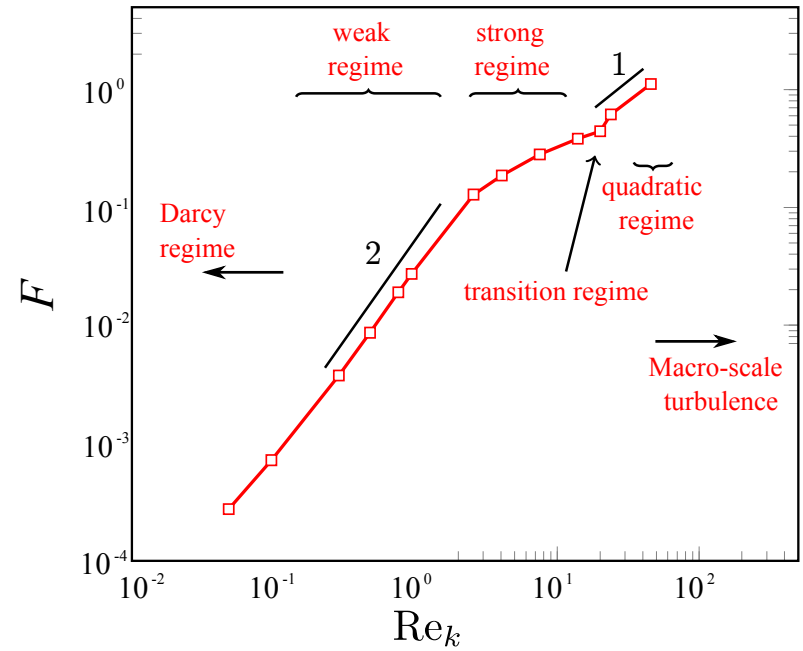
(passability)

- **Upscaling?**

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

⇓

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



Non Darcy regimes (Re>1)

- laminar inertia effects: theory → generalized Forchheimer equation

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

- Re → 0: Darcy, $\mathbf{F}=0$
- Re ~ 0: weak inertia, $\mathbf{F} \cdot \langle \mathbf{v}_\beta \rangle \sim \langle \mathbf{v}_\beta \rangle^3$ (Levy, Mei & Auriault, Firdaouss, ...)
- Re > 0: strong inertia, $\mathbf{F} \cdot \langle \mathbf{v}_\beta \rangle \sim \langle \mathbf{v}_\beta \rangle^2$ (Whitaker, 1996; Lasseux et al., 2011;...)



Weak Inertia

- **Solution following asymptotic expansions in Re**

$$\delta = \frac{\ell}{\nu_\beta} \nu = \text{Re}$$

$$\mathbf{v}^* = \frac{\tilde{\mathbf{v}}_\beta}{\nu} + \lambda, \quad p^* = \ell_\beta \frac{\tilde{p}_\beta}{\mu_\beta \nu}$$

$$\mathbf{v}^* = \mathbf{v}_0^* + \delta \mathbf{v}_1^* + \delta^2 \mathbf{v}_2^* + O(\delta^3)$$

$$p^* = p_0^* + \delta p_1^* + \delta^2 p_2^* + O(\delta^3)$$

- **1st correction?**

– **Periodic media:** $F_{\parallel} \sim \nu^2$

– **Periodic media+reversibility:** $F_{\parallel}^{(1)} = F_{\perp}^{(1)} = 0$

Wodié et Lévy, 1991; Mei et Auriault, 1991; Firdaouss et al., 1997
..... revisited by Pauthenet et al., 2017



Strong Inertia

• **Solution for** $\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \Rightarrow (\tilde{p}_\beta, \mathbf{v}_\beta) \Rightarrow \langle \mathbf{v}_\beta \rangle^\beta = v \boldsymbol{\lambda}$

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



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

P: rotation

F: non-linear scaling

$$\text{or } \nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} = -\varepsilon_\beta \mu_\beta (\mathbf{K}_D^{-1} \cdot \boldsymbol{\lambda} + \mathbf{f}) v$$

$$\mathbf{f} = K_\lambda^{-1} (F_\parallel \boldsymbol{\lambda} + F_\perp (\cos(\omega) \mathbf{n}_1 + \sin(\omega) \mathbf{n}_2))$$

$$\mathbf{n}_1 \times \mathbf{n}_2 = \boldsymbol{\lambda} \quad F_\parallel = \frac{\boldsymbol{\lambda} \cdot \mathbf{f}}{K_\lambda^{-1}} \quad K_\lambda^{-1} = \|\mathbf{K}_D^{-1} \cdot \boldsymbol{\lambda}\|$$

$$F_\perp = \|\mathbf{I} - \boldsymbol{\lambda} \boldsymbol{\lambda}\| \cdot \frac{\mathbf{f}}{K_\lambda^{-1}} \quad \omega = \left((\mathbf{I} - \boldsymbol{\lambda} \boldsymbol{\lambda}) \cdot \frac{\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g}}{\varepsilon_\beta \mu_\beta K_\lambda^{-1} v}, \mathbf{n}_1 \right)$$



Transition to inertia regimes: which Re number?

$$\text{Re} = \frac{\langle v_{\beta} \rangle^{\beta} \ell}{\nu_{\beta}}$$

- Literature discussion (see polemic in Lage et Antohe, 2000; etc...)

- $\ell = \sqrt{K}$?

– $K = \varepsilon d^2 / 32$ for a bundle of tubes (transition would change with porosity! → better

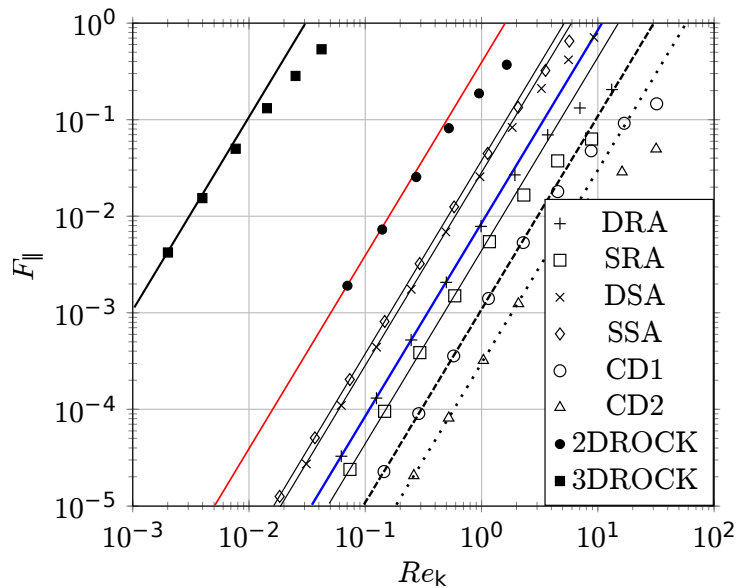
$$\ell = \sqrt{\frac{K}{\varepsilon}} \rightarrow \text{Re}_k$$

- Topological problem: array of cylinders → transition depends on the orientation → need a topological information!



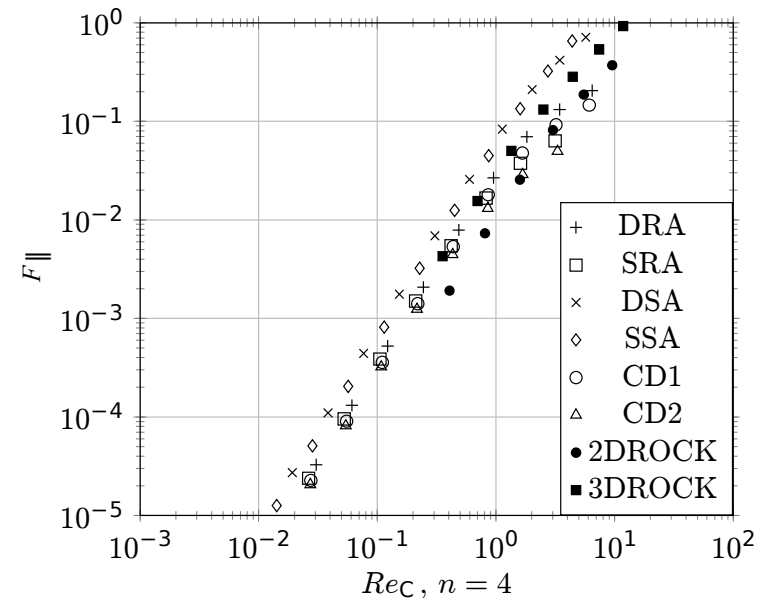
Transition to inertia effect: effect of topology (Pauthenet et al., 2017)

● If Re_k



(various media, rocks, ...:
Muljadi et al., 2016; etc...)

● Re_C



$$Re_C = \frac{v}{v_{\beta}} \sqrt{\frac{K_{\lambda}}{\varepsilon_{\beta}}} C_{\lambda}$$



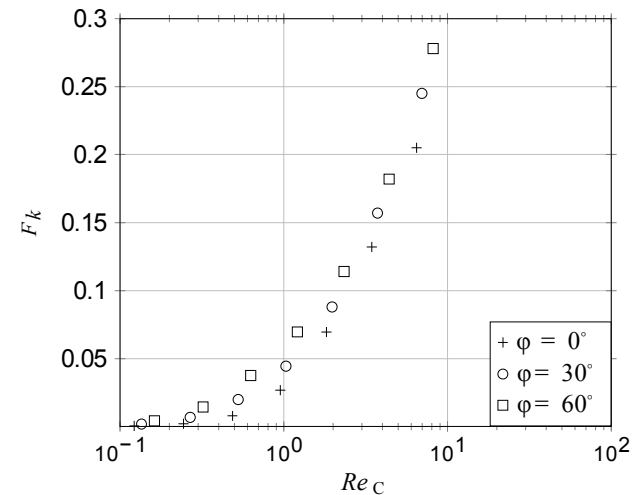
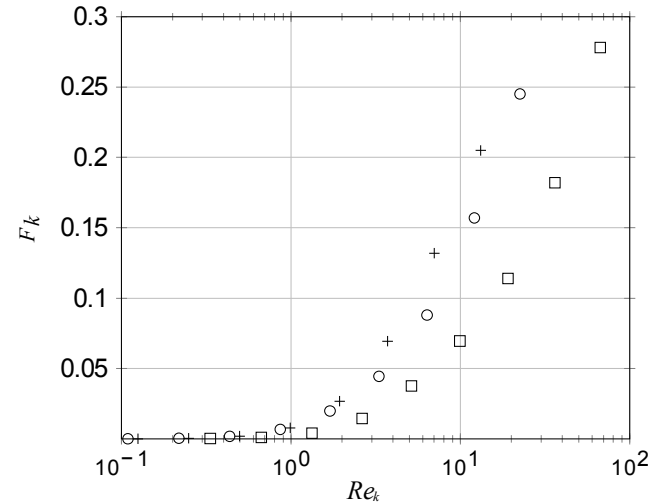
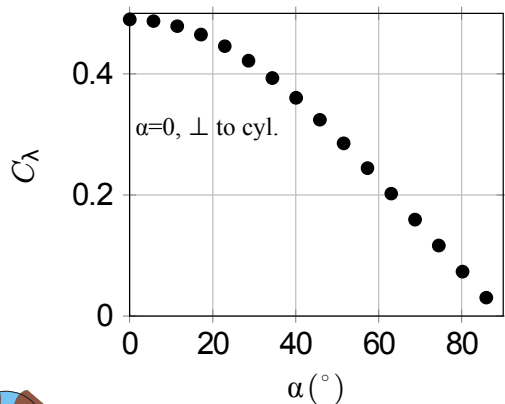
Topology effect (Ex.: array of Cylinder)

- **Tentative (open question)**

from Darcy closure

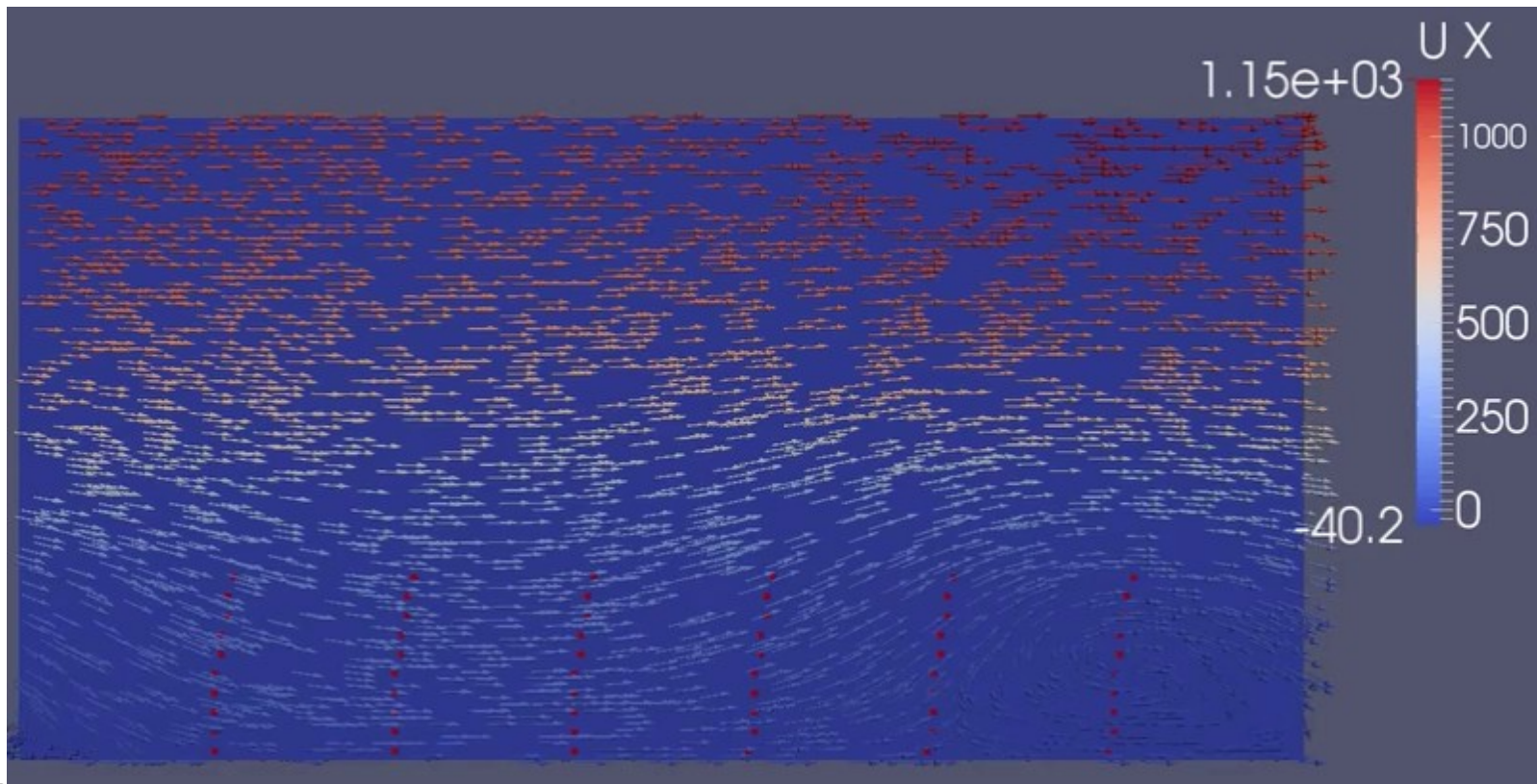
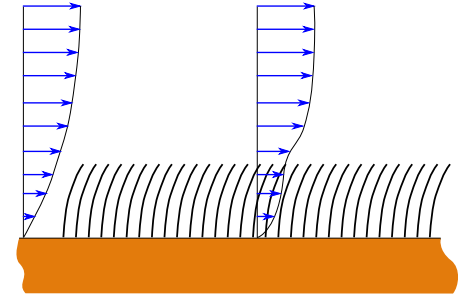
$$C_\lambda = \frac{\zeta(\mathbf{v}_0^* \cdot \nabla^* \mathbf{v}_0^*)}{\sqrt{\langle \nabla^* \mathbf{v}_0^* : T \nabla^* \mathbf{v}_0^* \rangle}^\beta} \sqrt{\frac{\lambda \cdot \mathbf{K}_D^{-1} \cdot \lambda}{K_\lambda^{-1}}}$$

$$\zeta(\mathbf{v}_0^* \cdot \nabla^* \mathbf{v}_0^*) = \langle \|\mathbf{v}_0^* \cdot \nabla^* \mathbf{v}_0^*\|^n \rangle \beta^{1/n}$$



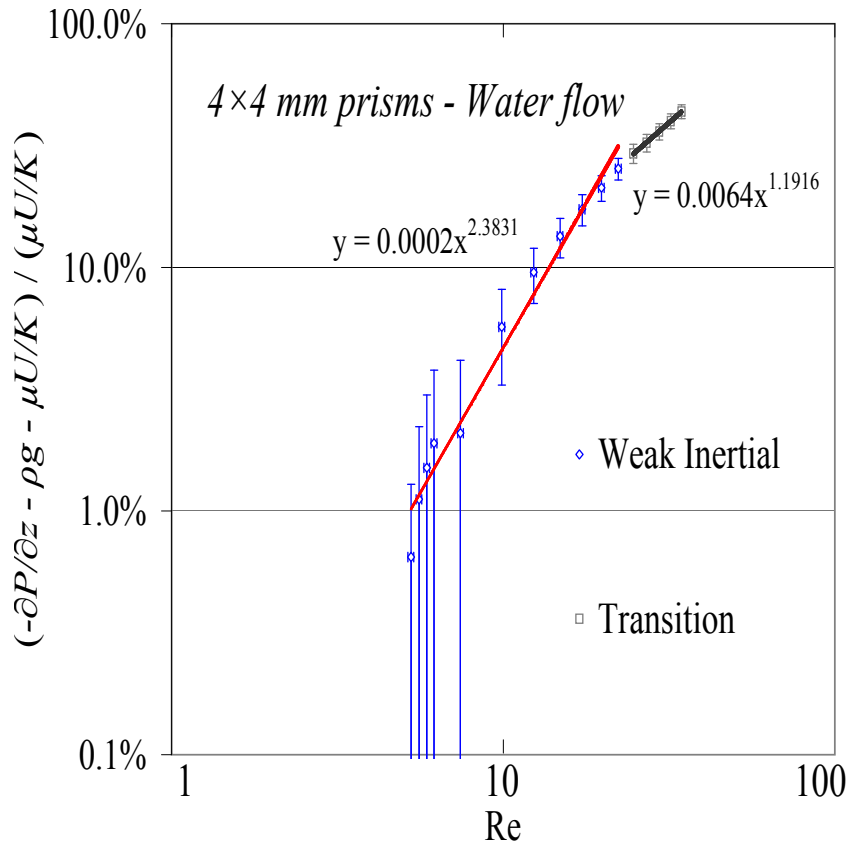
Example: canopy flow

Honami generation (Pauthenet, 2017)
...need \mathbf{K}_{app} for all fiber directions and \mathbf{V}_{β}

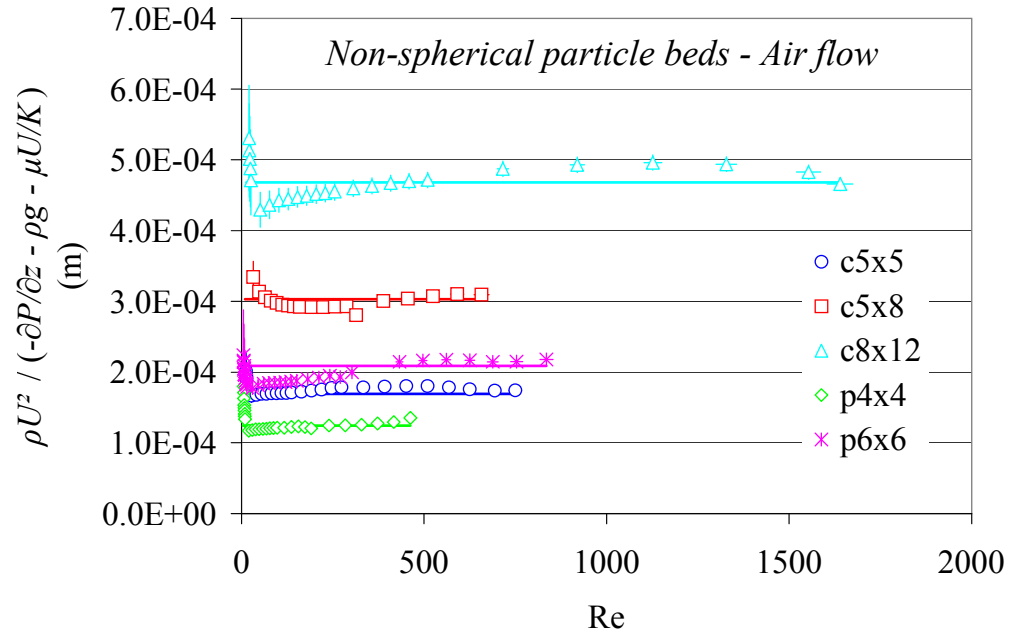


Experimental Evidence: inertia regime

Weak inertia



Strong inertia



Clavier et al., 2014



Note the importance of transition regimes!



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

- **Turbulence: time and spatial averaging (see book De Lemos, 2006; ...)**
 - Time and spatial averaging commute!
 - However: not necessarily the same result if sequential closure!?

$$\text{I. } \mathbf{v}_\beta \rightarrow \langle \mathbf{v}_\beta \rangle \rightarrow \overline{\langle \mathbf{v}_\beta \rangle}$$

$$\text{II. } \mathbf{v}_\beta \rightarrow \overline{\mathbf{v}_\beta} \text{ (RANS, ...)} \rightarrow \langle \overline{\mathbf{v}_\beta} \rangle$$

- For one-phase flow: 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...
- **Open: Simultaneous closure over $[R^3 \times R^t]$? More complex sequential closures ($t \rightarrow x \rightarrow t \rightarrow \dots$) depending on the hierarchy of scales?**
- **Open question for multiphase flow?**

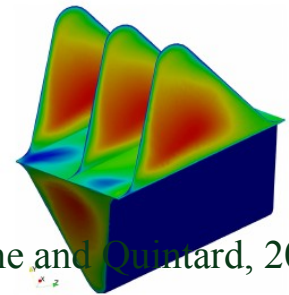


Turbulent flows in porous media (continued)

- Localized Turbulence: i.e., nearly periodic (see Jin et al., 2015 for DNS results)
 - Slow unsteady flows → generalized Forchheimer for time averaged pressure and velocity $\langle \mathbf{v}_\beta \rangle$ or $\langle \overline{\mathbf{v}_\beta} \rangle$
 - Spatial averaging of RANS models → generalized Forchheimer equation, F not necessarily $\sim \langle \mathbf{v}_\beta \rangle$ or $\langle \mathbf{v}_\beta \rangle^2$

Example: structured packings

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

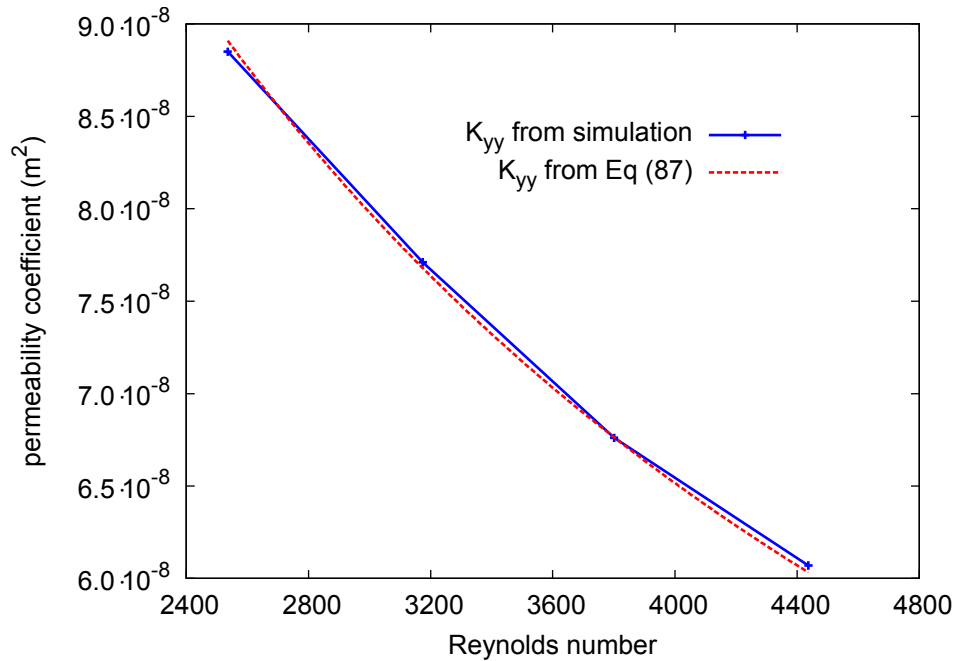
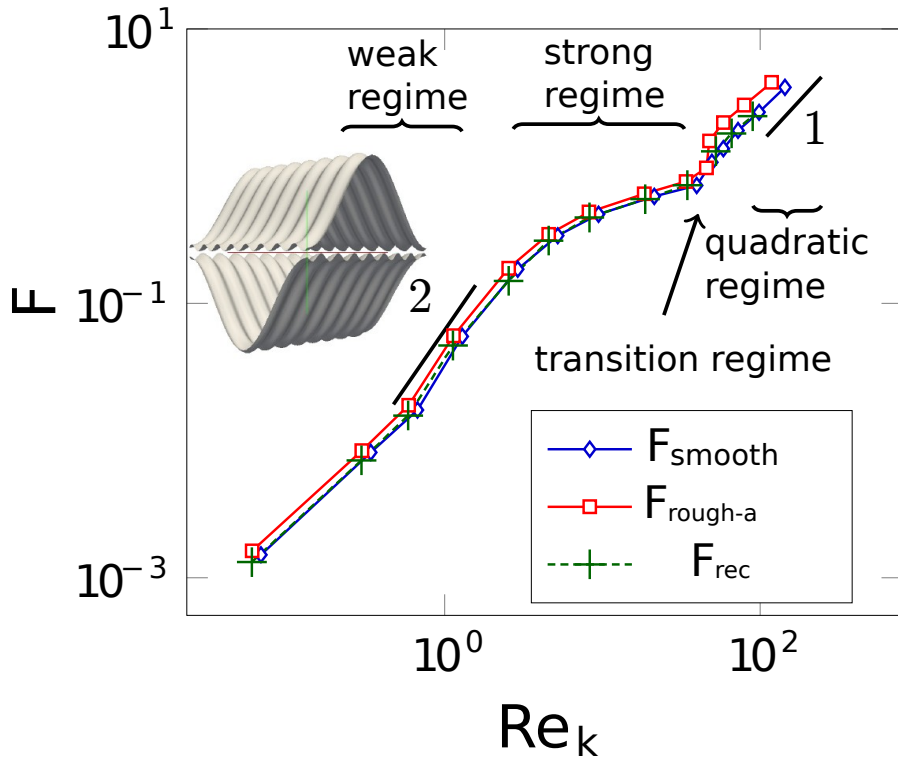


Soulaine and Quintard, 2014

- Porous media turbulence models (**beyond the scope of the lecture**)?
 - Pedras & De Lemos, Masuoka & Takatsu (1996), Nakayama & Kuwahara (1999), ...
 - note: useful for fluid/porous medium interface (D'Hueppe et al., 2012), deep inside the p.m. one may recover Darcy-Forchheimer regimes



Example : (Structured Packings)

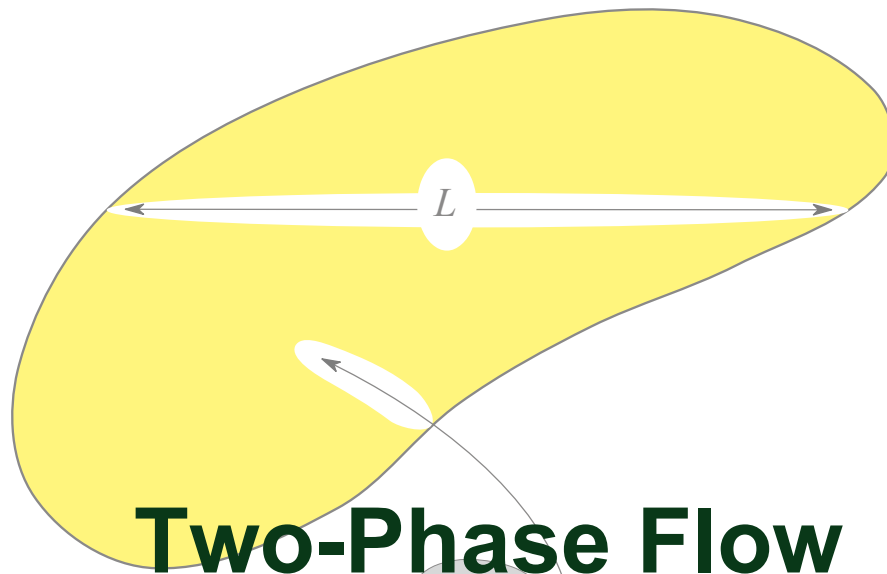


↑ Averaging of NS; Pasquier et al., 2016

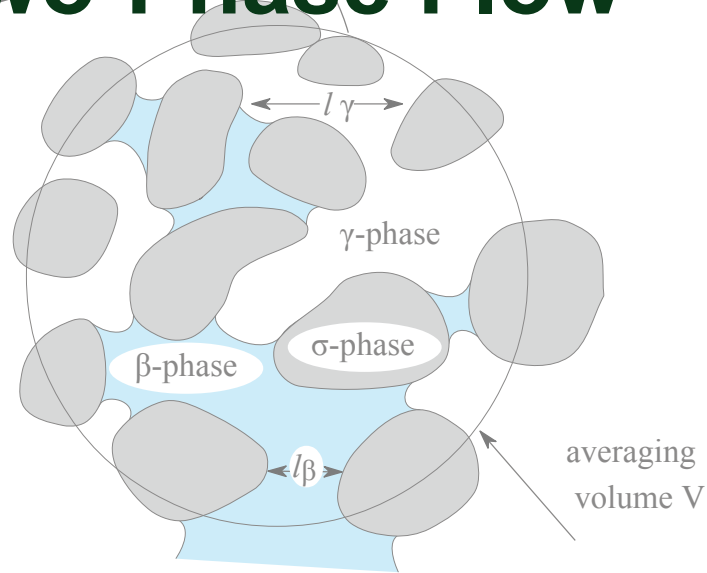
Averaging of RANS model; Soulaire & Quintard, 2014 ↗

$$\mathbf{K}^*(Re, \theta) \approx \begin{pmatrix} \frac{K_0}{1 + \beta_l Re} & 0 & 0 \\ 0 & \frac{K_0}{1 + \beta_l Re} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$





Two-Phase Flow



Two-Phase Flow

● Pore-scale

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

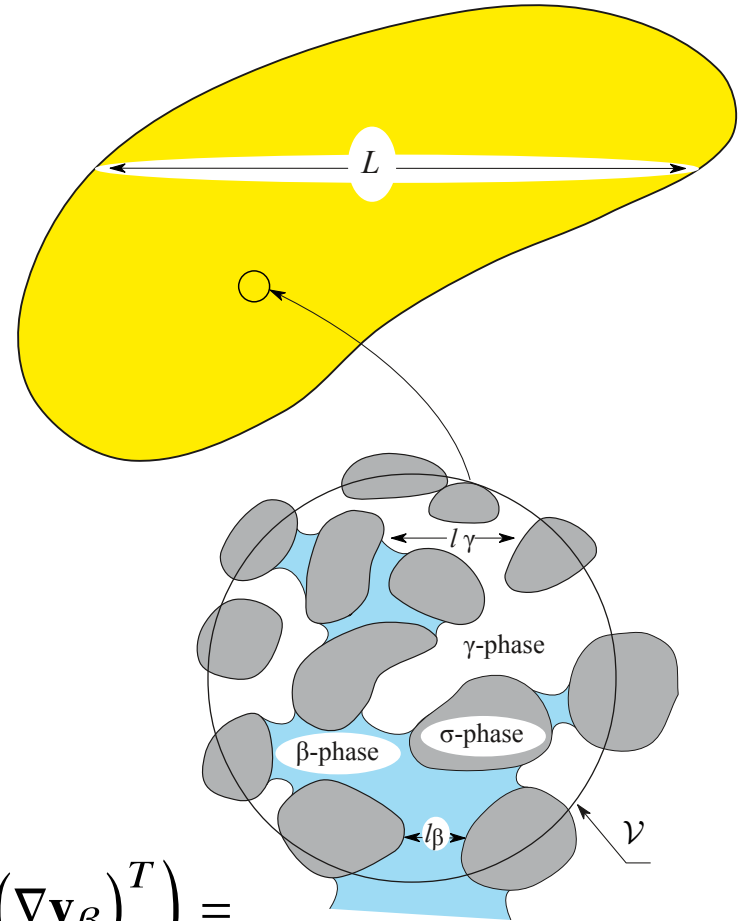
$$\frac{\partial \rho_\alpha \mathbf{v}_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha) = -\nabla p_\alpha + \rho_\alpha \mathbf{g} + \mu_\alpha \nabla^2 \mathbf{v}_\alpha \text{ in } V_\alpha \quad \alpha = \beta, \gamma$$

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

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

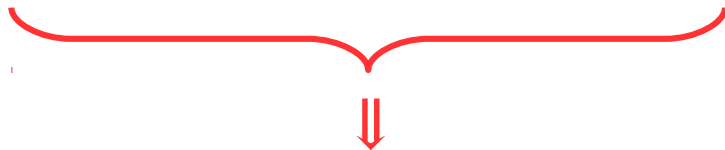
$$\text{B.C. 3 } \mathbf{v}_\beta = \mathbf{v}_\gamma \text{ at } A_{\beta\gamma}(t)$$

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

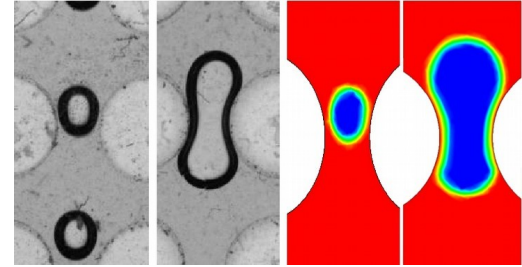


Note: complex and transient pore-scale flows

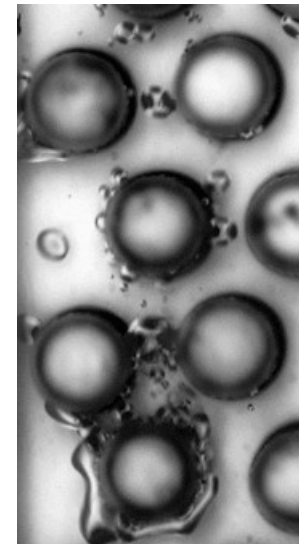
- Front propagation is in general time dependent!
- Specific features: Haines jumps, snap-off, ...
- Boiling, condensation



- Common practice: quasi-static approximation... $\langle \phi \rangle$ and not $\overline{\langle \phi \rangle}$
Justification: Ergodicity (not validated)?



Horgue et al.



See paper
Gourbil et al.

Sapin et al., 2016



DNS

- VOF, LBM, Cahn-Hilliard, SPH,: spurious velocities & convergence for high density and viscosity ratios, problems with wettability and Capillary number.
- Penalization (work with a phase indicator for the solid phase also; Raeni et al., 2012; Horgue et al., 2012)...
- Achieving numerical convergence is very difficult, though averages (e.g. effective properties) may be good for statistical reasons (one phase flow: Romeu & Noetinger, 1995...)
- Need large computational resources
- Alternative to DNS?
 - Macro-scale models (various types)
 - PNM (pore network models), dynamic PNM, Hybrid PNM

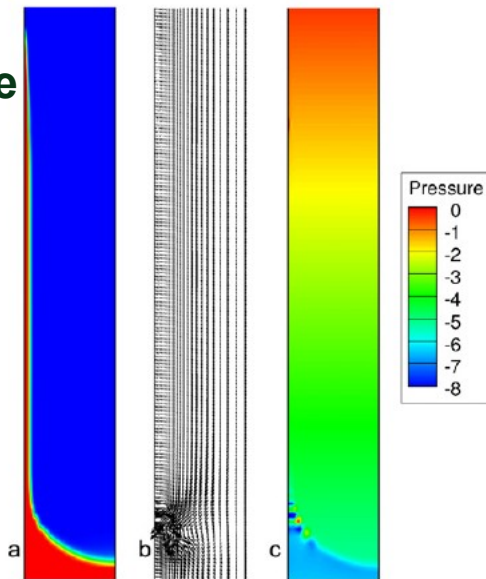
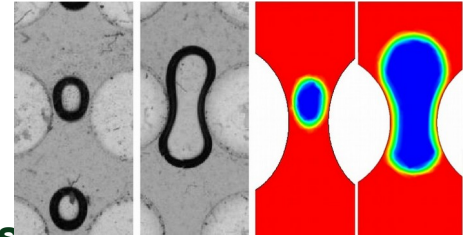


Fig. 6. Simulation of drainage with spurious currents along the meniscus curvature (HRIC, $Co = 1.00$, $Ca = 0.03$), (a) volume fraction, (b) velocity profile, (c) pressure distribution.

Horgue et al., 2012



Upscaling: quasi-static theory

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

● Example: Case of B.C. 4

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

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

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

+ Re, (We=Re×Ca) numbers

+ *Dynamic* Bond number

} If $\approx 0 \Rightarrow$

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

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

i.e., the classical capillary pressure theory!



Macro-Scale Models : Quasi-Static

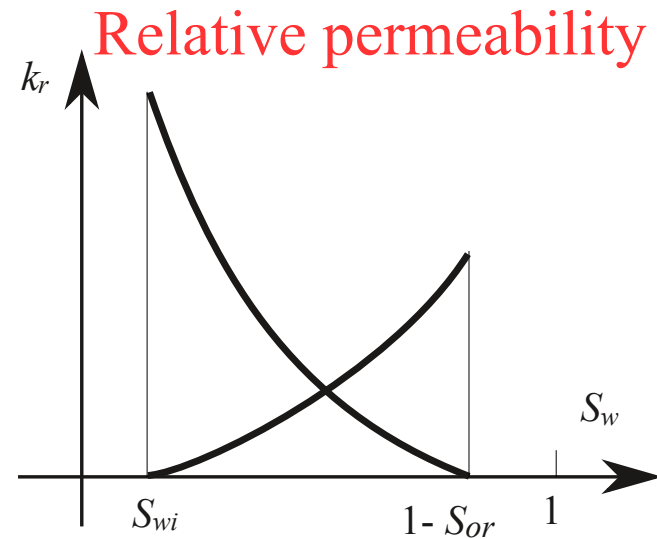
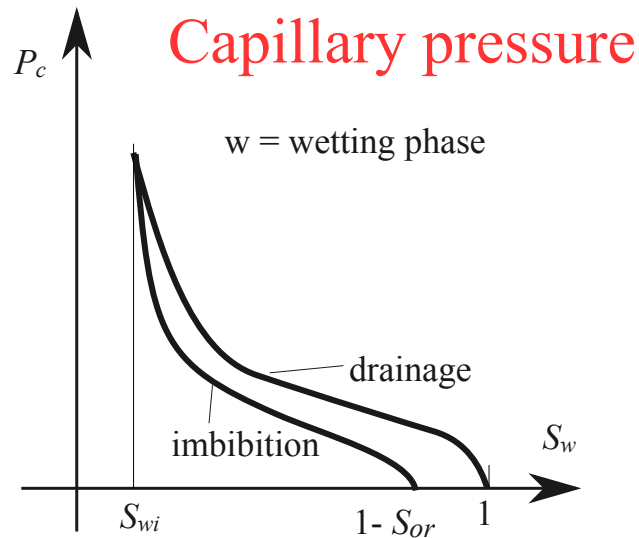
$$\mathbf{V}_\alpha = \langle \mathbf{v}_\alpha \rangle ; P_\alpha = \langle p_\alpha \rangle^\alpha ; \varepsilon_\alpha = \varepsilon S_\alpha \quad \alpha = \beta, \gamma$$

- **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

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

(Ex. : Whitaker, 1986)

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

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

Phase interaction 

Ex. : Two-Phase Poiseuille Flow

$$K_{ll} \approx K\alpha^2$$

$$K_{gg} \approx K\alpha^2$$

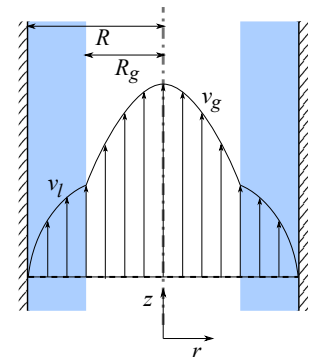
$$K_{lg} \approx \frac{\mu_g}{\mu_l} \frac{(1-\alpha)^2}{\alpha}$$

$$K_{gl} \approx \frac{\alpha}{1-\alpha}$$

$$\frac{\mu_g}{\mu_l} \rightarrow 0$$

$$\mu_l$$

$$\alpha = S_g$$



Inertia Effects

- Ergun (Heuristic): no-phase interaction terms

$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta \frac{1}{K k_{r\beta}} \mathbf{V}_\beta - \frac{\rho_\beta}{\eta \eta_\beta} \|\mathbf{V}_\beta\| \mathbf{V}_\beta \quad \text{Ergun, Fourar, Lenormand, ...}$$

- Schulenberg and Muler (1987) (Heuristic and )

Similar to theory for fluidized beds

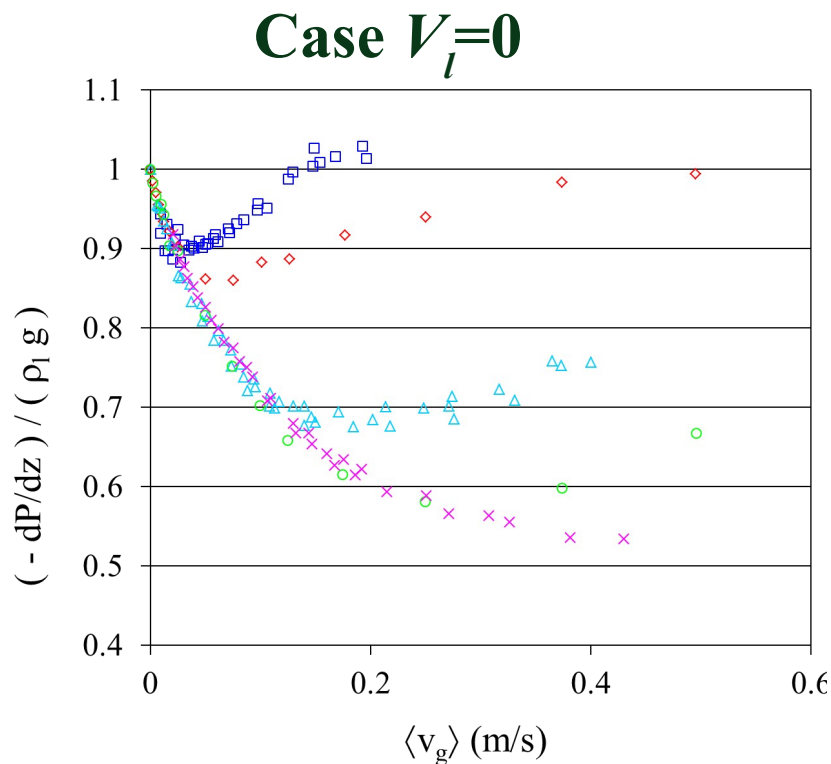
$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta \frac{1}{K k_{r\beta}} \mathbf{V}_\beta - \frac{\rho_\beta}{\eta \eta_\beta} \|\mathbf{V}_\beta\| \mathbf{V}_\beta + \frac{\mathbf{F}_{\beta\gamma}^S}{S_\beta}$$

- 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



from Clavier et al. (2015)

(IRSN: context of nuclear reactor severe accident)

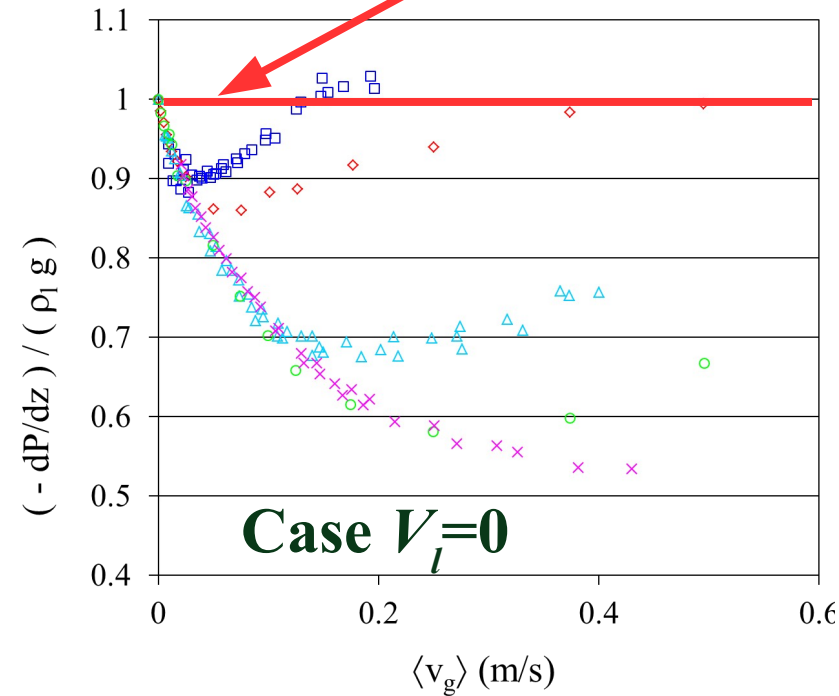
See also Taherzadeh & Saidi (2015)



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

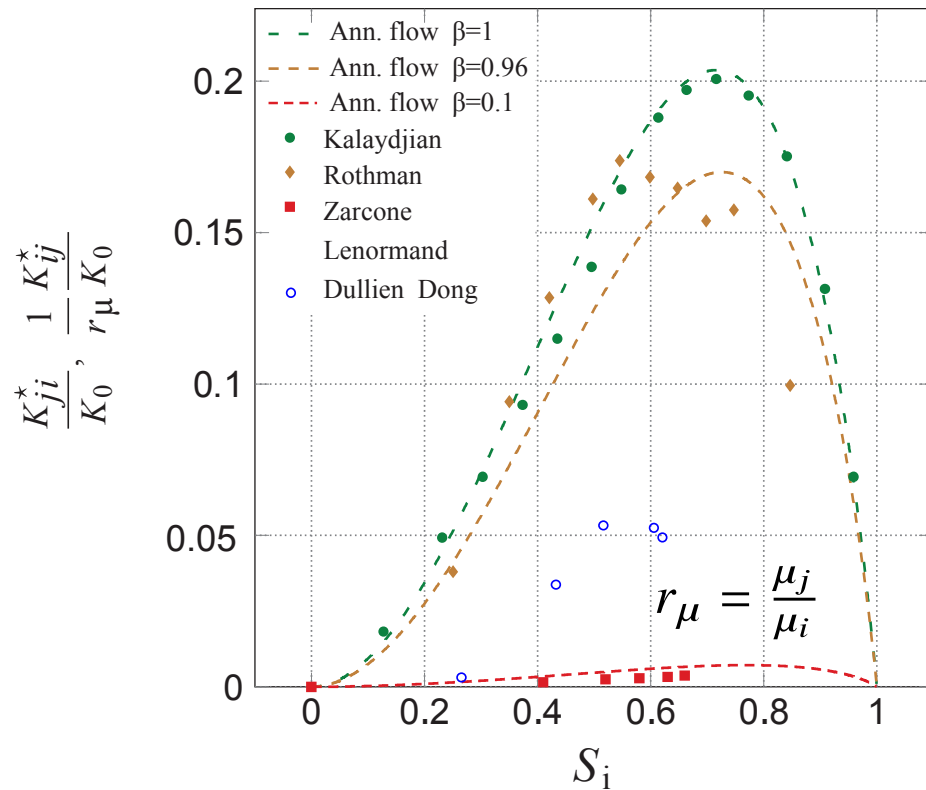


Impact of K_0

(Pasquier et al., 2017)

$$K_{ij} = \beta K_{ij} \text{ (annular 2-phase flow)}$$

(Pasquier et al., 2017)



$$\begin{pmatrix} U_i \\ U_j \end{pmatrix} + \mathcal{K}^\star \begin{pmatrix} \frac{\partial P}{\partial x} - \rho_i g \\ \frac{\partial P}{\partial x} - \rho_j g \end{pmatrix} = 0$$

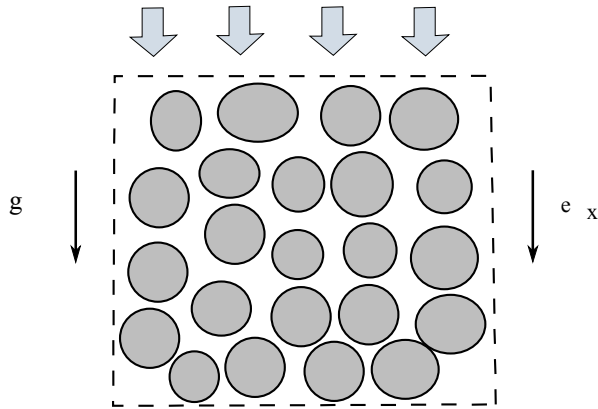
$$\begin{aligned} \mathcal{K}^\star &= \begin{pmatrix} K_{ii}^\star/\mu_i & K_{ij}^\star/\mu_j \\ K_{ji}^\star/\mu_i & K_{jj}^\star/\mu_j \end{pmatrix} \\ &= \frac{1}{1 - K_{ij}K_{ji}} \begin{pmatrix} K_{ii}/\mu_i & K_{jj}K_{ij}/\mu_j \\ K_{ii}K_{ji}/\mu_i & K_{jj}/\mu_j \end{pmatrix} \end{aligned}$$

$$\mathcal{N}_g = \frac{K_0 (\rho_i - \rho_j) g}{U \mu_i} \quad \text{Gravity number}$$



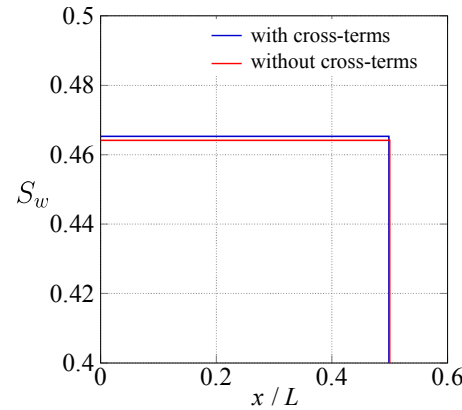
Effect of cross terms on the flow dynamic

$$\frac{\partial S_l}{\partial t} + \frac{\partial \mathcal{F}_l}{\partial S_l} \frac{\partial S_l}{\partial x} = 0$$

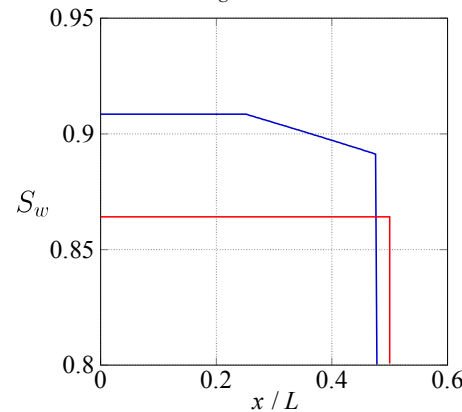


(a) Configuration 1: Imbibition

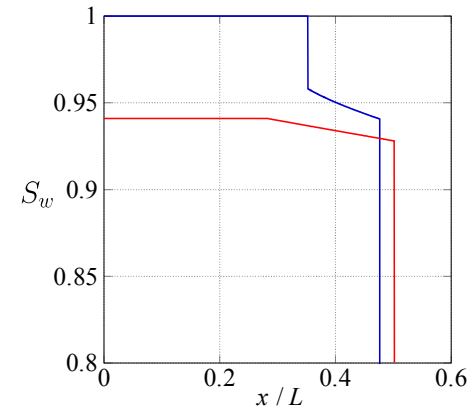
adapted Buckley-Leverett theory
(Pasquier et al., 2017)



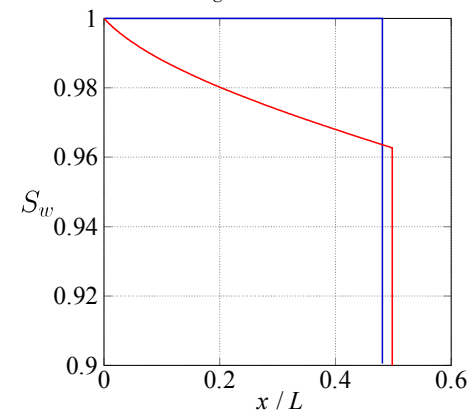
(b) $\frac{1}{N_g} = 0$



(d) $\frac{1}{N_g} = 0$



(f) $\frac{1}{N_g} = 0$

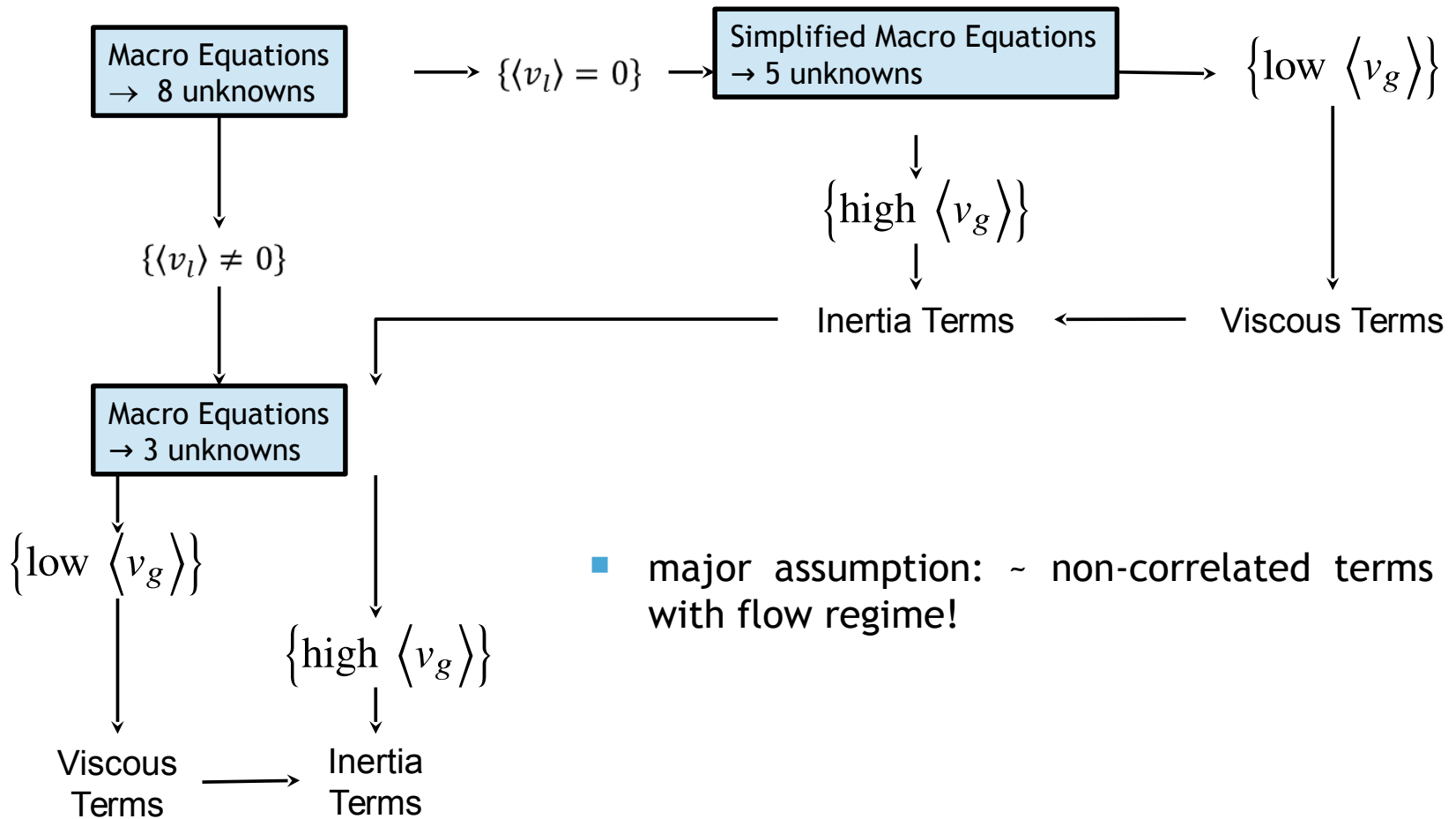


(h) $\frac{1}{N_g} = 1.1$



Estimation of multiphase parameters?

Ex. from IRSN experiments



Obtained correlations

$$K_{ll} = K (1 - \alpha)^3$$

$$K_{lg} = k_{lg} \frac{\mu_g (1 - \alpha)^2}{\mu_l \alpha}$$

$$f_{lg} = \frac{\alpha^3}{\alpha^3 + (1 - \alpha)^3}$$

$$F_{ll} = \frac{\rho_l K}{\mu_l \eta} \langle v_l \rangle$$

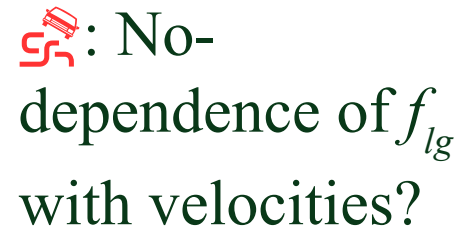
$$F_{lg} = K_{lg} f_{lg}$$

$$K_{gg} = K \alpha^4$$

$$K_{gl} = \frac{\mu_l}{\mu_g} \frac{K_{gg} K_{lg}}{K_{ll}}$$

$$F_{gg} = \frac{\rho_g K}{\mu_g \eta} \langle v_g \rangle$$

$$F_{gl} = f_{lg} \alpha^6$$

: No-dependence of f_{lg} with velocities?

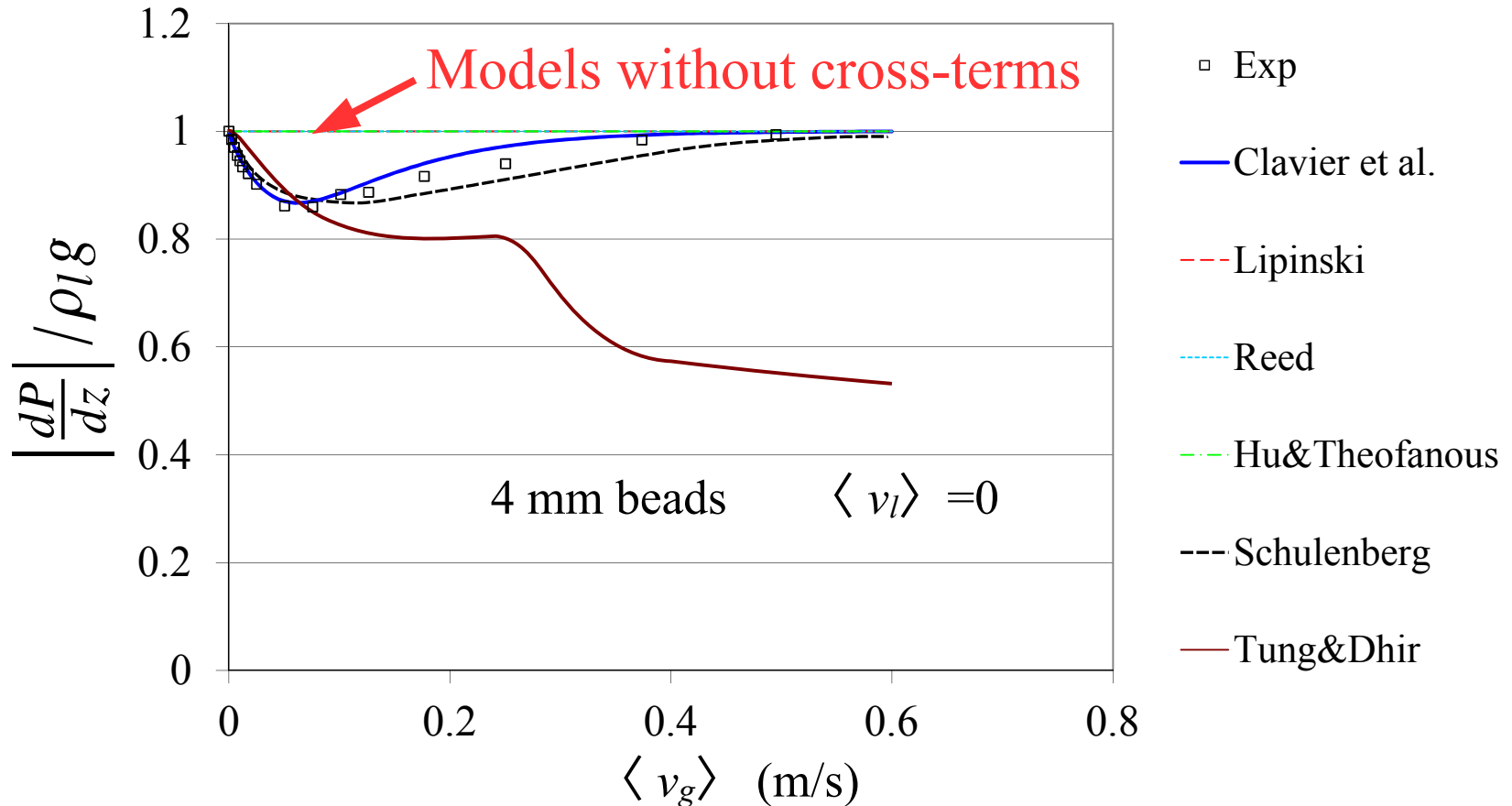
d (mm)	K (m2)	k_{lg}	k_{lg}/K
3.18 mm	8.89×10^{-9}	4	4.50×10^{-8}
4 mm	1.21×10^{-8}	5.5	4.56×10^{-8}
6.35 mm	3.18×10^{-8}	15	4.72×10^{-8}
8 mm	5.37×10^{-8}	23	4.28×10^{-8}
12.7 mm	1.96×10^{-7}	70	3.57×10^{-8}

d (mm)	n
3.18	9
4	7
6.35	3.2
8	2.5
12.70	2.2

Table 1: Best-fitting values of coefficient k_{lg}



Comparison to various models: pressure drop (dP)



...still an open problem!



More: Dynamic Models

- **impact of $\partial S/\partial t$, V_α , a_v ...**
 - 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_v as state variable, 1993), also Kalaydjian (1987)...
 - Phase field, Cahn-Hilliard (Cueto-Felgueroso & Juanes, 2009)...



Examples of dynamic equations

- Quintard & Whitaker, 1990

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

- Kalaydjian, Hassanizadeh & Gray, ...

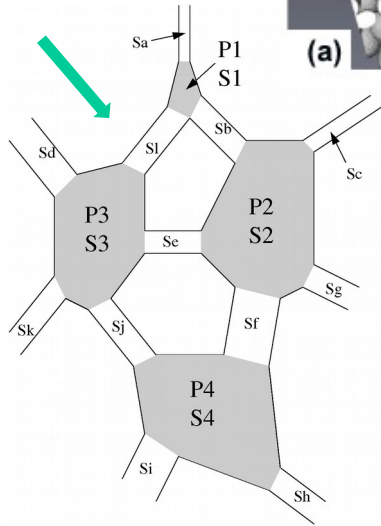
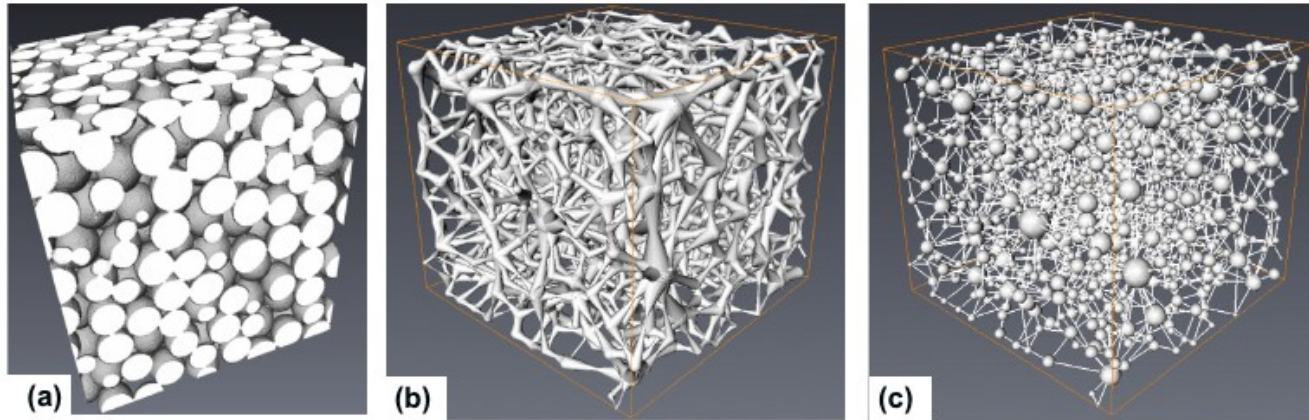
$$P_\gamma - P_\beta = p_c - L_1 \frac{\partial \varepsilon S_\beta}{\partial t}$$

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



PNM (Pore Network Model) : quasi-static

(reviews: Dullien, 1992;...; Jockar-Niasar & Hassanizadeh, 2012)



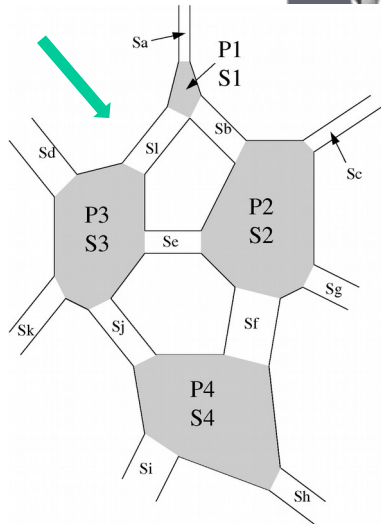
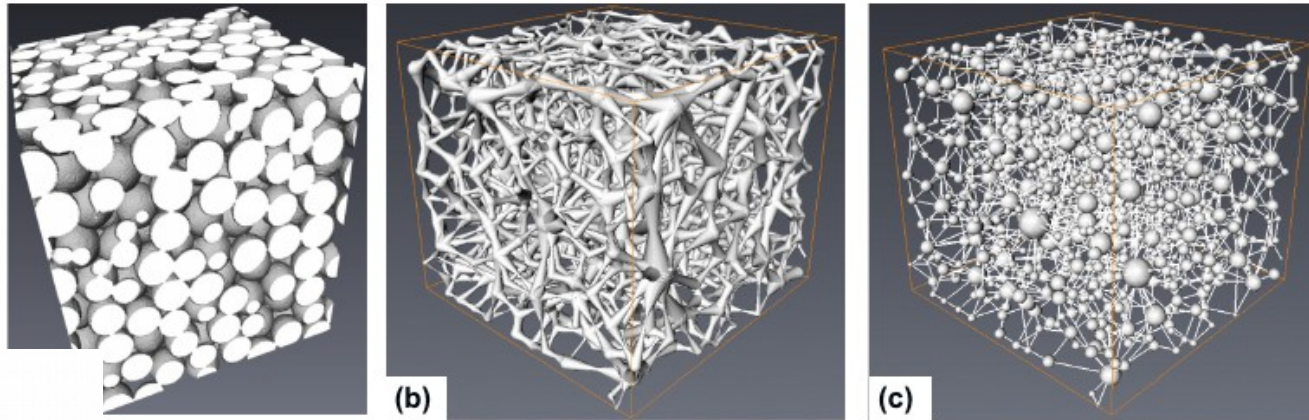
- Quasi-static rules → **Percolation theory**: vast literature and important results about flow patterns, etc.
- Used also to estimate k_r , P_c
- Drawback: structural properties are lost for other phases (e.g. solid phase)

Phase repartition according to capillary equilibrium



PNM - Dynamic

(See review: Jockar-Niasar & Hassanizadeh, 2012)



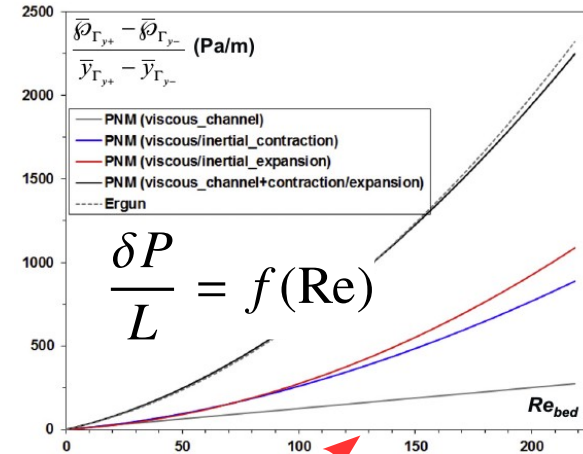
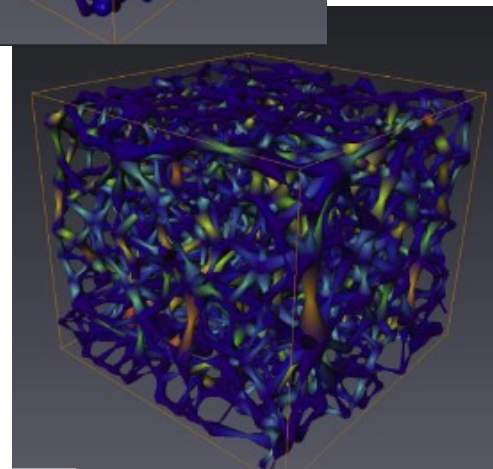
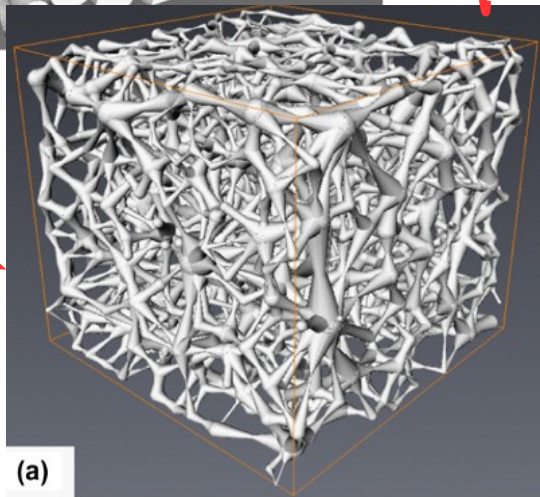
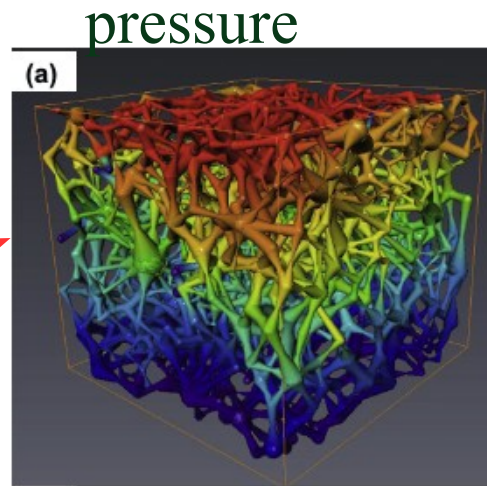
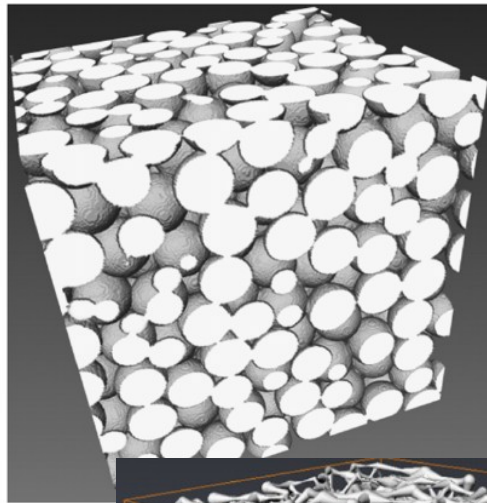
- Time dependent solution, solve for pressure field with approximate solutions for describing flow in connections
- Used to estimate k_r , P_c and other relations (hysteresis)

Pore-scale rules

(analytical: e.g. Poiseuille)



Example: application to the interpretation of tomographic images in the inertia regime



Larachi et al., 2014

velocity

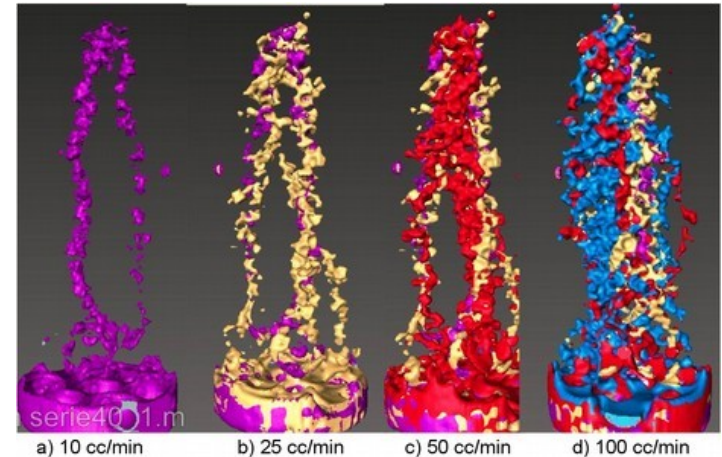


Mixed or Hybrid Models

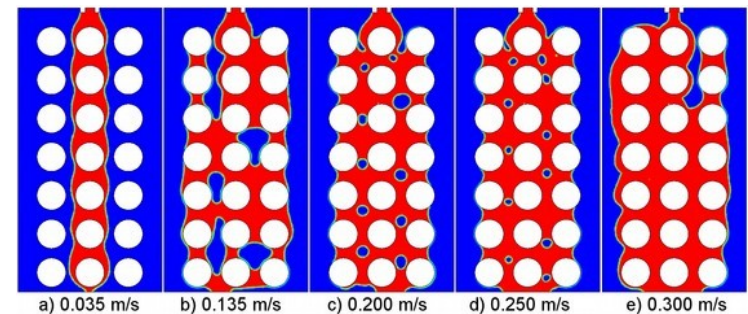
- Network models → a meso-scale representation!
- If low Re , Ca , Bo → percolation theory
- Otherwise: Coupling network model and Dynamic rules (which may come from local VOF simulations)

Melli & Scriven, 1991; Horgue et al. (PhD CIFRE/IFP/IMFT), 2012

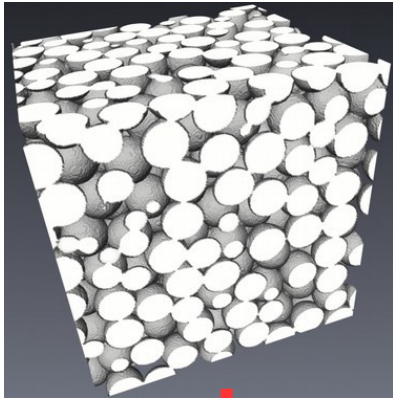
Trickle Bed (X-ray, IFP)



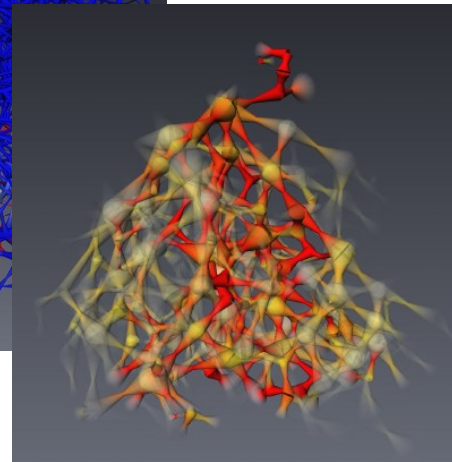
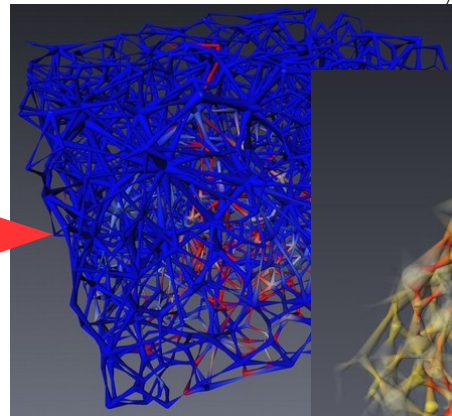
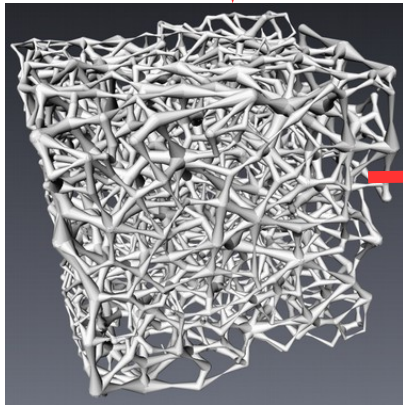
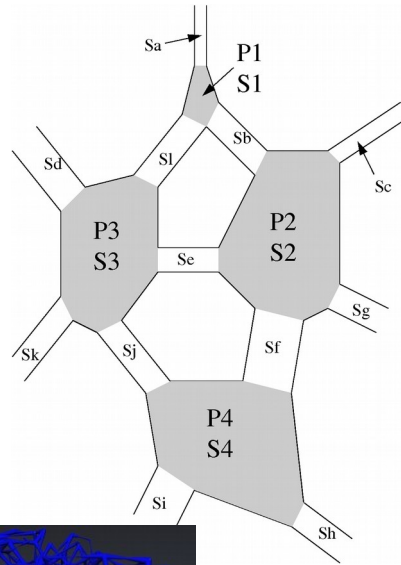
Micromodel experiments



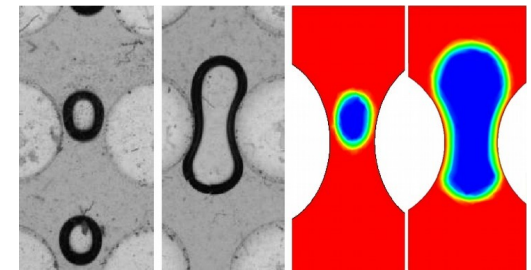
Mixed or Hybrid Models



Horgue
et al.,
2012

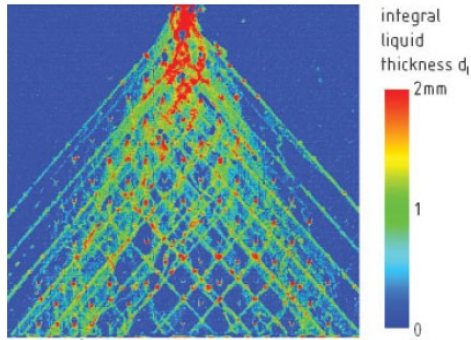


- 1.) Mass and momentum balance for the network
- 2.) Dynamic rules coming from local VOF simulations (or from experiments)



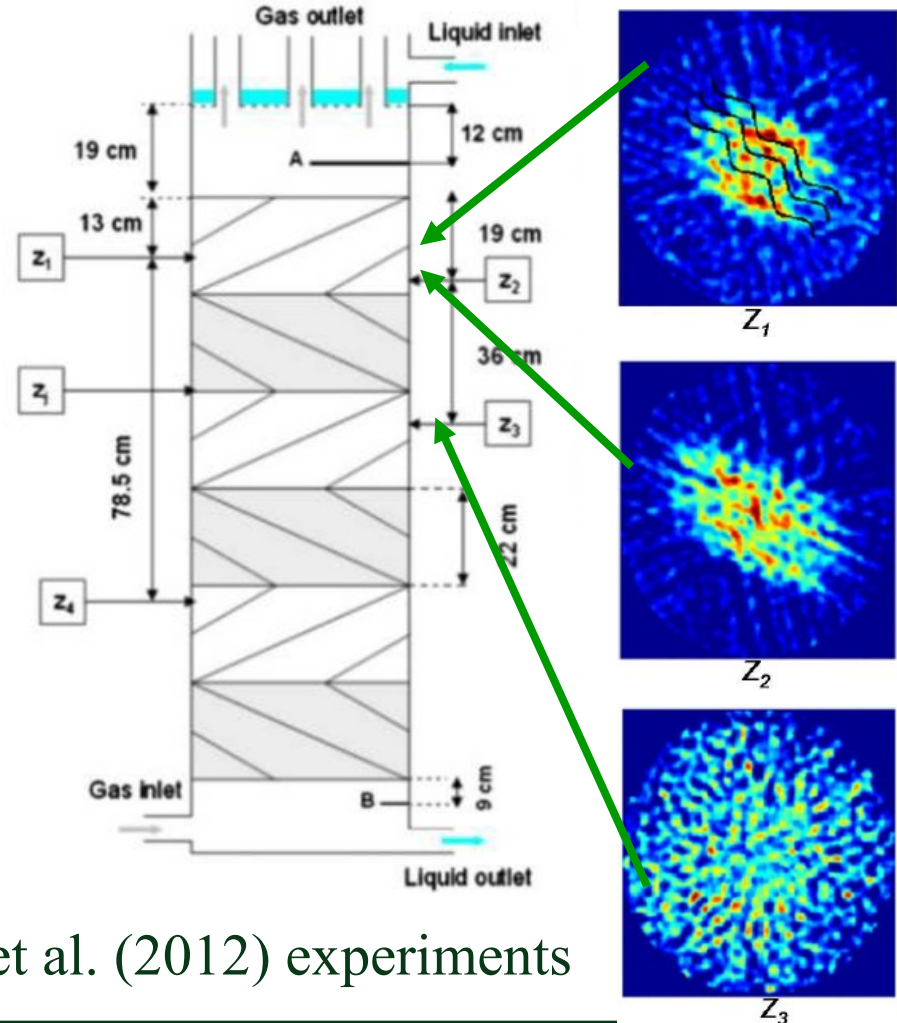
Macro-Scale Models with Phase “Splitting”

- Example: Flow through Structured Media



Mahr and Mewes (2007)

MellaPak (Sulzer Chemtech)



Fourati et al. (2012) experiments



Macro-Scale Models with Phase “Splitting”

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

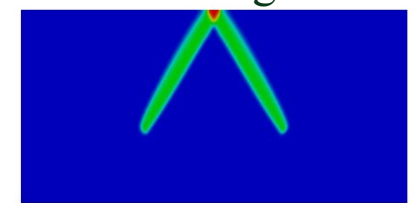
$$\varepsilon \frac{\partial S_{\beta_1}}{\partial t} + \nabla \cdot \mathbf{U}_{\beta_1} = \dot{m},$$

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

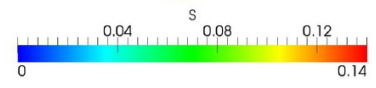
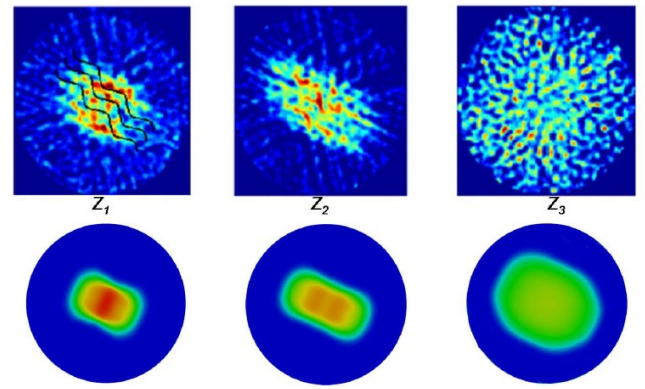
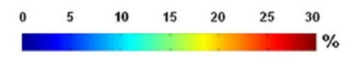
+ 3
momentum
equations

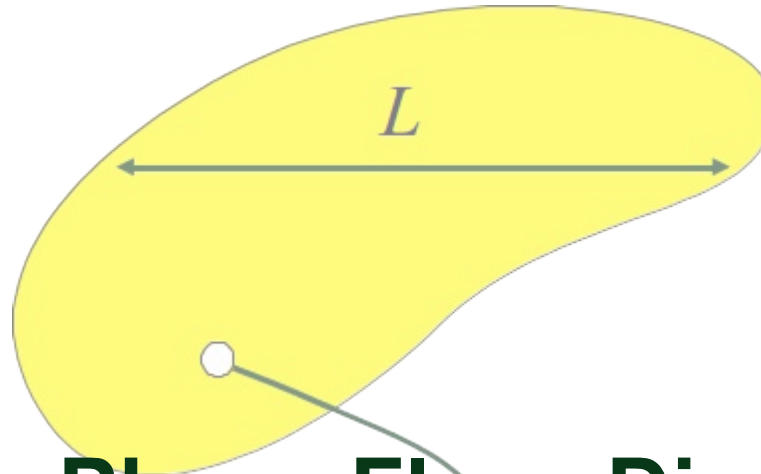
- Comparison with Fourati et al. (2012) experiments (Soullaine et al. 2014) → calibration of exchange term on the 1st stack**

Model with liquid phase splitting, no-exchange

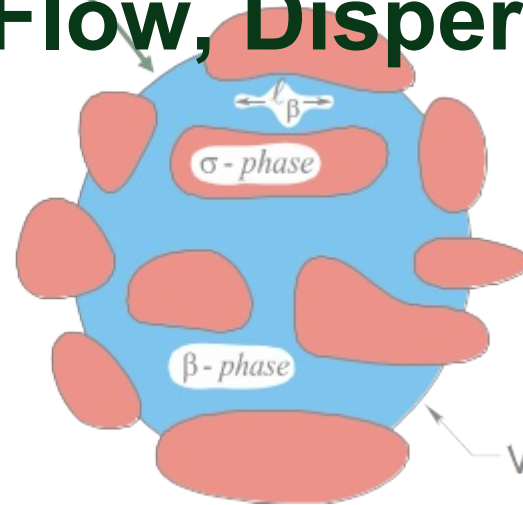


(b) t = 1 s





One-Phase Flow, Dispersion



Phenomenology

● Pore-Scale problem

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

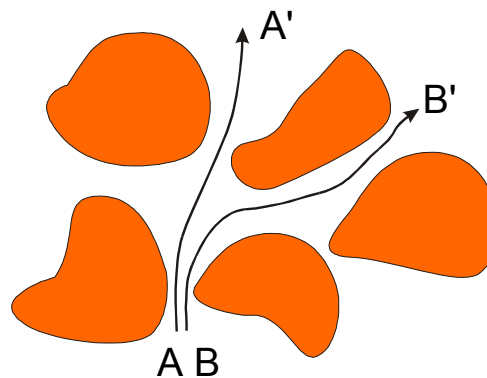
$$\frac{\partial c_\beta}{\partial t} + \nabla \cdot (c_\beta \mathbf{v}_\beta) = \nabla \cdot (D_\beta \nabla c_\beta)$$

B.C.1 $\mathbf{n}_{\beta\sigma} \cdot D_\beta \nabla c_\beta = 0$ at $A_{\beta\sigma}$ passive dispersion

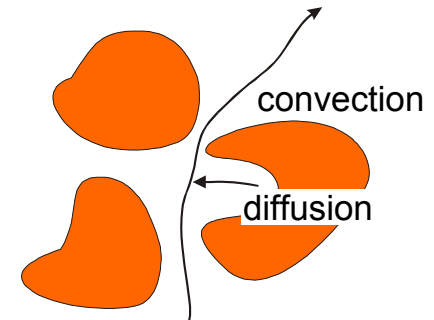
or B.C.1 $\mathbf{n}_{\beta\sigma} \cdot D_\beta \nabla c_\beta = f(c_\beta)$, at $A_{\beta\sigma}$ active dispersion



Taylor dispersion



Mechanical dispersion



Retardation due to dead-end pores



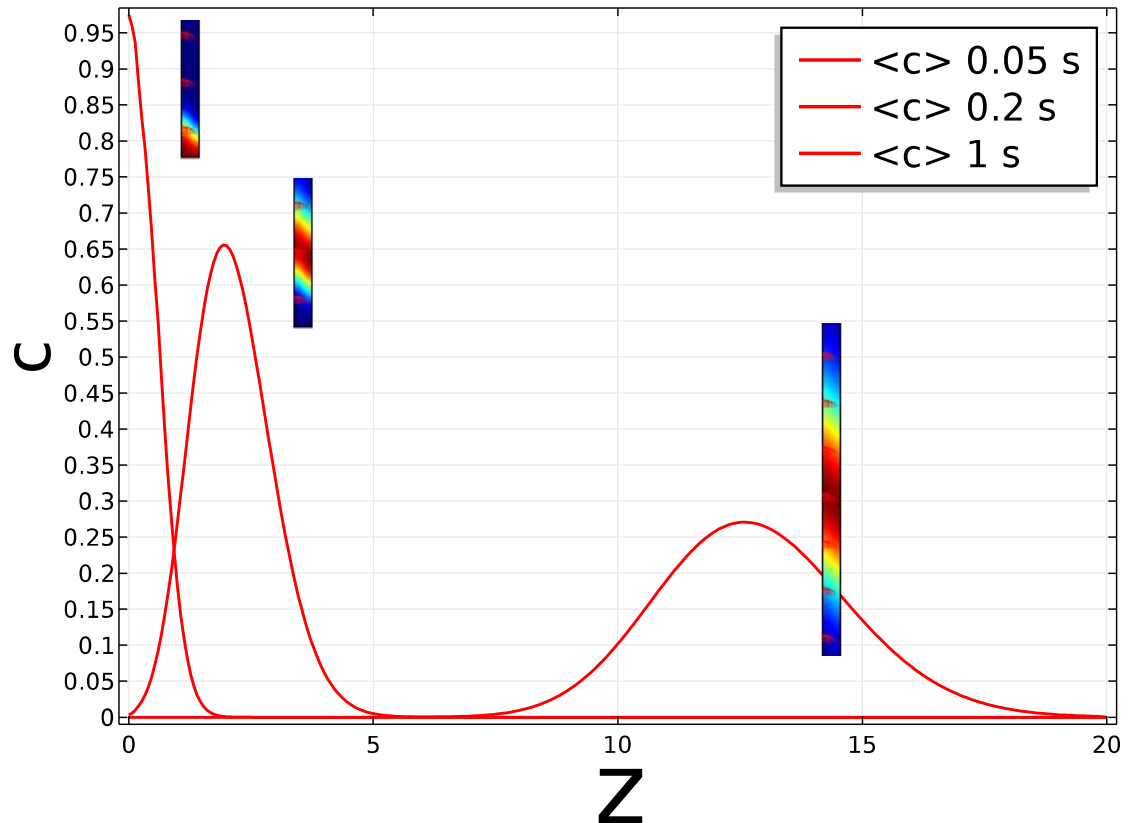
Taylor dispersion

$$\frac{\partial c_\beta}{\partial t} + \nabla \cdot (c_\beta \mathbf{v}_\beta) = \nabla \cdot (D_\beta \nabla c_\beta)$$

$$\text{B.C.1} \quad \mathbf{n}_{\beta\sigma} \cdot D_\beta \nabla c_\beta = 0 \quad \text{at } A_{\beta\sigma}$$

Which equation
for :

$$\langle c \rangle = \frac{1}{A} \int_A c \, dA ?$$



Macro-Scale Equations (tracer)

$$\nabla \cdot (\varepsilon_\beta \mathbf{U}_\beta) = \nabla \cdot (\mathbf{V}_\beta) = 0$$

$$\frac{\partial \varepsilon_\beta C_\beta}{\partial t} + \nabla \cdot (\varepsilon_\beta C_\beta \mathbf{U}_\beta) = \nabla \cdot (\varepsilon_\beta \mathbf{D}_\beta^* \cdot \nabla C_\beta)$$

Taylor dispersion : Tube : $D_\beta^* = D_\beta \left(1 + \frac{1}{192} \text{Pe}^2 \right)$ with $\text{Pe} = \frac{U_0 d}{D_\beta}$

Hele Shaw : $D_\beta^* = D_\beta \left(1 + \frac{1}{210} \text{Pe}^2 \right)$ with $\text{Pe} = \frac{U_0 b}{D_\beta}$

Linear dispersion :

$$\mathbf{D}_\beta^* = \mathbf{D}_0 + \alpha_T \|\mathbf{U}_\beta\| \mathbf{I} + (\alpha_L - \alpha_T) \frac{\mathbf{U}_\beta \mathbf{U}_\beta}{\|\mathbf{U}_\beta\|}$$

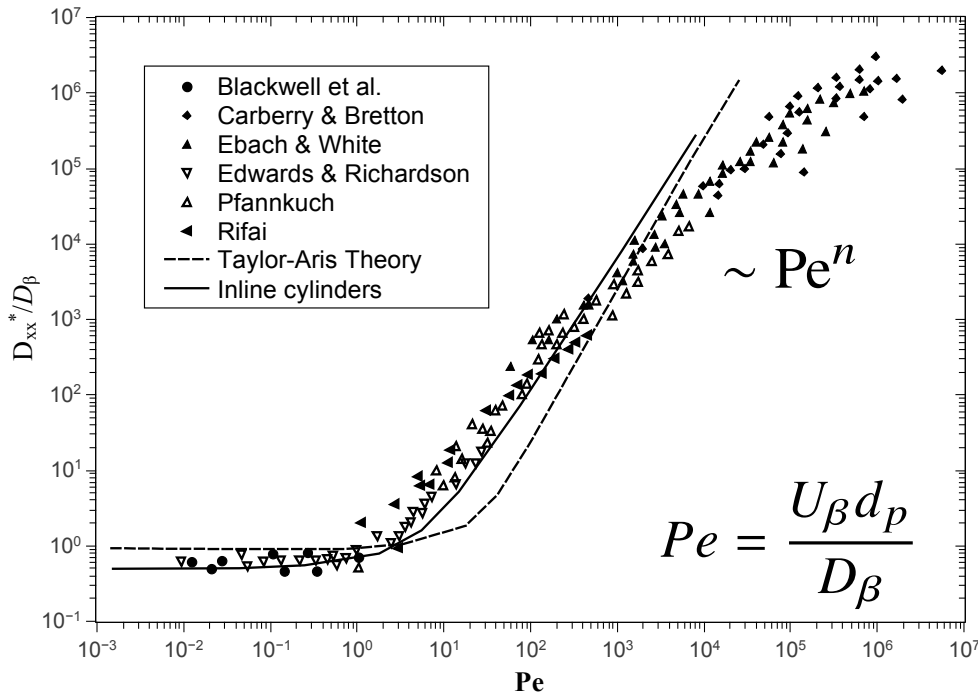
Longitudinal and transversal dispersivity

case $\mathbf{U} = U_0 \mathbf{e}_1$

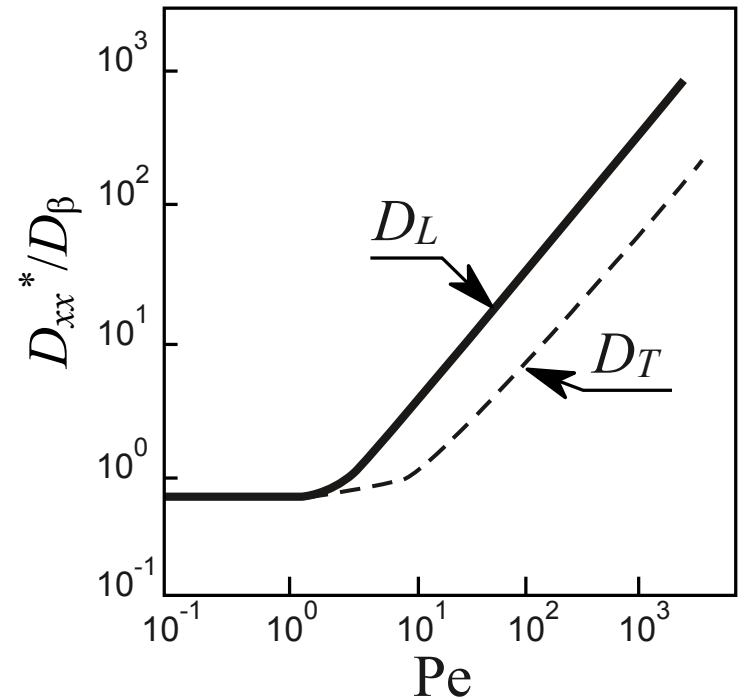
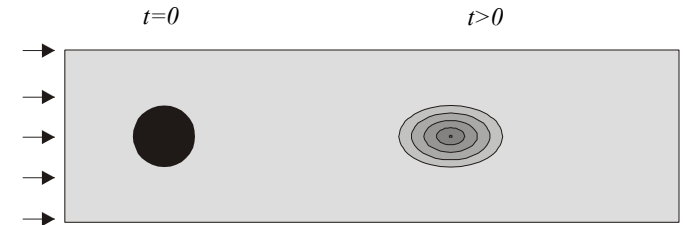
$$\mathbf{D}_\beta^* = \begin{bmatrix} \frac{D_\beta}{\tau} + \alpha_L U_0 & 0 & 0 \\ 0 & \frac{D_\beta}{\tau} + \alpha_T U_0 & 0 \\ 0 & 0 & \frac{D_\beta}{\tau} + \alpha_T U_0 \end{bmatrix}$$



Passive Dispersion



- $n=2$: Taylor dispersion
- $2 > n > 1$: from simple unit cells to highly disordered media



Active dispersion

- **Homogeneous source**

$$\frac{\partial c_\beta}{\partial t} + \nabla \cdot (c_\beta \mathbf{v}_\beta) = \nabla \cdot (D_\beta \nabla c_\beta) - k_\beta c_\beta$$

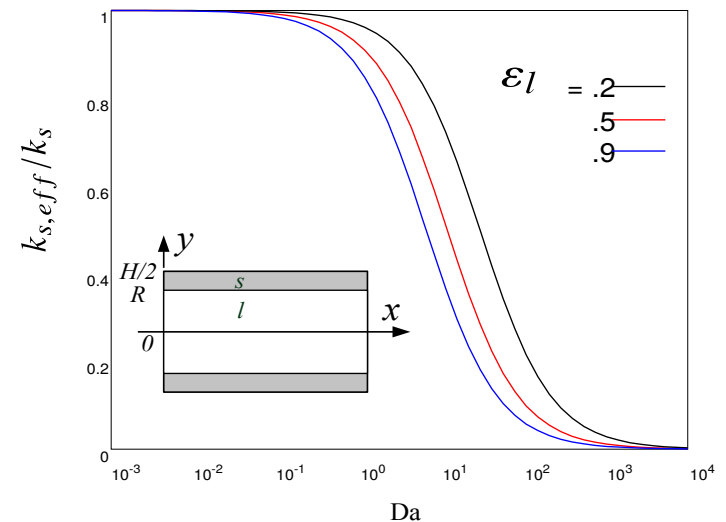
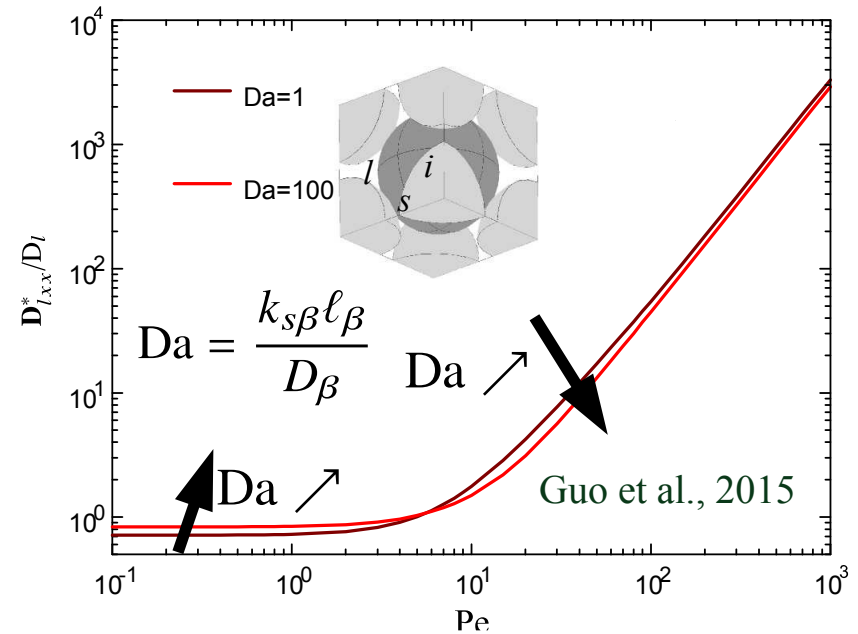
$$\Rightarrow \frac{\partial \varepsilon_\beta C_\beta}{\partial t} + \nabla \cdot (C_\beta \mathbf{V}_\beta) = \nabla \cdot (\varepsilon_\beta \mathbf{D}_\beta^* \cdot \nabla C_\beta) - \varepsilon_\beta k_\beta C_\beta$$

- **Heterogeneous source**

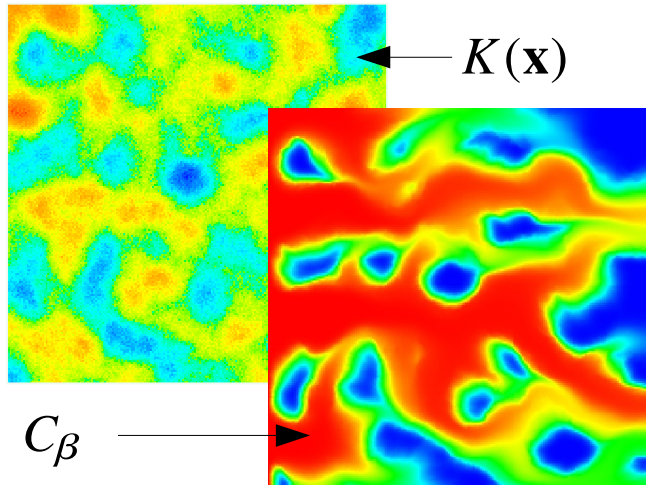
B.C. 1 $\mathbf{n}_{\beta\sigma} \cdot (D_\beta \nabla c_\beta) = -k_{s\beta} c_\beta$ at $A_{\beta\sigma}$

$$\frac{\partial \varepsilon_\beta C_\beta}{\partial t} + \nabla \cdot (C_\beta \mathbf{V}_\beta + \dots) = \nabla \cdot (\varepsilon_\beta \mathbf{D}_\beta^* \cdot \nabla C_\beta) - K_{\beta\sigma}$$

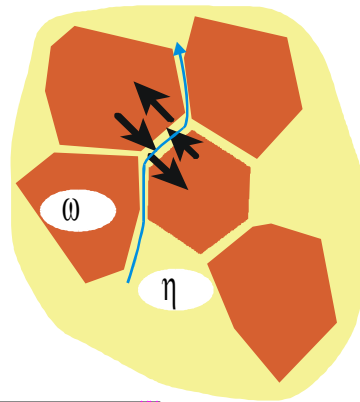
$$K_{\beta\sigma} = \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-D_\beta \nabla c_\beta) dA = a_v k_{s\beta,eff}$$



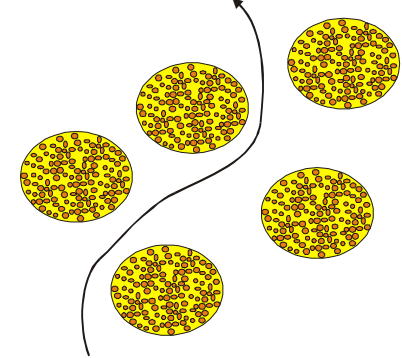
Abnormal dispersion, double-porosity models, ...



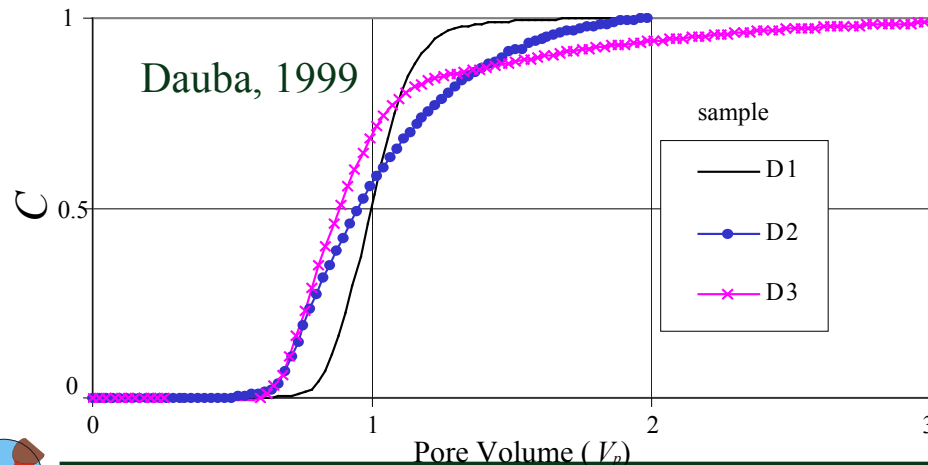
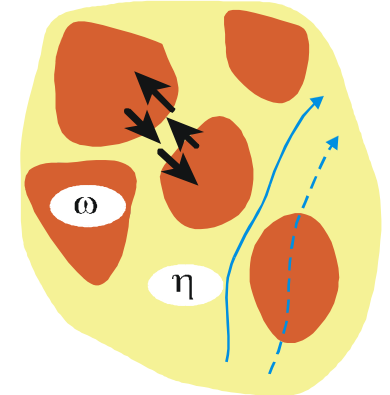
Fractured media



macro-porosity/micro-porosity



mobile/immobile
or
mobile/mobile



Non-Locality: a Simple Example

- Heterogeneous diffusion: Coupled micro-macro problem

$$\left\{ \begin{array}{l} \frac{\partial \tilde{T}}{\partial t} = \nabla \cdot (k \nabla \tilde{T}) + \nabla \cdot (\tilde{k} \nabla \langle T \rangle) - \nabla \cdot \langle k \nabla \tilde{T} \rangle \quad \text{micro} \\ \frac{\partial \langle T \rangle}{\partial t} = \nabla \cdot (\langle k \rangle \nabla \langle T \rangle + \langle k \nabla \tilde{T} \rangle) \quad \text{macro} \end{array} \right.$$

- Solution in Laplace space

$$f_{LT}(p) = \int_0^{\infty} e^{-pt} f(t) dt$$



Solution in the Laplace Space

- **Micro-scale and macro-scale equations (IC: uniform field)**

$$\left\{ \begin{array}{ll} p\tilde{T}_{LT} = \nabla \cdot (k\nabla\tilde{T}_{LT}) + \nabla \cdot (\tilde{k}\nabla\langle T\rangle_{LT}) - \nabla \cdot \langle k\nabla\tilde{T}_{LT} \rangle & \text{micro} \\ p\langle T\rangle_{LT} = \nabla \cdot (\langle k \rangle \nabla \langle T \rangle_{LT} + \langle k\nabla\tilde{T}_{LT} \rangle) & \text{macro} \end{array} \right.$$

- **Closure** $\tilde{T}_{LT} = p\mathbf{b}_{LT} \cdot \nabla \langle T \rangle_{LT}$

$$p\mathbf{b}_{LT} = \nabla \cdot (k\nabla\mathbf{b}_{LT}) + \frac{1}{p}\nabla \cdot \tilde{k}\mathbf{I} - \nabla \cdot \langle k\nabla\mathbf{b}_{LT} \rangle \quad +\text{period.}, \dots$$

- **Macro-scale Equation**

$$p\langle T \rangle_{LT} = \nabla \cdot (\langle k \rangle \nabla \langle T \rangle_{LT} + \langle k\nabla(p\mathbf{b}_{LT} \cdot \nabla \langle T \rangle_{LT}) \rangle)$$



Transient / Steady-State Closure (~asymptotic behavior)

- **Transient Closure**

$$\tilde{T} = \int_0^t \left. \frac{\partial \mathbf{b}}{\partial \tau} \right|_{\tau} \cdot \nabla \langle T \rangle |_{t-\tau} d\tau = \frac{\partial \mathbf{b}}{\partial t} * \cdot \nabla \langle T \rangle$$

$$\frac{\partial \mathbf{b}}{\partial t} = \nabla \cdot (k \nabla \mathbf{b}) + \nabla \cdot \tilde{\mathbf{k}} \mathbf{I} - \nabla \cdot \langle k \nabla \mathbf{b} \rangle$$

+period., ...

- **Steady-State closure**

$$\mathbf{b} = \text{const.} = \lim_{t \rightarrow \infty} \mathbf{b}(t) = \mathbf{b}_{\infty}$$

$$\tilde{T} = \mathbf{b}_{\infty} \cdot \nabla \langle T \rangle$$

$$\frac{\partial \langle T \rangle}{\partial t} = \nabla \cdot \left(\mathbf{K}_{eff} * \cdot \nabla \langle T \rangle \right)$$

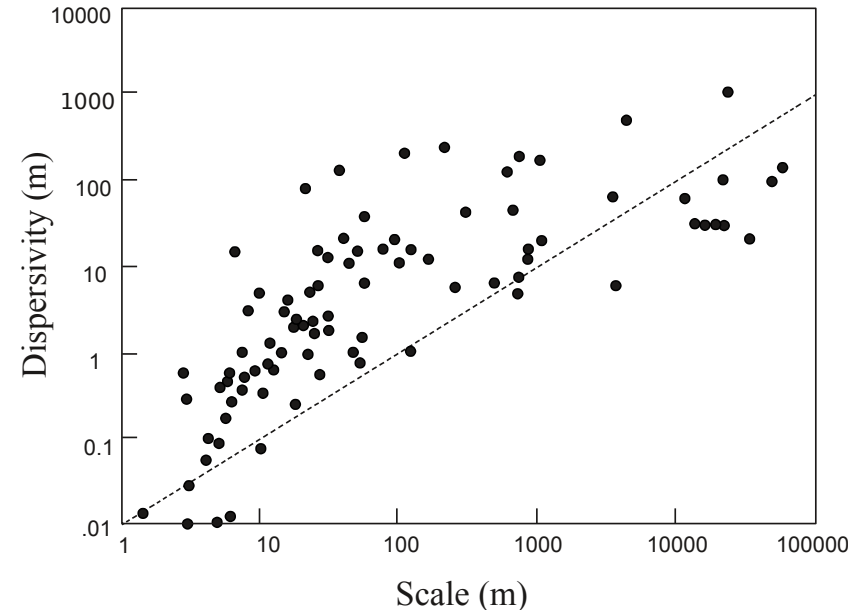
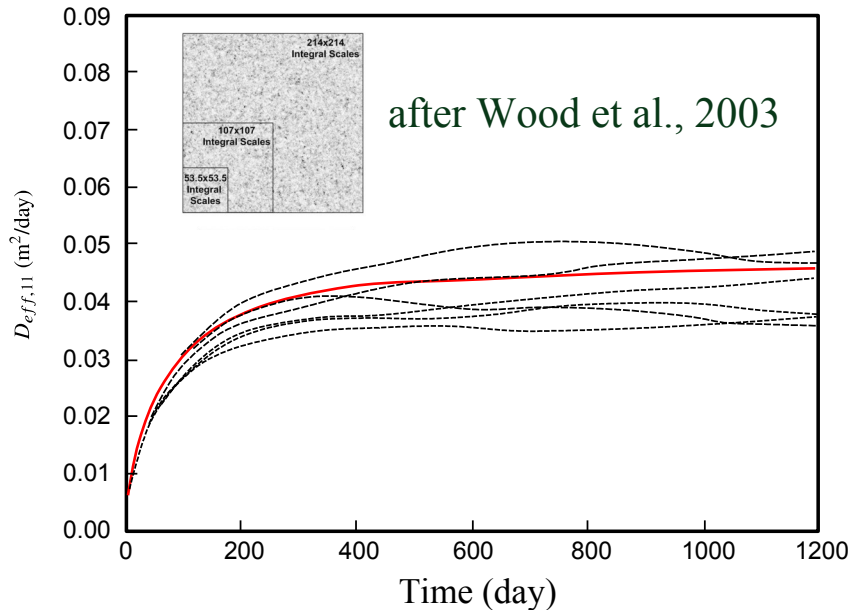
$$\frac{\partial \langle T \rangle}{\partial t} = \nabla \cdot \left(\mathbf{K}_{eff}^{\infty} \cdot \nabla \langle T \rangle \right)$$

with $\mathbf{K}_{eff} = \langle k \rangle \mathbf{I} + \left\langle k \nabla \frac{\partial \mathbf{b}}{\partial t} \right\rangle$

$$\mathbf{K}_{eff}^{\infty} = \langle k \rangle \mathbf{I} + \langle k \nabla \mathbf{b}_{\infty} \rangle$$



Abnormal dispersion in heterogeneous media



Long time/length for reaching « Fickian » dispersion !

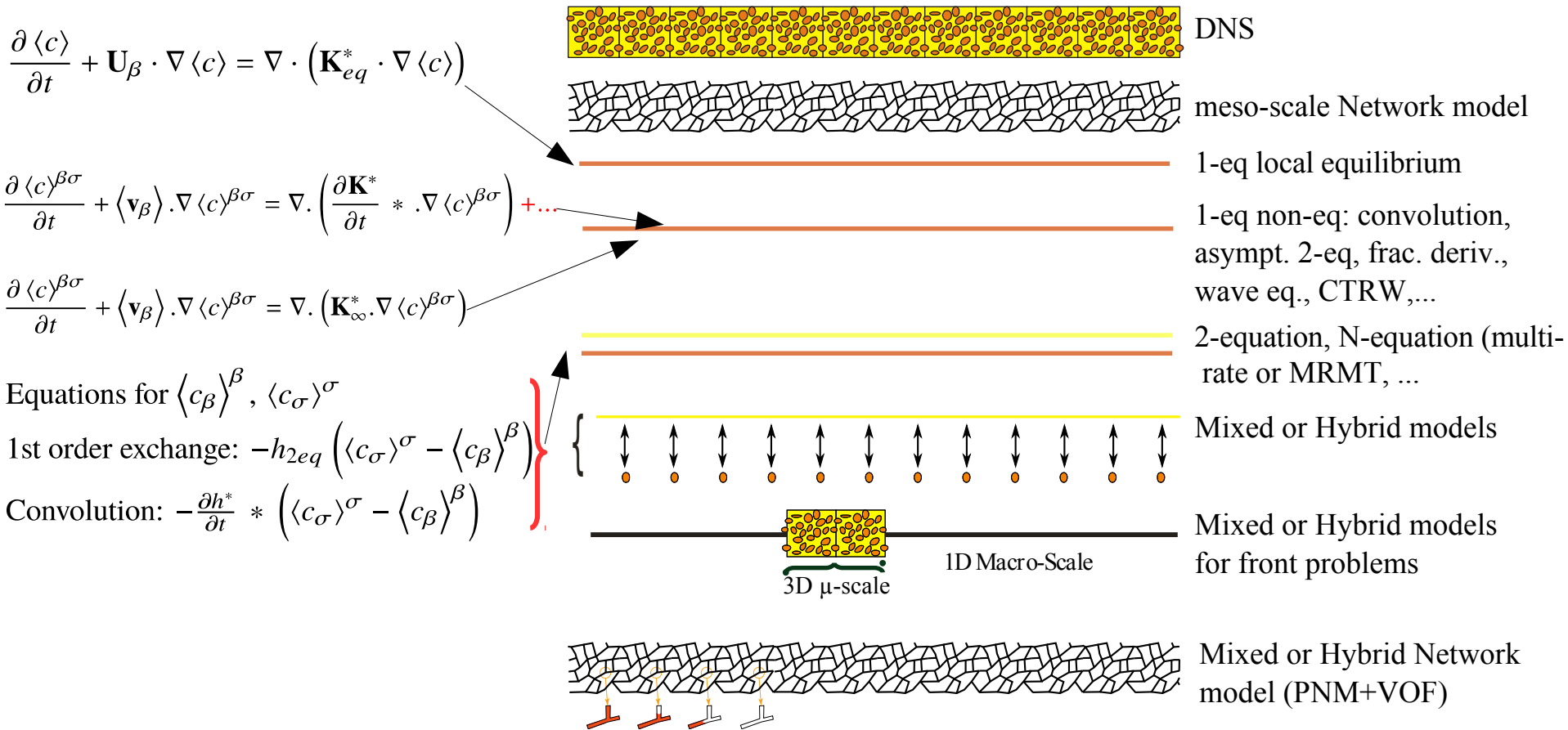
Dispersivity appears length-scale dependent ! (Gelhar and Axness, 1983)

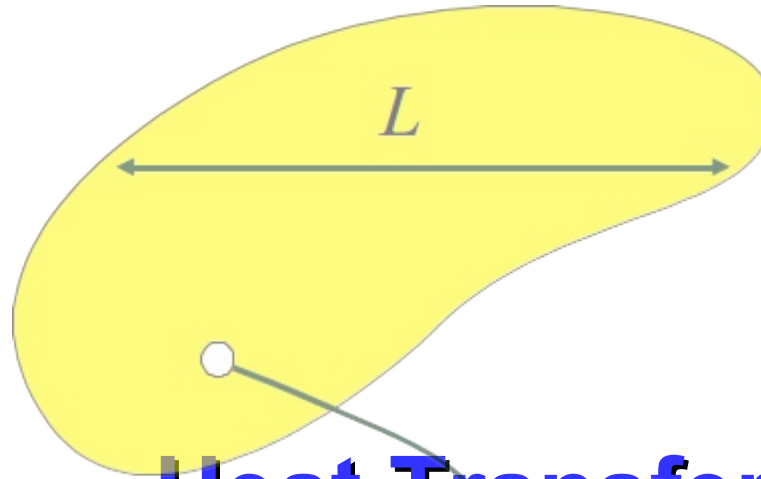
→ advice: keep as much heterogeneities as possible !



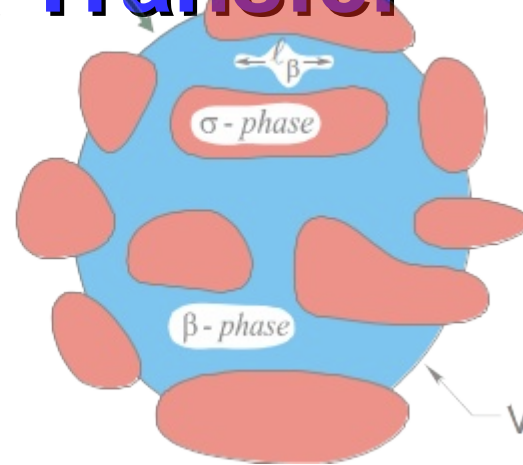
Various models available

Ex.: two-region



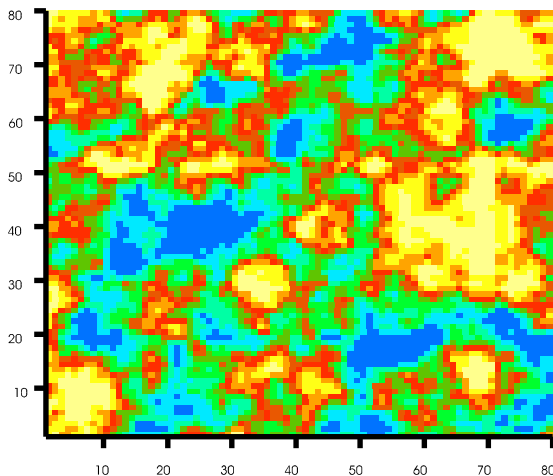


Heat Transfer

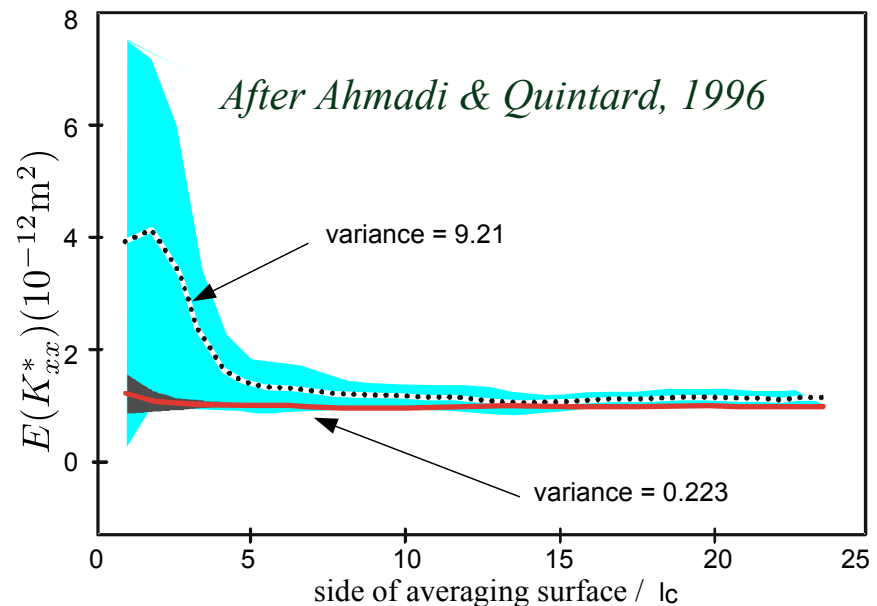


(recall) Diffusion in a heterogenous system : Effective Conductivity

$$\nabla \cdot (\mathbf{k}(x) \cdot \nabla T) = 0 \quad \Rightarrow \quad \left\{ \begin{array}{l} \nabla \cdot (\mathbf{K}_{eff} \cdot \nabla \mathcal{T}) = 0 \\ \mathcal{T} = \langle T \rangle \\ \mathbf{K}_{eff} = \langle \mathbf{k} \rangle + \langle \mathbf{k} \cdot \nabla \mathbf{b} \rangle \end{array} \right. \quad \nabla \cdot (\mathbf{k} \cdot \nabla \mathbf{b}) = -\nabla \cdot \tilde{\mathbf{k}} + \dots$$



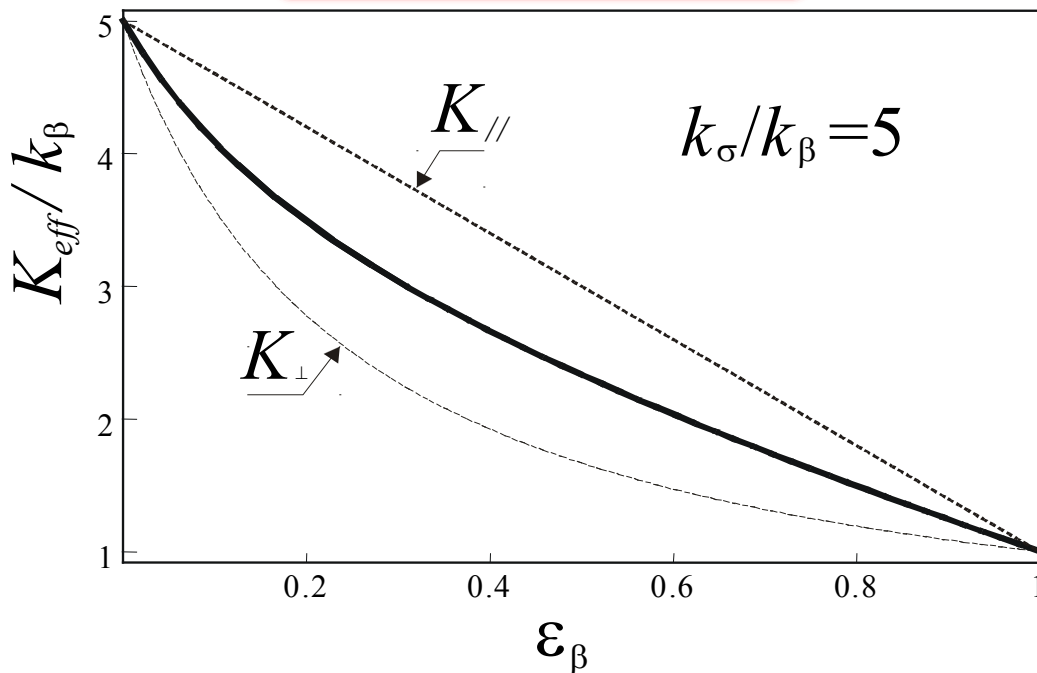
log-normal $k(x)$, spatially correlated



Bounds

Wiener, 1912: $\frac{1}{K_{\perp}} = \frac{\varepsilon_{\sigma}}{k_{\sigma}} + \frac{\varepsilon_{\beta}}{k_{\beta}}$; $K_{\parallel} = \varepsilon_{\sigma}k_{\sigma} + \varepsilon_{\beta}k_{\beta}$

$$K_{\perp} \leq K_{eff} \leq K_{\parallel}$$



Maxwell, 1873

$$K_{eff} = \varepsilon_{\sigma}k_{\sigma} + \varepsilon_{\beta}k_{\beta} - \frac{\varepsilon_{\sigma}\varepsilon_{\beta}(k_{\sigma} - k_{\beta})^2}{\varepsilon_{\beta}k_{\sigma} + \varepsilon_{\sigma}k_{\beta} + 2k_{\beta}}$$

See also Poisson, Mosotti, Lorenz

Landau and Lifshitz
(1960)

$$K_{eff} = K_{\parallel}^{2/3} K_{\perp}^{1/3}$$



Bounds...

Hashin & Shtrikman, 1963 (isotropic media): $k_\beta > k_\sigma$ d , space dimension

$$\varepsilon_\sigma k_\sigma + \varepsilon_\beta k_\beta - \frac{\varepsilon_\sigma \varepsilon_\beta (k_\beta - k_\sigma)^2}{\varepsilon_\beta k_\sigma + \varepsilon_\sigma k_\beta + k_\sigma (d-1)} \leq K_{eff} \leq \varepsilon_\sigma k_\sigma + \varepsilon_\beta k_\beta - \frac{\varepsilon_\sigma \varepsilon_\beta (k_\beta - k_\sigma)^2}{\varepsilon_\beta k_\sigma + \varepsilon_\sigma k_\beta + k_\beta (d-1)}$$

Lichtenecker, 1926: $K_{eff} = k_\sigma^{\varepsilon_\sigma} k_\beta^{\varepsilon_\beta}$

Bruggeman (1935): $\sum_i \varepsilon_i \frac{k_i - k_{eff}}{k_i + (d-1)k_{eff}} = 0$ Spherical inclusions

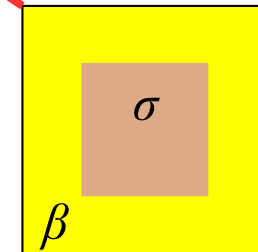
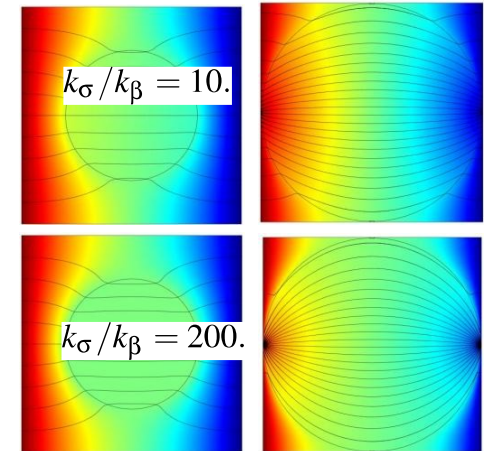
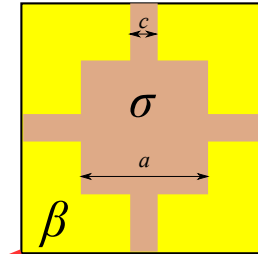
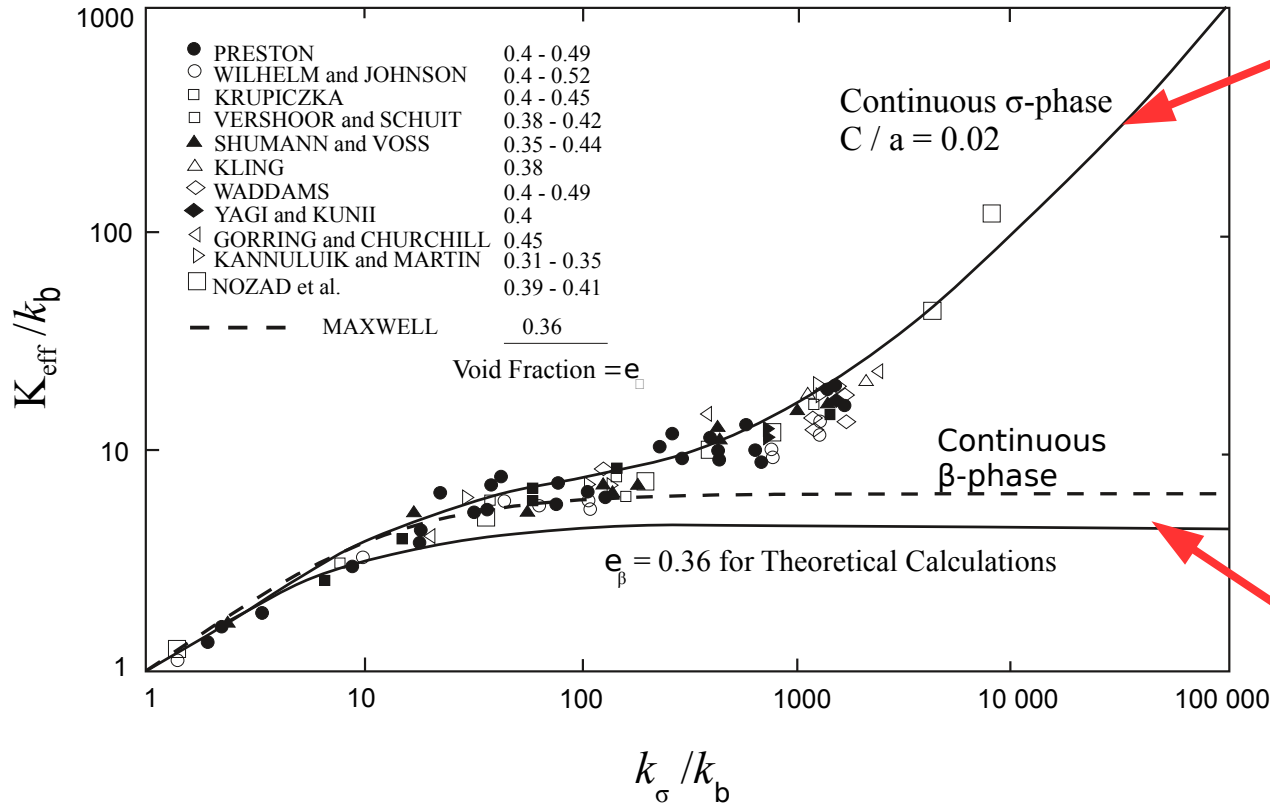
see: *Cellular and Porous Materials: Thermal Properties Simulation and Prediction*, Edited by Andreas Ochsner, Graeme E. Murch, and Marcelo J.S. de Lemos, WILEY, 2008.

Hashin, Z. & Shtrikman, S. A., Variational approach to the theory of the elastic behaviour of multiphase materials, *Journal of the Mechanics and Physics of Solids*, 1963, 11, 127 - 140

...numerous literature!



Effect of contact points

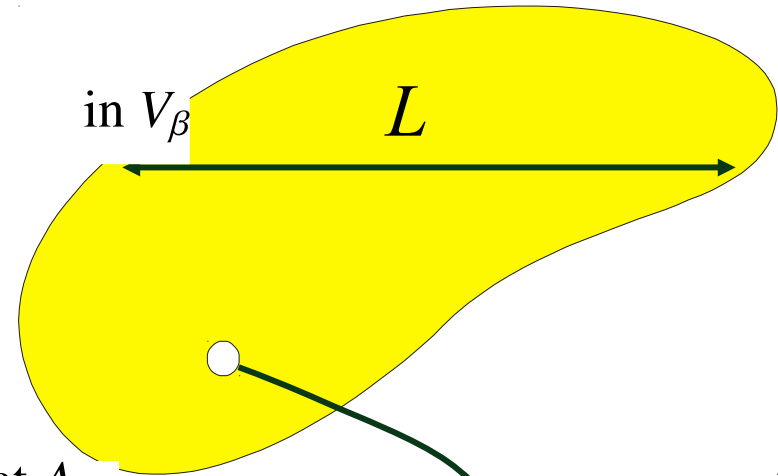


(Nozad et al., 1985)



Two-Phase, Unsteady Problem

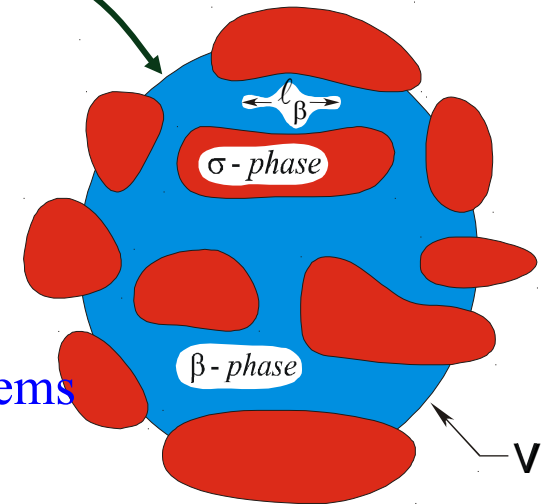
$$(\rho c_p)_\beta \frac{\partial T_\beta}{\partial t} + (\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla T_\beta = \nabla \cdot (k_\beta \nabla T_\beta) \quad \text{in } V_\beta$$



$$\text{B.C.1} \quad T_\beta = T_\sigma \quad \text{at } A_{\beta\sigma}$$

$$\text{B.C.2} \quad -\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla T_\beta = -\mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla T_\sigma \quad \text{at } A_{\beta\sigma}$$

$$\rho_\sigma C_\sigma \frac{\partial T_\sigma}{\partial t} = \nabla \cdot (k_\sigma \nabla T_\sigma) \quad \text{in } V_\sigma$$



Note: decoupled mass and momentum balance problems
 → Darcy, Darcy-Brinkman, etc...



Macro-scale Temperatures

- Temperature not additive: ~OK to use phase average

$$\mathcal{T}_\beta = \langle T_\beta \rangle^\beta = \frac{1}{\mathcal{V}_\beta} \int_{\mathcal{V}_\beta} T_\beta dV$$

$$\mathcal{T}_\sigma = \langle T_\sigma \rangle^\sigma = \frac{1}{\mathcal{V}_\sigma} \int_{\mathcal{V}_\sigma} T_\sigma dV$$

- Mixture Temperature

$$\langle T \rangle^{\beta\sigma} = \frac{\left(\varepsilon_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta + (\rho c_p)_\sigma \langle T_\sigma \rangle^\sigma \right)}{\left(\varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma \right)}$$

- Phenomenology

- Contrast of parameters → different regimes

- Local equilibrium :

$$\langle T_\beta \rangle^\beta = \langle T_\sigma \rangle^\sigma = \langle T \rangle = \langle T \rangle^{\beta\sigma}$$

- Non-equilibrium models



Upscaling (eqs for β -phase)

$$T_\beta = \langle T_\beta \rangle^\beta + \tilde{T}_\beta \quad T_\sigma = \langle T_\sigma \rangle^\sigma + \tilde{T}_\sigma$$

Micro:

$$(\rho c_p)_\beta \frac{\partial \tilde{T}_\beta}{\partial t} + (\rho c_p)_\beta \tilde{\mathbf{v}}_\beta \cdot \nabla \langle T_\beta \rangle^\beta + (\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla \tilde{T}_\beta = \nabla \cdot (k_\beta \nabla \tilde{T}_\beta) - \varepsilon_\beta^{-1} \nabla \cdot \left(k_\beta \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_\beta dA \right) - \varepsilon_\beta^{-1} k_\beta \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \nabla \tilde{T}_\beta dA$$

Macro:

$$\underbrace{\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t}}_{\text{accumulation}} + \underbrace{\varepsilon_\beta (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle^\beta \cdot \nabla \langle T_\beta \rangle^\beta}_{\text{convection}} = \underbrace{\nabla \cdot \left[k_\beta \left(\varepsilon_\beta \nabla \langle T_\beta \rangle^\beta + \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_\beta dA \right) \right]}_{\text{conduction}} - \underbrace{(\rho c_p)_\beta \nabla \cdot \langle \tilde{\mathbf{v}}_\beta \tilde{T}_\beta \rangle}_{\text{dispersion}} + \underbrace{\frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla T_\beta dA}_{\text{interfacial flux}}$$

spatial and time non-locality!



Upscaling: BCs, time scales

$$\text{B.C.:} \quad \tilde{T}_\beta = \tilde{T}_\sigma - \underbrace{\left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right)}_{\text{source term}}$$

$$-\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \tilde{T}_\beta - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \langle T_\beta \rangle^\beta}_{\text{source term}} = -\mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \tilde{T}_\sigma - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \langle T_\sigma \rangle^\sigma}_{\text{source term}}$$

different time-scales: if (but not sufficient condition...)

$$\left(\frac{(\rho c_p)_\beta l_\beta^2}{k_\beta} \approx \frac{(\rho c_p)_\sigma l_\sigma^2}{k_\sigma} \right) \ll \left(\frac{\varepsilon_\beta (\rho c_p)_\beta L^2}{K_\beta^*} \approx \frac{\varepsilon_\sigma (\rho c_p)_\sigma L^2}{K_\sigma^*} \right)$$

→ **local equilibrium**



I - Local Equilibrium \rightarrow 1-Eq model

$$\langle T_\beta \rangle^\beta = \langle T_\sigma \rangle^\sigma = \langle T \rangle = \langle T \rangle^{\beta\sigma} \quad (\text{Carbonell \& Whitaker, 84; Nozad et al, 85; ...})$$

$$\varepsilon_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta + \varepsilon_\sigma (\rho c_p)_\sigma \langle T_\sigma \rangle^\sigma = (\rho c_p)^* \langle T \rangle \quad (\rho c_p)^* = \varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma$$

Closure: $\tilde{T}_\beta = \mathbf{b}_\beta \cdot \nabla \langle T \rangle + O(\ell^2/L^2) \quad \tilde{T}_\sigma = \mathbf{b}_\sigma \cdot \nabla \langle T \rangle + O(\ell^2/L^2)$

$$(\rho c_p)^* \frac{\partial \langle T \rangle}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta \mathbf{U}_\beta \cdot \nabla \langle T \rangle = \nabla \cdot (\mathbf{K}_{eff} \cdot \nabla \langle T \rangle)$$

with: $\left\{ \begin{array}{l} \mathbf{U}_\beta = \langle \mathbf{v}_\beta \rangle^\beta \\ \mathbf{K}_{eff} = (\varepsilon_\beta k_\beta + \varepsilon_\sigma k_\sigma) \mathbf{I} + \underbrace{\frac{(k_\beta - k_\sigma)}{V} \int_{A_{\beta\sigma}} (\mathbf{n}_{\beta\sigma} \mathbf{b}_\beta) dA}_{\text{tortuosity}} - \underbrace{(\rho c_p)_\beta \langle \tilde{\mathbf{v}}_\beta \mathbf{b}_\beta \rangle}_{\text{dispersion}} \end{array} \right.$



LE Closure Problem

dispersion

$$(\rho c_p)_{\beta} \tilde{\mathbf{v}}_{\beta} + (\rho c_p)_{\beta} \mathbf{v}_{\beta} \cdot \nabla \mathbf{b}_{\beta} = k_{\beta} \nabla^2 \mathbf{b}_{\beta} \quad \text{in } V_{\beta}$$

$$\begin{aligned} \text{B.C.1} \quad -\mathbf{n}_{\beta\sigma} \cdot k_{\beta} \nabla \mathbf{b}_{\beta} - \mathbf{n}_{\beta\sigma} k_{\beta} = \\ -\mathbf{n}_{\beta\sigma} \cdot k_{\sigma} \nabla \mathbf{b}_{\sigma} - \mathbf{n}_{\beta\sigma} k_{\sigma} \quad \text{at } A_{\beta\sigma} \end{aligned}$$

$$\text{B.C.2} \quad \mathbf{b}_{\beta} = \mathbf{b}_{\sigma} \quad \text{at } A_{\beta\sigma}$$

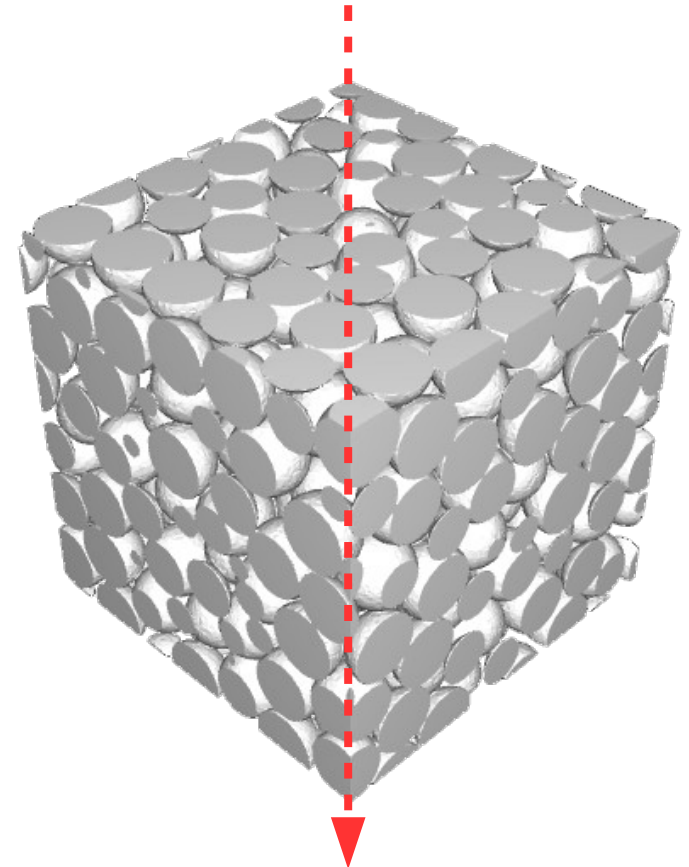
$$0 = k_{\sigma} \nabla^2 \mathbf{b}_{\sigma} \quad \text{in } V_{\sigma}$$

$$\mathbf{b}_{\beta}(\mathbf{x} + \mathbf{l}_i) = \mathbf{b}_{\beta}(\mathbf{x}) ; \mathbf{b}_{\sigma}(\mathbf{x} + \mathbf{l}_i) = \mathbf{b}_{\sigma}(\mathbf{x})$$

$$\langle \mathbf{b}_{\beta} \rangle = 0 ; \langle \mathbf{b}_{\sigma} \rangle = 0$$

tortuosity

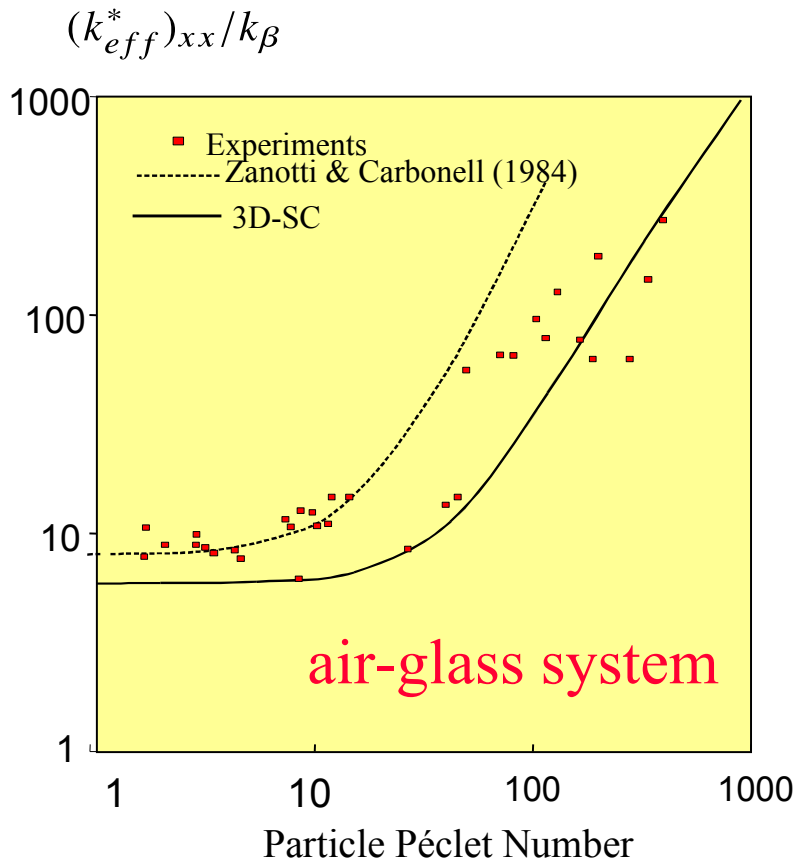
solve for \mathbf{b}



compute \mathbf{K}_{eff}



Application: Thermal Dispersion

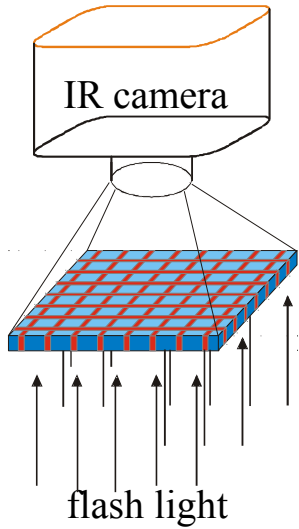


Quintard et al., 1997

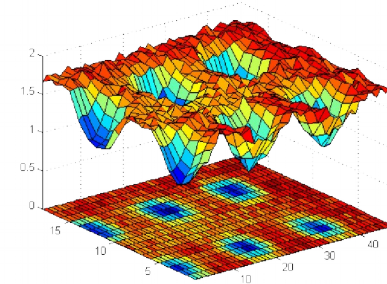
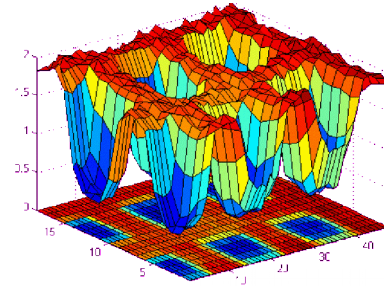
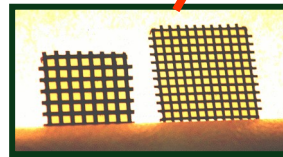
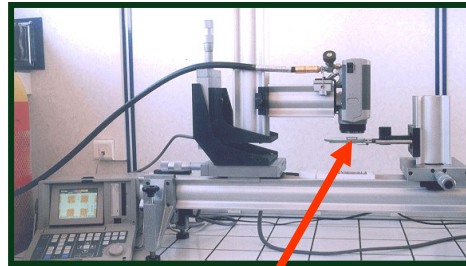
- **experiments:** Yagi et al., 1960; Gunn and De Souza, 1974
- Zanotti & Carbonell, 1984: fitted at low Pe, square root dependence at large Pe (Taylor's dispersion)
- Quintard & al., 1997: 3D results



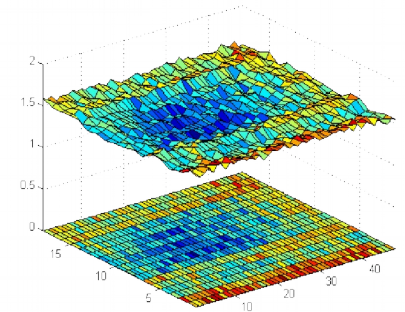
Example of Non-Equilibrium



Ramond et al., 98



$t \rightarrow \infty$



II - Local Non-Equilibrium: Various closures for 2-Eq models

- **transient closure** (→ convolution product, at least in time)

$$\begin{aligned}\tilde{T}_\beta &= -\frac{\partial s_\beta}{\partial t} * \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \frac{\partial \mathbf{b}_{\beta\beta}}{\partial t} * \nabla \langle T_\beta \rangle^\beta + \frac{\partial \mathbf{b}_{\beta\sigma}}{\partial t} * \nabla \langle T_\sigma \rangle^\sigma + \dots \\ \tilde{T}_\sigma &= +\frac{\partial s_\sigma}{\partial t} * \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + \frac{\partial \mathbf{b}_{\sigma\beta}}{\partial t} * \nabla \langle T_\beta \rangle^\beta + \frac{\partial \mathbf{b}_{\sigma\sigma}}{\partial t} * \nabla \langle T_\sigma \rangle^\sigma + \dots\end{aligned}$$

- **quasi-steady closure**

$$\begin{aligned}\tilde{T}_\beta &= -s_\beta \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \mathbf{b}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + \dots \\ \tilde{T}_\sigma &= +s_\sigma \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + \mathbf{b}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + \dots\end{aligned}$$

- **other ...** Hsu (1999), Nakayama, ... *DeGroot & Straatman, 2011*

$$\tilde{T}_\beta = -s_\beta \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \mathbf{b}_\beta \cdot \nabla \langle T_\beta \rangle^\beta + \dots$$

- **n-th order closure** (see Davit and Quintard, 2014, for n=2)



Local Non-Equilibrium Models: 1st order 2-Eq model

- Volume averaging theory, 1st order, quasi-steady closure

(Carbonell & Whitaker, 84; Zanotti & Carbonell, 84; Quintard & Whitaker, 93, 95, 97; Quintard et al., 96;

$$\varepsilon_{\beta} (\rho c_p)_{\beta} \frac{\partial \langle T_{\beta} \rangle^{\beta}}{\partial t} + (\rho c_p)_{\beta} \langle \mathbf{v}_{\beta} \rangle \cdot \nabla \langle T_{\beta} \rangle^{\beta} - \dots = \nabla \cdot \left(\mathbf{K}_{\beta\beta}^* \cdot \nabla \langle T_{\beta} \rangle^{\beta} + \dots \right) + q_{\beta\sigma}$$

$$\varepsilon_{\sigma} (\rho c_p)_{\sigma} \frac{\partial \langle T_{\sigma} \rangle^{\sigma}}{\partial t} - \dots = \nabla \cdot \left(\mathbf{K}_{\sigma\sigma}^* \cdot \nabla \langle T_{\sigma} \rangle^{\sigma} + \dots \right) - q_{\beta\sigma}$$

$$q_{\beta\sigma} = -h_{2eq} \left(\langle T_{\beta} \rangle^{\beta} - \langle T_{\sigma} \rangle^{\sigma} \right) + \dots$$

Similar to heuristic models if no non-conventional terms (in red)!



Various estimates for the 1st order exchange coefficient (diffusive case)!

Consequence: various values from inverse methods with \neq objective functions

	Stratified System	2D-Rectangular System	3D-Parallelepiped System	
Linked to 1st eigenvalue	Asymptotic Value	$\pi^2 k_\sigma / l^2$	$\pi^2 k_\sigma \left(\frac{2}{l^2} \right)$	$\pi^2 k_\sigma \left(\frac{3}{l^2} \right)$
Parabolic profile, also literature on LDF models, Liaw et al. (1979)	Warren & Root (1963)	$12 k_\sigma / l^2$	$16 k_\sigma \left(\frac{2}{l^2} \right)$	$20 k_\sigma \left(\frac{3}{l^2} \right)$
Linear Hat profile	Kazemi et al. (1976, 1992)	$4 k_\sigma / l^2$	$4 k_\sigma \left(\frac{1}{l_x^2} + \frac{1}{l_y^2} \right)$	$4 k_\sigma \left(\frac{1}{l_x^2} + \frac{1}{l_y^2} + \frac{1}{l_z^2} \right)$
Linked to harmonic mean of eigenvalues!	Quintard & Whitaker (1992)	$12 k_\sigma / l^2$	$14.22 k_\sigma \left(\frac{1}{l_x^2} + \frac{1}{l_y^2} \right)$	$16.54 k_\sigma \left(\frac{1}{l_x^2} + \frac{1}{l_y^2} + \frac{1}{l_z^2} \right)$



III - 2-Eq Asymptotic Behavior (mixture temperature)

$$\left(\varepsilon_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta + \varepsilon_\sigma (\rho c_p)_\sigma \langle T_\sigma \rangle^\sigma \right) = \left(\varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma \right) \langle T \rangle^{\beta\sigma}$$

- $t \rightarrow \infty$ for a semi- or infinite medium (see Zanotti & Carbonell, 1984; Davit et al., 2010):

$$\left(\varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma \right) \frac{\partial \langle T \rangle^{\beta\sigma}}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta U_\beta \frac{\partial \langle T \rangle^{\beta\sigma}}{\partial x} = (K_\infty^*)_{xx} \frac{\partial^2 \langle T \rangle^{\beta\sigma}}{\partial x^2}$$

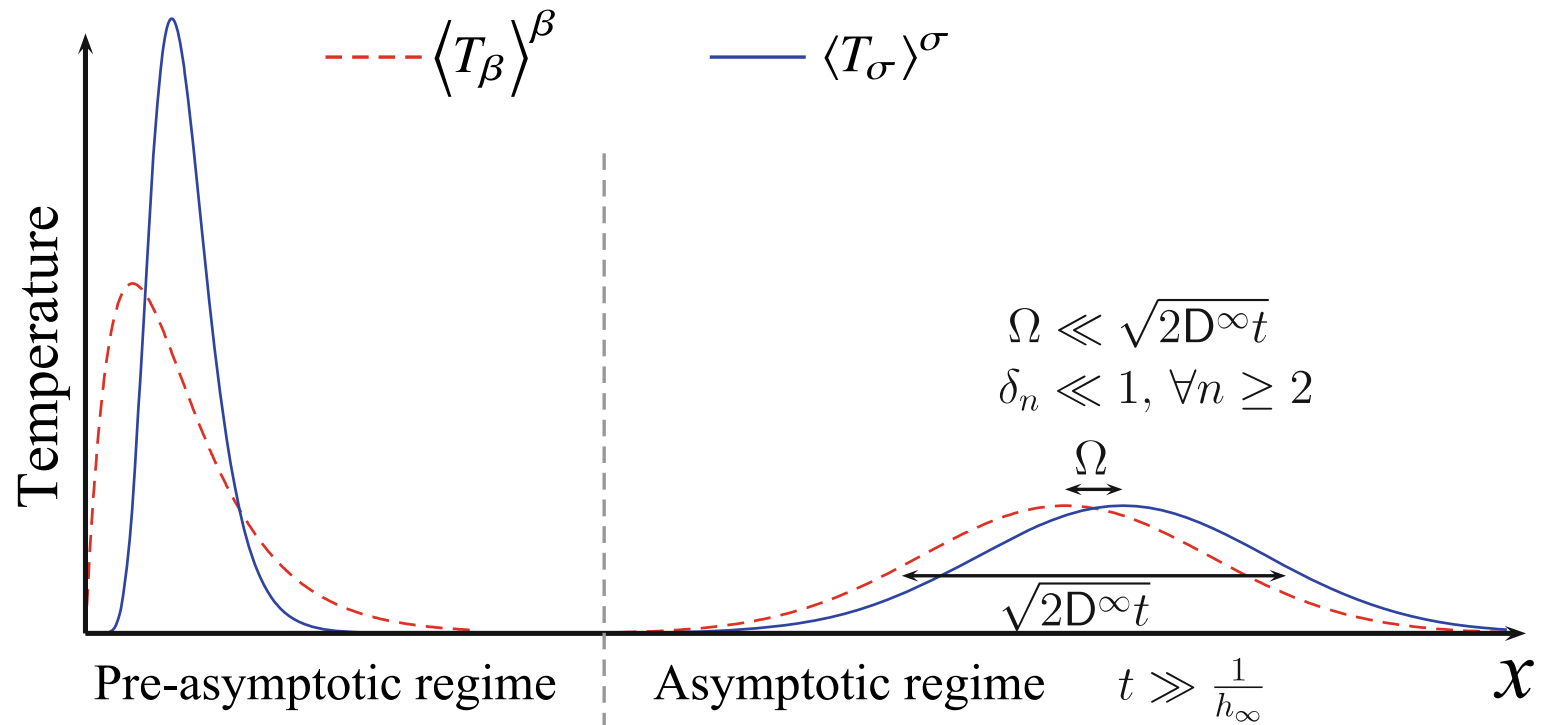
$$(K_\infty^*)_{xx} = (K_{\beta\beta}^*)_{xx} + (K_{\beta\sigma}^*)_{xx} + (K_{\sigma\beta}^*)_{xx} + (K_{\sigma\sigma}^*)_{xx} + \frac{\left(\varepsilon_\beta (\rho c_p)_\beta \varepsilon_\sigma (\rho c_p)_\sigma U_\beta \right)^2}{h_{2eq} \left(\varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma \right)^2}$$

$$\neq K_{eff} = K_{\beta\beta}^* + K_{\beta\sigma}^* + K_{\sigma\beta}^* + K_{\sigma\sigma}^*$$

→ good test for the choice of ... h_{2eq} !



2-Eq Asymptotic Behavior (mixture temperature)



from Zanotti & Carbonell, 1984; Davit et al., 2010 (moment analysis)



IV - 1-Eq Non-Equilibrium Model

(Chella et al., 1998; Moyne et al., 2000; Quintard et al., 2001; Davit et al., 2010; ~Brenner's method)

- **Mixture Temperature:**
$$\langle T \rangle^{\beta\sigma} = \frac{\left(\varepsilon_{\beta} (\rho c_p)_{\beta} \langle T_{\beta} \rangle^{\beta} + (\rho c_p)_{\sigma} \langle T_{\sigma} \rangle^{\sigma} \right)}{\left(\varepsilon_{\beta} (\rho c_p)_{\beta} + \varepsilon_{\sigma} (\rho c_p)_{\sigma} \right)}$$

- **New decomposition:**
$$\hat{T}_{\beta} = T_{\beta} - \langle T \rangle^{\beta\sigma}$$

- **Specific Closure:**

$$\hat{T}_{\beta} = \mathbf{b}_{\beta}^{\infty} \cdot \nabla \langle T \rangle^{\beta\sigma} \qquad \hat{T}_{\sigma} = \mathbf{b}_{\sigma}^{\infty} \cdot \nabla \langle T \rangle^{\beta\sigma}$$

- **same equation and effective property as asymptotic eq.**

→ Direct Estimation of \mathbf{K}_{∞}^* (see proof in Davit et al., 2010, if proper closure problem!)

- see Moyne et al. for relation with homogenization theory



V - Better Non-Equilibrium models (N-eq., multi-rate models)

- **Multi-rate (Brusseau et al., 1989;...); N-equation (Landereau et al., 1998) → a practical alternative to time convolution**

$$\varepsilon_{\beta}(\rho c_p)_{\beta} \frac{\partial \langle T_{\beta} \rangle^{\beta}}{\partial t} = \nabla \cdot (K_{\beta} \nabla \langle T_{\beta} \rangle^{\beta}) - \sum_n b_n (\langle T_{\beta} \rangle^{\beta} - T_{\sigma n})$$

$$\varepsilon_{\sigma}(\rho c_p)_{\sigma} \frac{\partial T_{\sigma n}}{\partial t} = -k_{\sigma} \lambda_n (T_{\sigma n} - \langle T_{\beta} \rangle^{\beta}) \quad n = 1, 2, ..$$

Example: 3-eqs

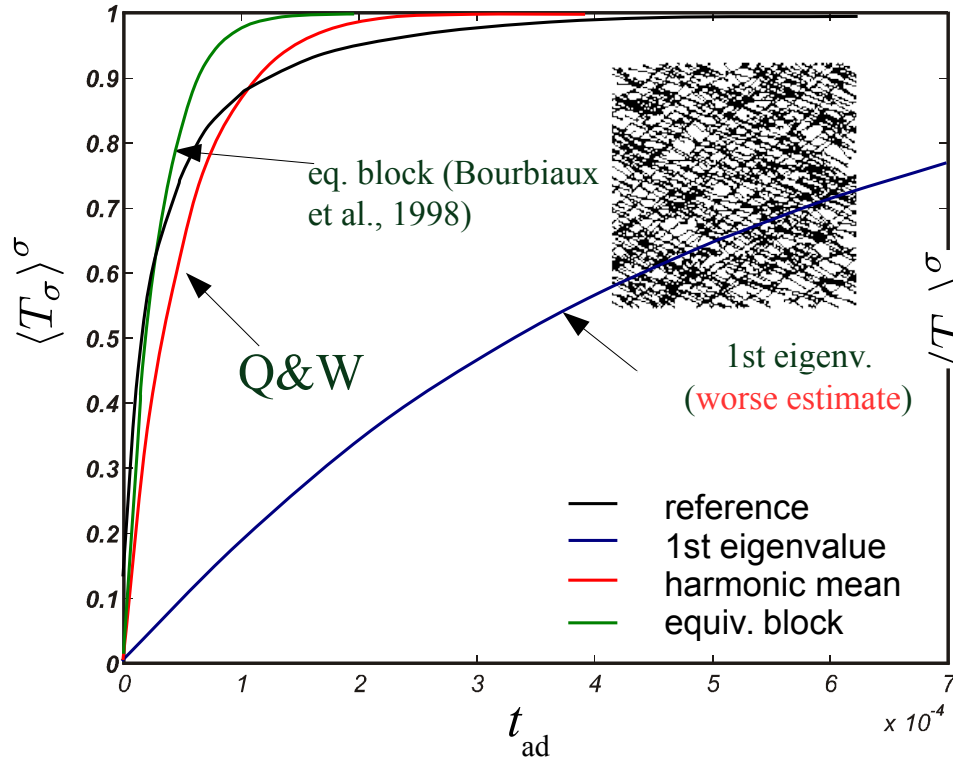
$$T_{\sigma 1}, T_{\sigma r}$$

with λ_1, λ_r (from the harmo. mean of the remaining eigenv.)

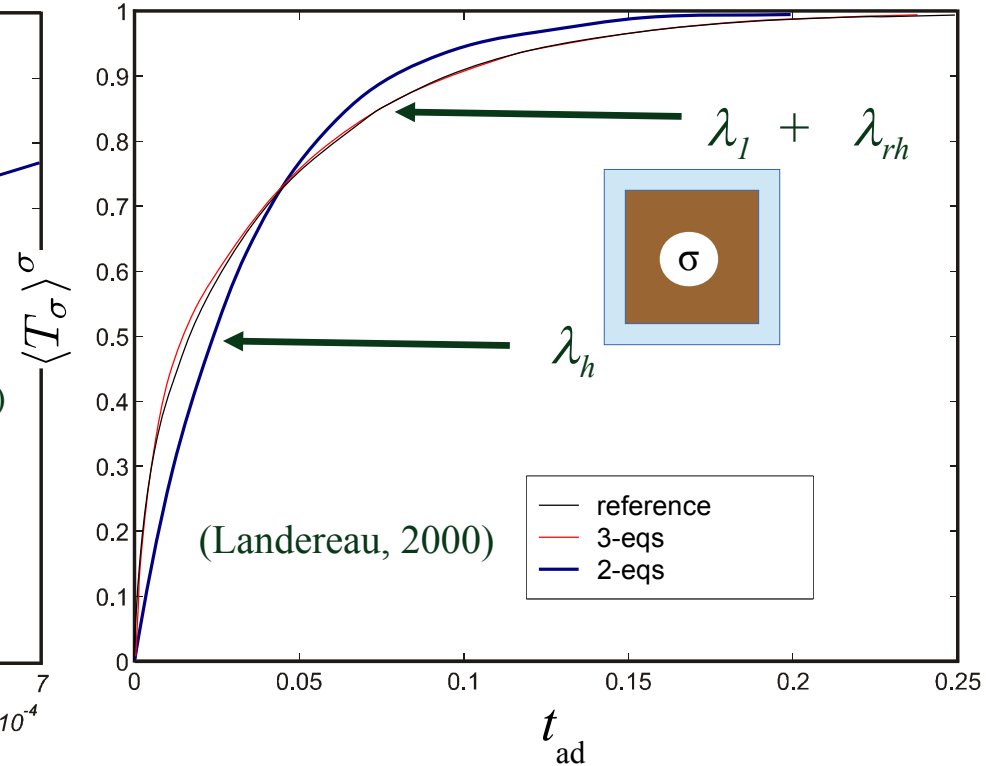


Examples: fractured media

(also for Darcy's law with slightly compressible fluid)



Tests with various h_{2eq}




Test with 3-Eq model



VI - Mixed Model (diffusion, $k_\sigma \ll k_\beta$, dispersed σ -phase; De Swaan, 1976;)

(if homogenization theory use $k_\sigma = \varepsilon^2 k_\beta$)

$$\underbrace{\langle T_\beta \rangle^\beta + \tilde{T}_\beta}_{O(\frac{l_\beta}{L} \langle T_\beta \rangle^\beta)} = T_\sigma \Rightarrow \underbrace{\langle T_\beta \rangle^\beta}_{\text{macro-scale}} = \underbrace{T_\sigma}_{\text{micro-scale}}$$

Macro-	$\varepsilon_\beta (\rho C_p)_\sigma \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} = \nabla \cdot (\mathbf{K}_\beta^* \cdot \nabla \langle T_\beta \rangle^\beta) - \varphi_{\beta\sigma}$	
Micro-	$(\rho c_p)_\sigma \frac{\partial T_\sigma}{\partial t} = \nabla \cdot (k_\sigma \nabla T_\sigma) \quad \text{in } V_\sigma \quad T_\sigma = \langle T_\beta \rangle^\beta, \text{ at } A_{\beta\sigma}$	

general solution:
$$T_\sigma(\mathbf{x}, t) = \int_0^t \left. \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} \right|_{t-\tau} \bar{T}_\sigma(\mathbf{x}, \tau) d\tau$$

→ involves spectrum of eigenvalues & eigenfunctions → $h(t, BC, IC)$!

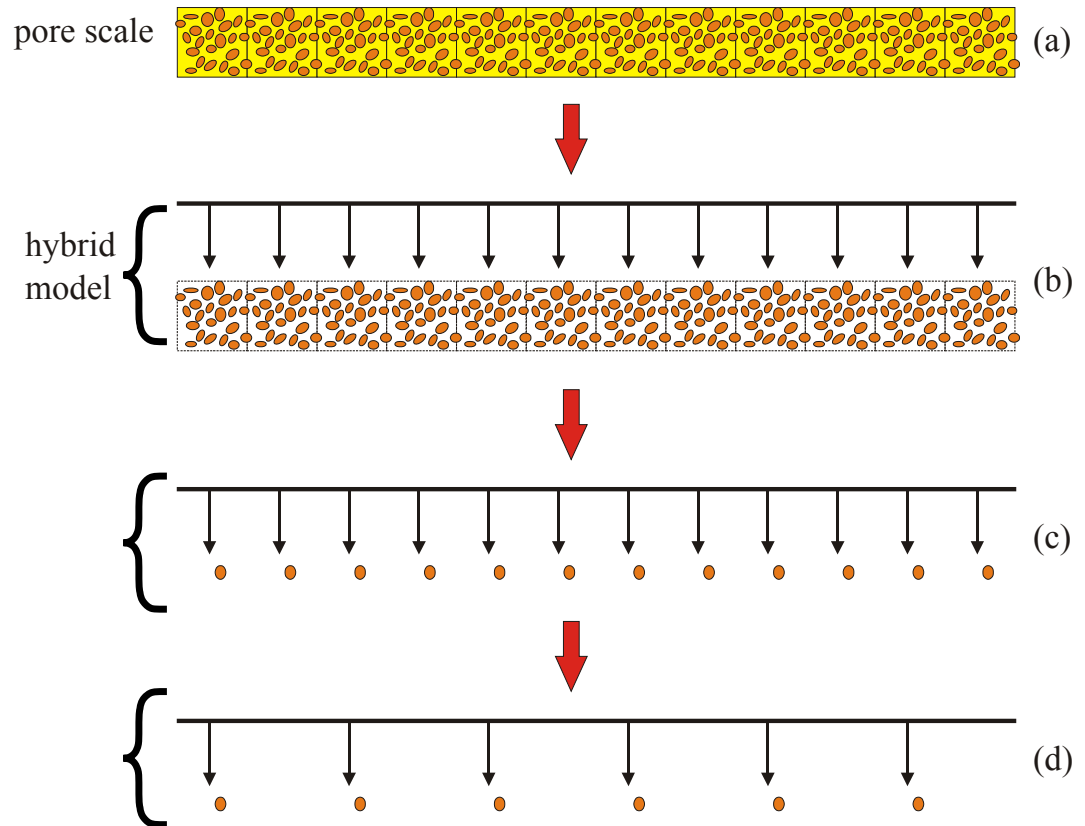


Mixed Model: Practical Implementation

-Direct Numerical Simulation (Heavy computations)

-Mixed Model, Full UC (still Heavy Comp.)

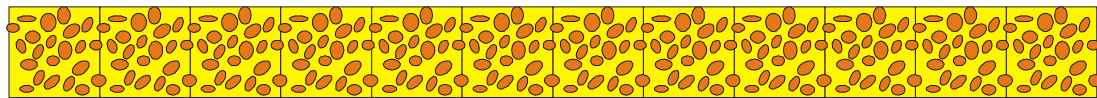
-Mixed Model, Representative Matrix Block,...



...in some cases Analytical Solutions may be available



Summary: a schematic representation of the various models



DNS



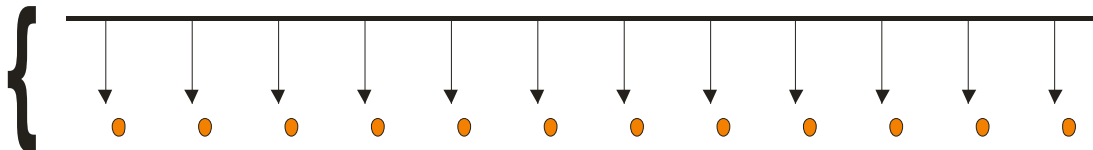
1-eq local equilibrium



1 equation (convolution, or asymptotic behavior of the 2-eq. model, fractional derivative, Telegraph eq., CTRW ...)



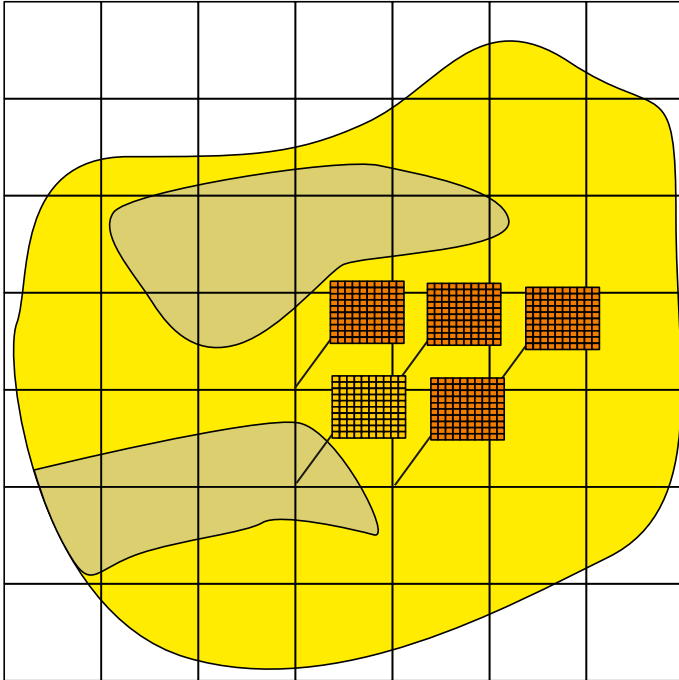
2-equation, N-equation (multi-rate or MRMT, etc...)



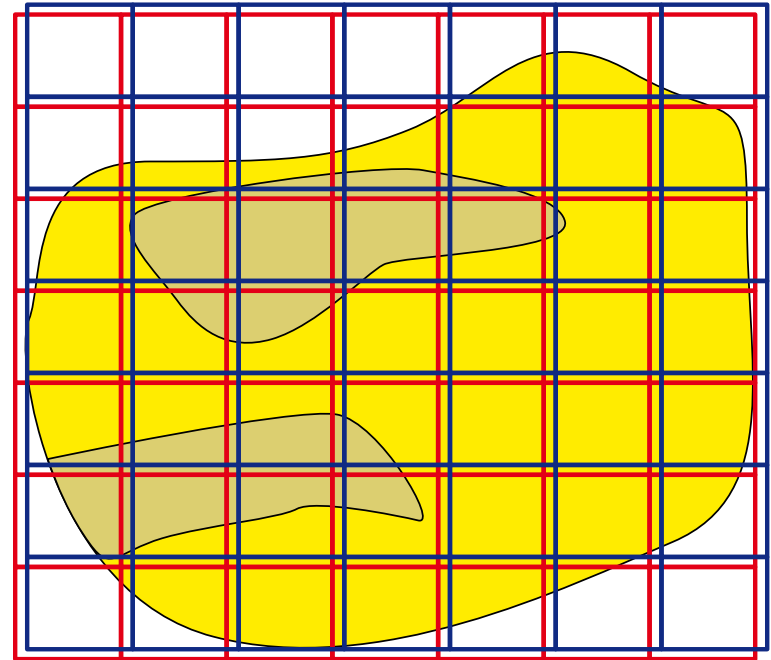
Mixed models



Numerical implementation



Mixed or hybrid models



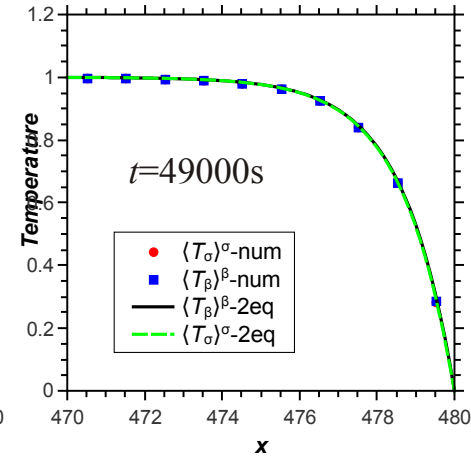
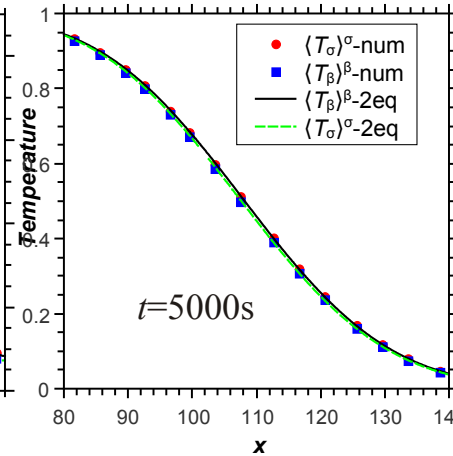
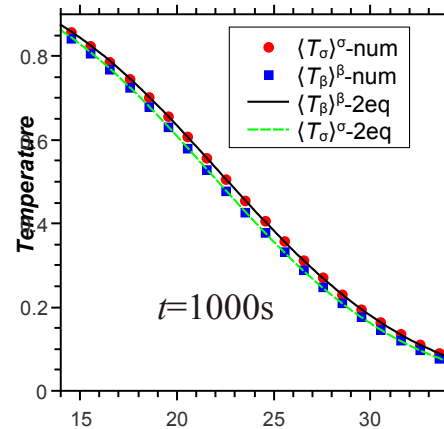
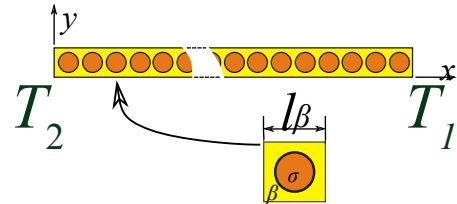
2-eq models

 **Keep heterogeneities as much as possible to avoid abnormal dispersion in the local model !**

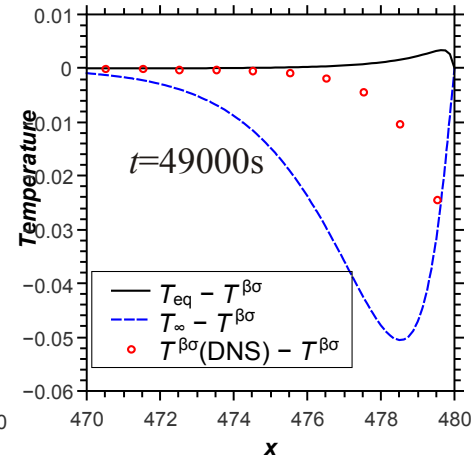
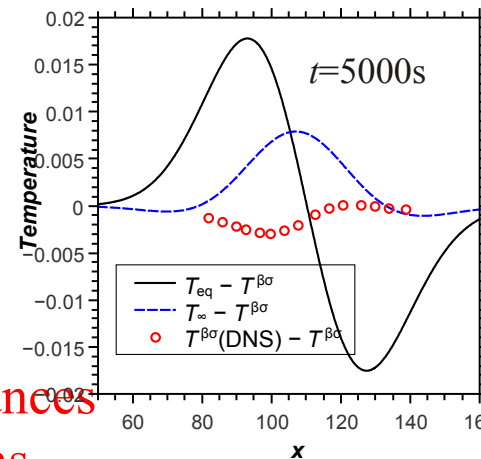


Important: transitions between the various models!

(Davarzani et al., 2010; Davit & Quintard, 2014)



- $t \sim 0$ non-homogenizable or specific treatment
- $t > 0$ LNE models
- $t \gg 0$ (if enough length): 1-Eq asymptotic model
- $t \rightarrow \infty$ (revert to 1eq-LE if finite domain, because of Dirichlet condition)



Conclusions:

- 1-Eq asymp. not valid in all circumstances
- 2-Eq robust for dealing with transitions



More on homogenization and Local Non-equilibrium model

- **Pernin, 1984:** $-\mathbf{n}_{\beta\sigma} \cdot k_{\beta} \nabla T_{\beta} = h (T_{\beta} - T_{\sigma})$ at $A_{\beta\sigma}$
 - recover a 2-eq. model
 - drawback: h must be a solution not an assumption!
- **if $k_{\sigma} = (l/L)^2 k_{\beta}$ (Hornung, Arbogast, ...):**
 - mixed model
 - may recover 2-eq model through approx. solution (but 1st eigenvalue a very bad solution!)
- **$k_{\sigma} = (l/L) k_{\beta}$: at 1st order obtain 2-Eq model**
see double expansion in Bertin et al., 2000



Simple coupled problems (non-linear properties, one-side coupling, ...)



Non-Linear Properties

- **Approximation**

$$\left. \begin{aligned} k_\beta &= F(T_\beta) = F(\langle T_\beta \rangle^\beta) + \frac{\partial F}{\partial T_\beta}(\langle T_\beta \rangle^\beta) \tilde{T}_\beta + \dots \\ \tilde{T}_\beta &= O\left(\frac{l_\beta}{L} \langle T_\beta \rangle^\beta\right) * \end{aligned} \right\} k_\beta = F(T_\beta) \approx F(\langle T_\beta \rangle^\beta)$$

- **Consequence: closure and effective properties depend on *parameter* $\langle T_\beta \rangle^\beta$**

* not always the case : example $\tilde{\mathbf{v}}_\beta \approx \langle \mathbf{v}_\beta \rangle^\beta$



Coupled problems, a simple example: transport with Soret effect

- one-side coupling (T_β , known problem):

$$\tilde{T}_\beta = \mathbf{b}_{T\beta} \cdot \nabla \langle T \rangle \quad ; \quad \tilde{T}_\sigma = \mathbf{b}_{T\sigma} \cdot \nabla \langle T \rangle$$

$$\frac{\partial c_\beta}{\partial t} + \nabla \cdot (c_\beta \mathbf{v}_\beta) = \nabla \cdot (D_\beta \nabla c_\beta + D_{T\beta} \nabla T_\beta)$$

- Closure (Lacabanne et al., 2002; Davarzani et al., 2010, 2011, ext. for $Pe \neq 0$):

$$\tilde{c}_\beta = \mathbf{b}_{C\beta} \cdot \nabla \langle c_\beta \rangle^\beta + \mathbf{b}_{S\beta} \cdot \nabla \langle T \rangle$$

problem involves $\mathbf{b}_{T\beta}$!

$$\mathbf{v}_\beta \cdot \nabla \mathbf{b}_{S\beta} = D_\beta \nabla^2 \mathbf{b}_{S\beta} + D_{T\beta} \nabla^2 \mathbf{b}_{T\beta}$$

$$\text{BC: } -\mathbf{n}_{\beta\sigma} \cdot (D_\beta \nabla \mathbf{b}_{S\beta} + D_{T\beta} \nabla \mathbf{b}_{T\beta}) = \mathbf{n}_{\beta\sigma} \cdot D_{T\beta}, \text{ at } A_{\beta\sigma}$$

etc... 😊!



Coupled problems, a simple example: transport with Soret effect

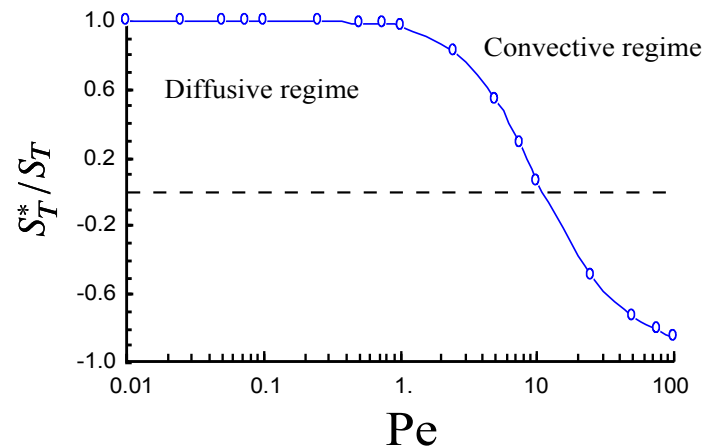
- **macro-equation:**

$$\frac{\partial \varepsilon_\beta \langle c_\beta \rangle^\beta}{\partial t} + \nabla \cdot \left(\varepsilon_\beta \langle \mathbf{v}_\beta \rangle^\beta \langle c_\beta \rangle^\beta \right) = \nabla \cdot \left(\varepsilon_\beta \mathbf{D}_\beta^* \cdot \nabla \langle c_\beta \rangle^\beta + \varepsilon_\beta \mathbf{D}_{T\beta}^* \cdot \nabla \langle T \rangle \right)$$

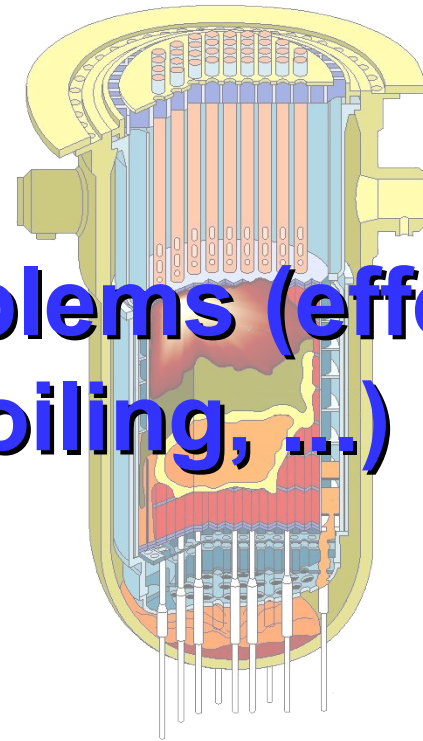
- **Results for Soret Coefficient:** $S_T = D_{T\beta} / D_\beta$
 $S_T^* = D_{T\beta}^* / D_\beta^*$

$$\frac{\mathbf{D}_\beta^*}{D_\beta} = \frac{\mathbf{D}_{T\beta}^*}{D_{T\beta}} \sim \frac{1}{\tau} \text{ if } \text{Pe} = 0$$

results validated against
experiments (Pe=0) and DNS!



Complex coupled problems (effect of source terms, boiling, ...)



Potential strong coupling: Effect of source terms

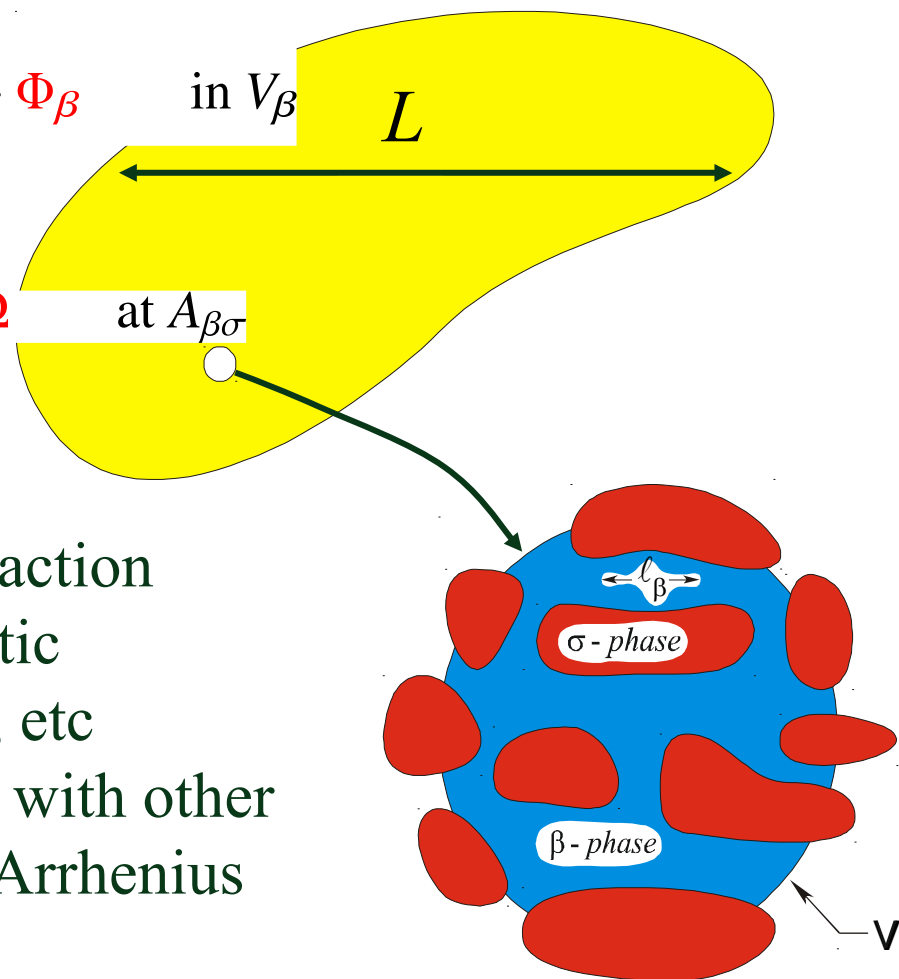
$$(\rho c_p)_\beta \frac{\partial T_\beta}{\partial t} + (\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla T_\beta = \nabla \cdot (k_\beta \nabla T_\beta) + \Phi_\beta \quad \text{in } V_\beta$$

$$\text{B.C.1} \quad T_\beta = T_\sigma \quad \text{at } A_{\beta\sigma}$$

$$\text{B.C.2} \quad -\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla T_\beta = -\mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla T_\sigma - \Omega \quad \text{at } A_{\beta\sigma}$$

$$(\rho c_p)_\sigma \frac{\partial T_\sigma}{\partial t} = \nabla \cdot (k_\sigma \nabla T_\sigma) + \Phi_\sigma \quad \text{in } V_\sigma$$

- applications: chemical reaction (combustion, ...), magnetic induction, nuclear safety, etc
- strong potential coupling with other transport problems (like Arrhenius reaction rates, radiation)



Coupled micro- and macro-scale problems

$$\underbrace{\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t}}_{\text{accumulation}} + \underbrace{\varepsilon_\beta (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle^\beta \cdot \nabla \langle T_\beta \rangle^\beta}_{\text{convection}} = \nabla \cdot \underbrace{\left[k_\beta \left(\varepsilon_\beta \nabla \langle T_\beta \rangle^\beta + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_\beta dA \right) \right]}_{\text{conduction}}$$

$$- \underbrace{(\rho c_p)_\beta \nabla \cdot \langle \tilde{\mathbf{v}}_\beta \tilde{T}_\beta \rangle}_{\text{dispersion}} + \underbrace{\frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla T_\beta dA}_{\text{interfacial flux}} + \underbrace{\varepsilon_\beta \langle \Phi_\beta \rangle^\beta}_{\text{homogeneous thermal source}}$$

$$\varepsilon_\sigma (\rho c_p)_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} = \nabla \cdot \left[k_\sigma \left(\varepsilon_\sigma \nabla \langle T_\sigma \rangle^\sigma + \frac{1}{V} \int_{A_{\sigma\beta}} \mathbf{n}_{\sigma\beta} \tilde{T}_\sigma dA \right) \right] + \frac{1}{V} \int_{A_{\sigma\beta}} \mathbf{n}_{\sigma\beta} \cdot k_\sigma \nabla T_\sigma dA + \varepsilon_\sigma \langle \Phi_\sigma \rangle^\sigma$$

Note: B.C.2 gives

$$\frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla T_\beta dA = \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla T_\sigma dA + a_v \langle \Omega \rangle_{\beta\sigma}$$

$$a_v = \frac{1}{V} \int_{A_{\beta\sigma}} dA \quad (\text{specific area}) \quad \frac{1}{V} \int_{A_{\beta\sigma}} \Omega dA = a_v \langle \Omega \rangle_{\beta\sigma} \quad \varepsilon_\beta = \frac{V_\beta}{V}$$



Pore-Scale Deviation Problem

$$(\rho c_p)_\beta \frac{\partial \tilde{T}_\beta}{\partial t} + (\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla \tilde{T}_\beta + \underbrace{(\rho c_p)_\beta \tilde{\mathbf{v}}_\beta \cdot \nabla \langle T_\beta \rangle^\beta}_{\text{source}} = \nabla \cdot (k_\beta \nabla \tilde{T}_\beta) - \frac{\varepsilon_\beta^{-1}}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \tilde{T}_\beta dA + \tilde{\Phi}_\beta$$

$$\text{B.C.1} \quad \tilde{T}_\beta = \tilde{T}_\sigma - \underbrace{(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma)}_{\text{source}}, \quad \text{at } A_{\beta\sigma}$$

$$\text{B.C.2} \quad \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \tilde{T}_\beta = \mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \tilde{T}_\sigma - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \langle T_\beta \rangle^\beta}_{\text{source}} - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \langle T_\sigma \rangle^\sigma}_{\text{source}} + \underbrace{\langle \Omega \rangle_{\beta\sigma}}_{\text{source}} + \tilde{\Omega}, \quad \text{at } A_{\beta\sigma}$$

$$(\rho c_p)_\sigma \frac{\partial \tilde{T}_\sigma}{\partial t} = \nabla \cdot (k_\sigma \nabla \tilde{T}_\sigma) - \frac{\varepsilon_\sigma^{-1}}{V} \int_{A_{\sigma\beta}} \mathbf{n}_{\sigma\beta} \cdot k_\sigma \nabla \tilde{T}_\sigma dA + \tilde{\Phi}_\sigma$$

with $\Omega = \langle \Omega \rangle_{\beta\sigma} + \tilde{\Omega}, \quad \Phi_\sigma = \langle \Phi_\sigma \rangle^\sigma + \tilde{\Phi}_\sigma$

Note: no source terms for homogeneous heat sources if Φ constant
 → no impact on effective properties!



Macro-scale models

- Local equilibrium

$$(\rho c_p)^* \frac{\partial \langle T \rangle}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle^\beta \cdot \nabla \langle T \rangle = \nabla \cdot (\mathbf{K}_{eff} \cdot \nabla \langle T \rangle) + a_V \langle \Omega \rangle_{\beta\sigma} + \varepsilon_\sigma \langle \Phi_\sigma \rangle^\sigma + \varepsilon_\beta \langle \Phi_\beta \rangle^\beta$$

- 2eq model (Quintard & Whitaker, Hdbk Porous Media, 2000; Davit and Quintard, Hdbk Porous Media, 2015)

$$\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle^\beta \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \nabla \cdot (\mathbf{K}_{\beta\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\beta\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma) - a_V h (\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma) + a_V \xi \Omega + \varepsilon_\beta \langle \Phi_\beta \rangle^\beta + \dots$$

distribution coefficient 

see extension to radiative heat transfer (Leroy et al., 2013), application to combustion (Chen et al., 2014), ...

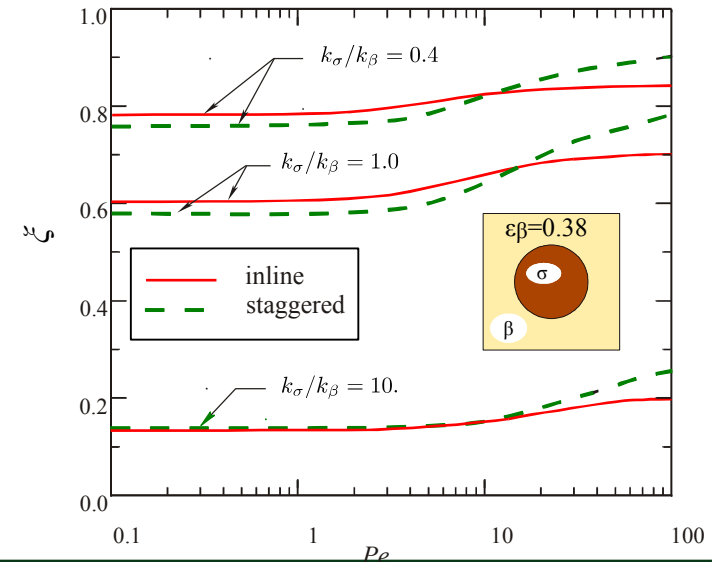
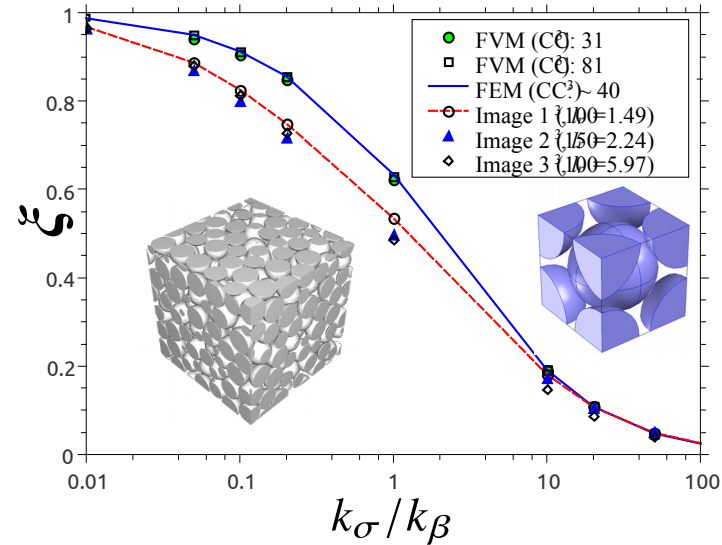


Calculation of ξ

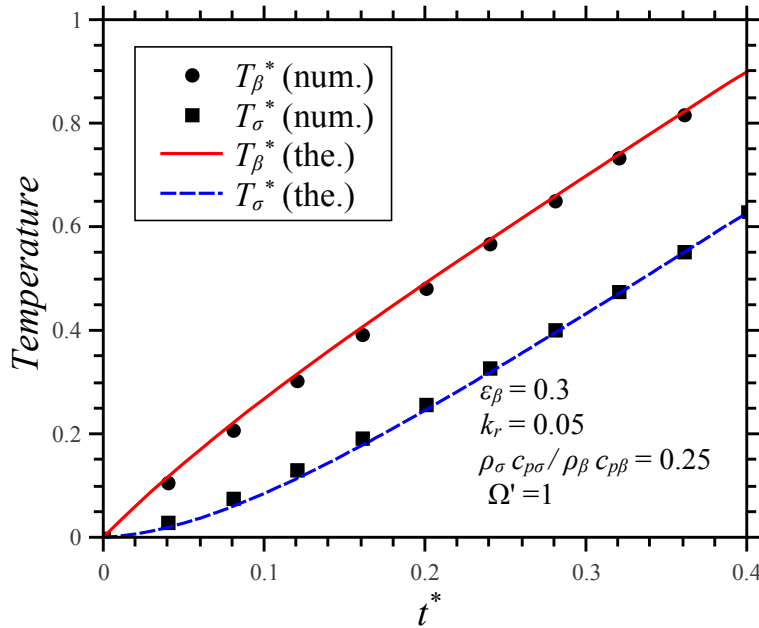
- if $k_\sigma / k_\beta \rightarrow \infty, \xi \rightarrow 0$
- if $k_\sigma / k_\beta \rightarrow 0, \xi \rightarrow 1$

- Moderate influence of Péclet number
- $REV > d_p$?
- Role of a_v ?

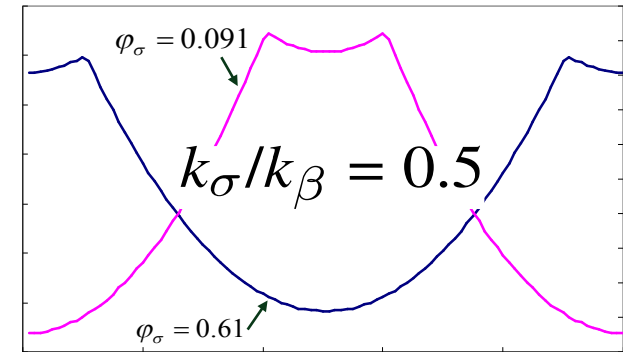
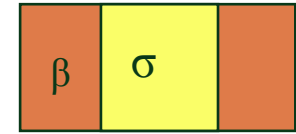
Warning!
Engng practice: $\xi \rightarrow 0$



0D “experiment”: example of stratified UC



DNS



$$\varphi_\sigma = \left(\frac{\varepsilon_\sigma (\rho c_p)_\sigma}{\varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma} \right)$$

$$\lim_{t \rightarrow \infty} \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) = \frac{\xi \varepsilon_\sigma (\rho c_p)_\sigma - (1 - \xi) \varepsilon_\beta (\rho c_p)_\beta}{h_{2eq} \left(\varepsilon_\sigma (\rho c_p)_\sigma + \varepsilon_\beta (\rho c_p)_\beta \right)} a_v \Omega$$

- The more conductive material has not necessarily the highest average T
- Note: Good test for the theory for both h_{2eq} and ξ



Example: Combustion

Yang et al., TiPM, 2015

$$\Omega = A_0 e^{-E/RT_{int}} \times H_{rxn}$$

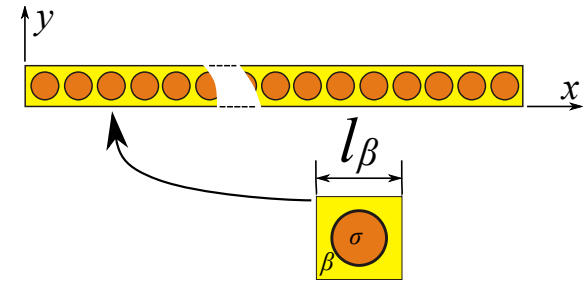
$$\begin{aligned} \varepsilon (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} + (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \\ \nabla \cdot \left(\mathbf{K}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma \right) - h_{2eq} \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) \\ + \varepsilon_\beta \langle \Phi_\beta \rangle^\beta + a_V \xi \left(1 + w \frac{E}{R (\langle T_\sigma \rangle^\sigma)^2} \right) A_0 e^{-E/R \langle T_\sigma \rangle^\sigma} H_{rxn} \end{aligned}$$

with

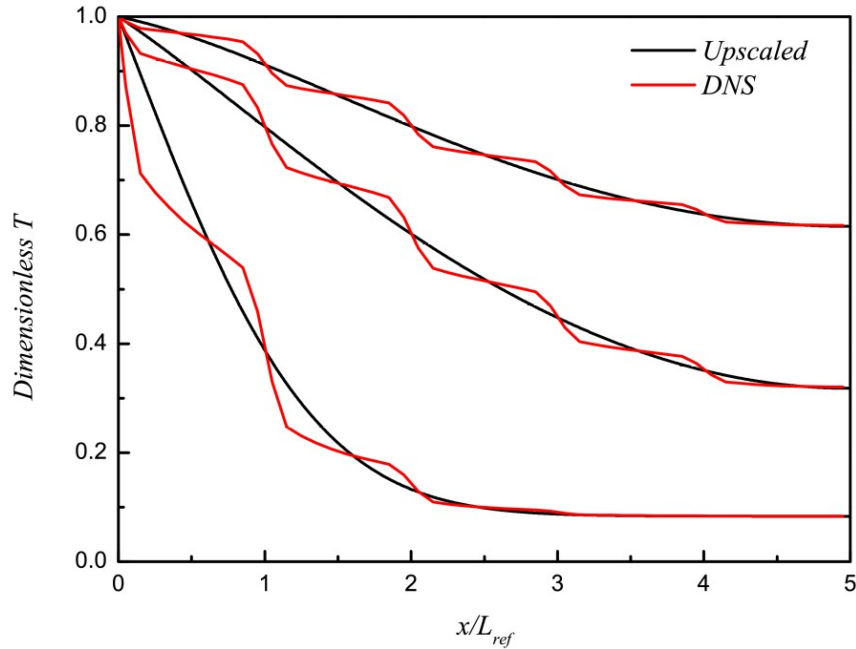
$$w \approx \frac{\frac{E}{R (\langle T_\beta \rangle^\beta)^2} e^{-E/R \langle T_\beta \rangle^\beta} \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) - \left(e^{-E/R \langle T_\sigma \rangle^\sigma} - e^{-E/R \langle T_\beta \rangle^\beta} \right)}{\frac{E}{R (\langle T_\sigma \rangle^\sigma)^2} e^{-E/R \langle T_\sigma \rangle^\sigma} - \frac{E}{R (\langle T_\beta \rangle^\beta)^2} e^{-E/R \langle T_\beta \rangle^\beta}}$$



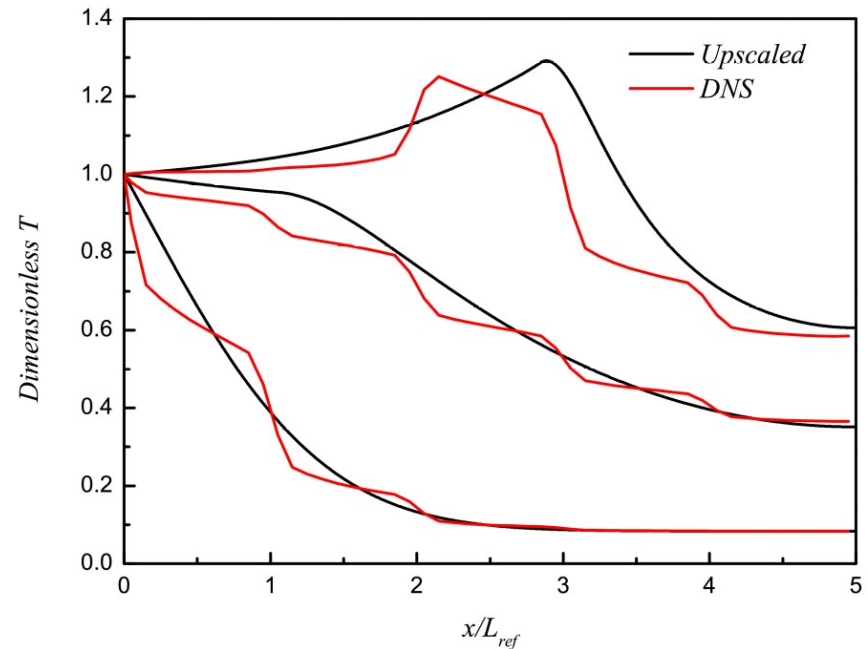
Example: Combustion



Yang et al., TiPM, 2015



$$Da = \frac{A_0 e^{-E/R\langle T_\sigma \rangle^\sigma} l_\sigma}{k_\sigma / (\rho c_p)_\sigma}$$



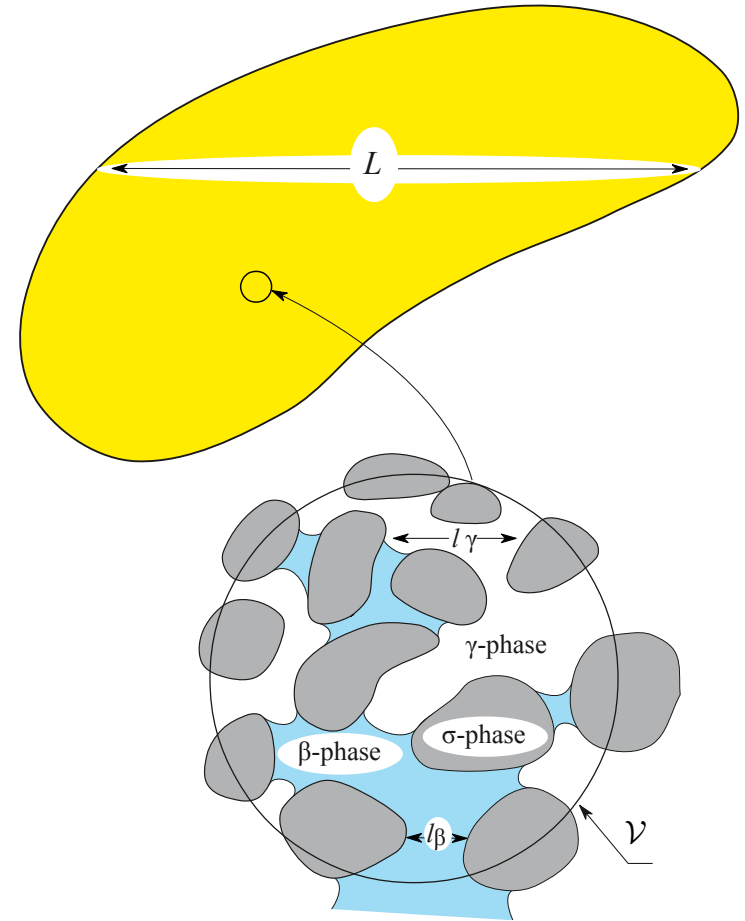
Two-Phase Flow with Phase Change

Case with no inert gas!

$\left\{ \begin{array}{l} \text{Mass balances+Momentum balances} \\ \text{+Energy balances} \end{array} \right.$

Specific Bcs at $A_{\beta\gamma}$:

$$\left\{ \begin{array}{l} T_\gamma = T_\beta = T_{sat}(p) \\ \mathbf{n}_{\beta\gamma} \cdot \left(\rho_\gamma (\mathbf{v}_{\gamma v} - \mathbf{w}_{\beta\gamma}) \delta h_{\beta\gamma} \right) \\ \quad - \mathbf{n}_{\beta\gamma} \cdot (k_\gamma \nabla T_\gamma) = -\mathbf{n}_{\beta\gamma} \cdot (k_\beta \nabla T_\beta) \end{array} \right.$$

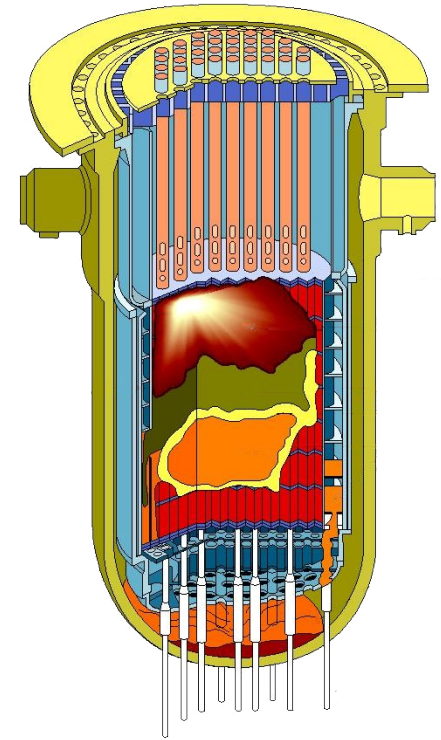


If Local Eq.: $\mathcal{T}_\beta = \mathcal{T}_\gamma = \mathcal{T}_\sigma = T_{sat}(P)$ (not always observed!)



☢ Nuclear LOCA accident

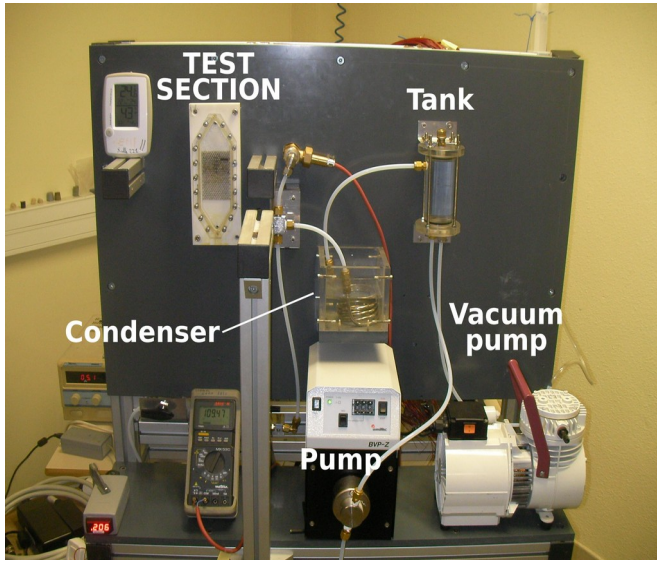
- Important source term in the solid phase → local non-equilibrium !
- Decoupled 2-phase flow, quasi-steady → Generalized Darcy-Forchheimer? (time-space ergodicity?)
- 3-T model, extension of 2-T model: Berthoud & Valette (1994); Petit et al. (1999); Duval et al. (2004);...based on quasi-steady approx.
- Heuristic: time averaging of averaged equations → porous media Nukiyama curves (see Sapin et al., 2014)



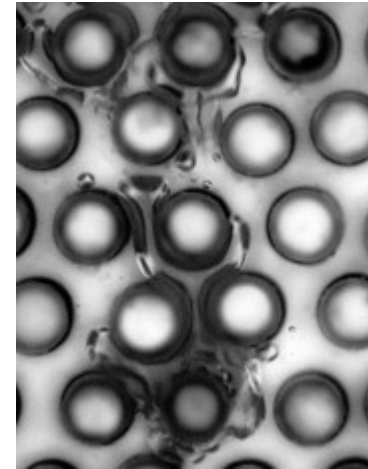
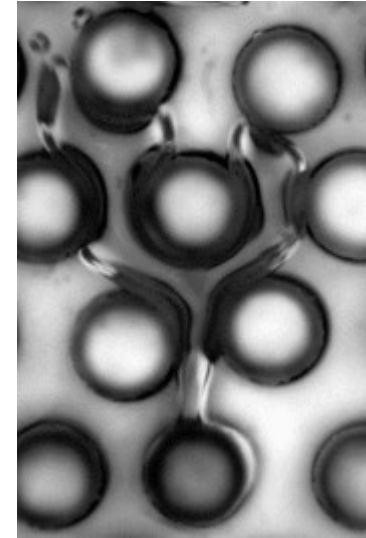
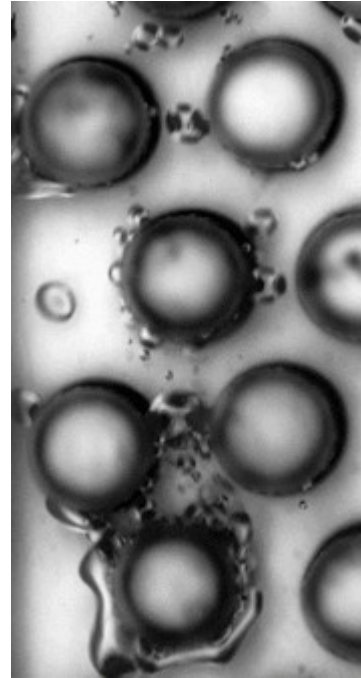
Highly open problem!



Pore-Scale Experimentations



Video in slow motion!

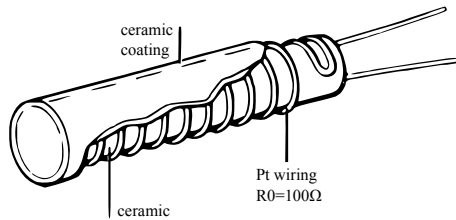


Sapin et al., 2014

Nucleate Boiling

Film Boiling

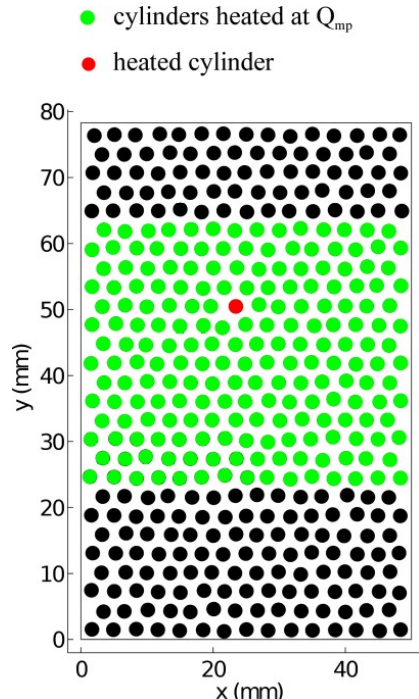
Intense Boiling



Need time-averaging!



Porous Media Nukiyama Curves



$$Q_{mp} = 20 \text{ mW}$$

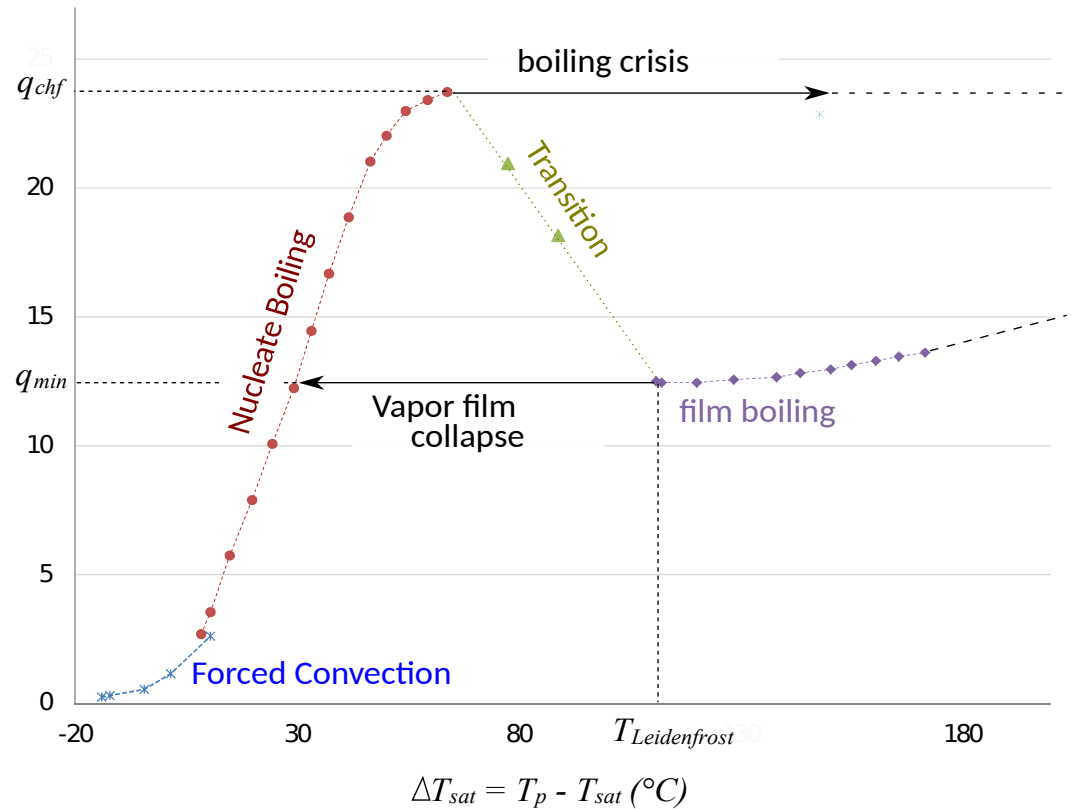
$$T_l = 24.4^\circ\text{C}$$

$$P = 1.181 \text{ bar}$$

$$T_{sat} = f(P) = 39.9^\circ\text{C}$$

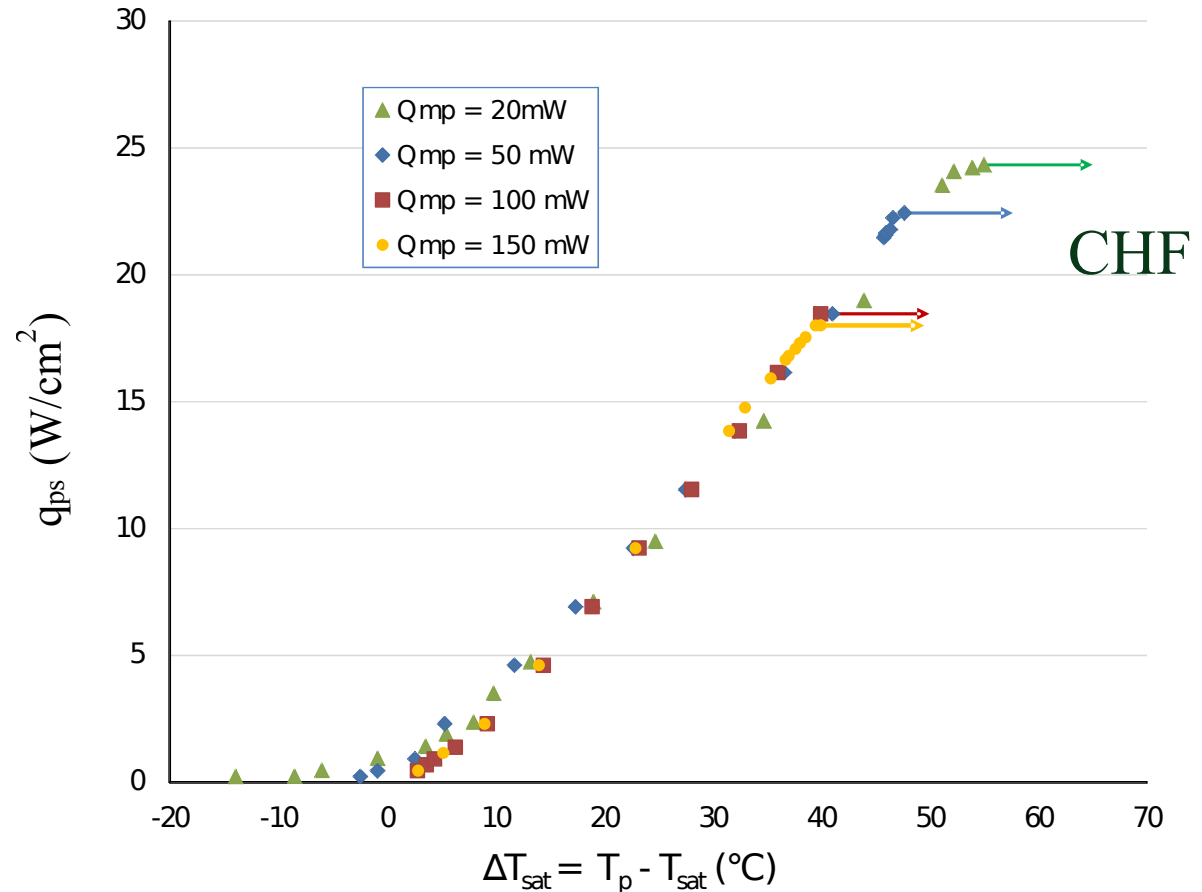
$$v_l = 3.4 \text{ mm/s}$$

Wall flux
 $q_{ps} \text{ (W/cm}^2\text{)}$

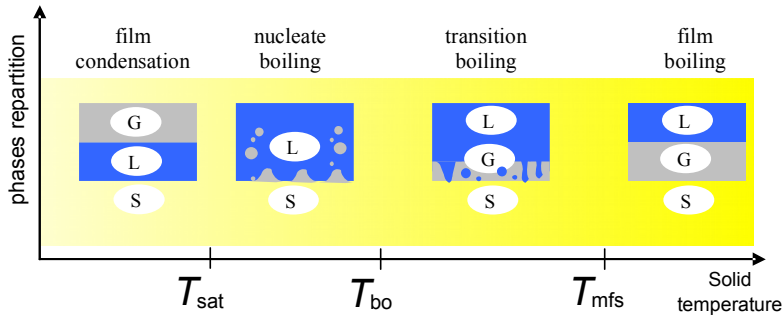


Critical Flux

Surrounding heating changes critical flux!
...but the behavior up to CHF seems to be unaffected (contrary to modeling guess)?!



Macro-Scale Model?



Bachrata et al., 2013 (implemented in CATHARE Safety code)

Need effective properties as a function of saturations, temperatures, velocities !

$$H_i = \langle h_i \rangle^i ; \alpha = S_g$$

$$\frac{\partial \varepsilon_g \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{V}_g) = \dot{m}$$

$$\frac{\partial \varepsilon_l \rho_l}{\partial t} + \nabla \cdot (\rho_l \mathbf{V}_l) = -\dot{m}$$

$$\dot{m} = -\frac{1}{V} \int_{A_{gl}} \mathbf{n}_{gl} \cdot \rho_g (\mathbf{v}_g - \mathbf{w}) dA$$

$$\frac{\partial (\alpha \varepsilon \rho_g H_g)}{\partial t} + \nabla \cdot (\alpha \varepsilon \rho_g \mathbf{V}_g H_g) = \nabla \cdot (\mathbf{K}_g^* \cdot \nabla \mathcal{T}_g) + \dot{m}_{lg} h_g^{sat} + Q_{sg} - Q_{gi}$$

$$\frac{\partial ((1 - \alpha) \varepsilon \rho_l H_l)}{\partial t} + \nabla \cdot ((1 - \alpha) \varepsilon \rho_l \mathbf{V}_l H_l) = \nabla \cdot (\mathbf{K}_l^* \cdot \nabla \mathcal{T}_l) - \dot{m}_{lg} h_l^{sat} + Q_{sl} - Q_{li}$$

$$\frac{\partial ((1 - \varepsilon) \rho_s H_s)}{\partial t} = \nabla \cdot (\mathbf{K}_s^* \cdot \nabla \mathcal{T}_s) - Q_{sl} - Q_{sg} - Q_{si} + \omega_s$$

$$Q_{\beta i} = h_{\beta i} (\mathcal{T}_\beta - T_{sat}) ; Q_{s\beta} = h_{s\beta} (\mathcal{T}_s - \mathcal{T}_\beta)$$

$$\dot{m}_{lg} h_{lg} = Q_{si} + Q_{gi} + Q_{li}$$

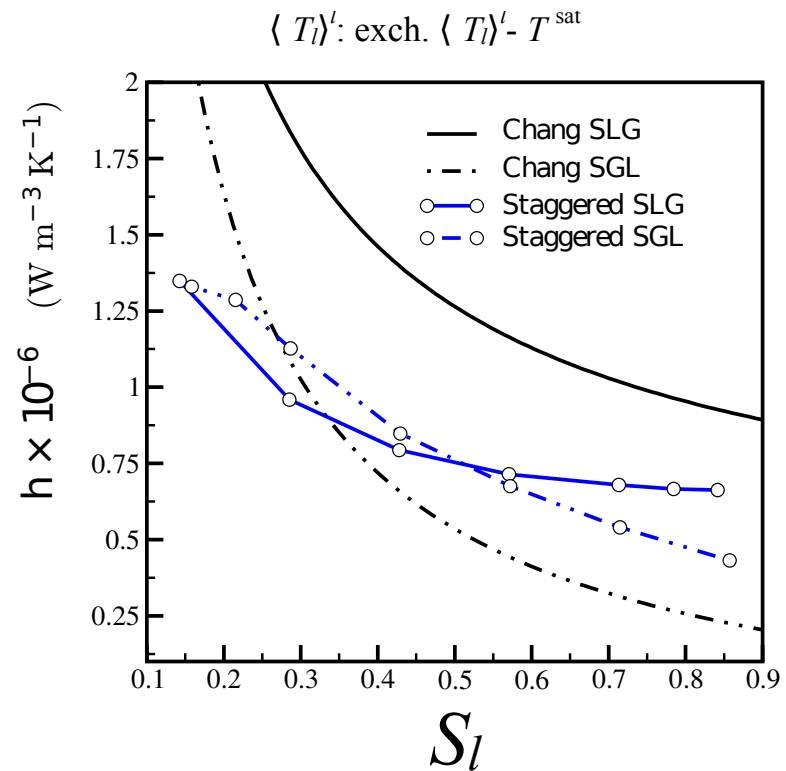
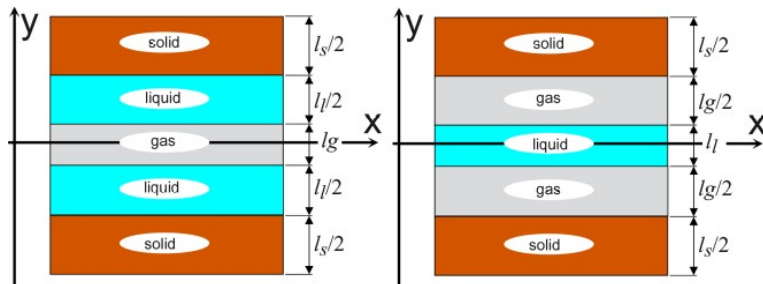
+ generalized Forchheimer



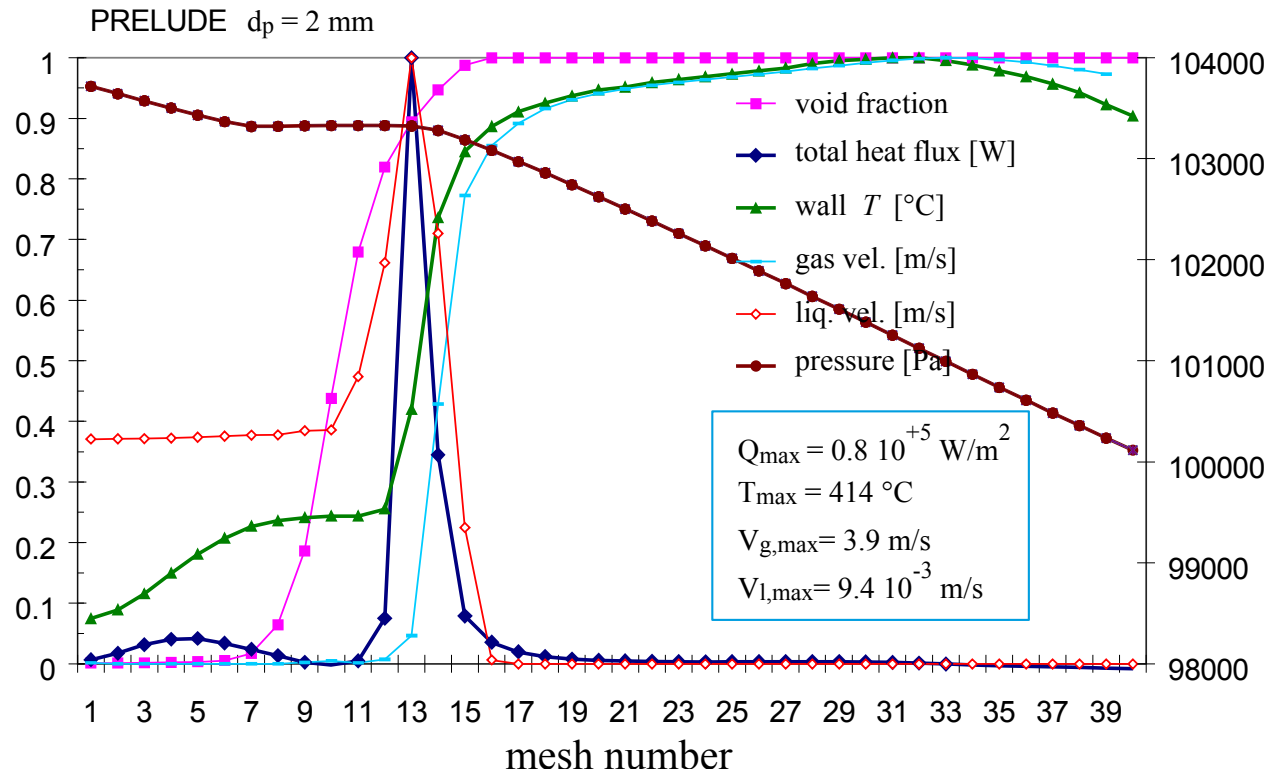
Heat Exchange Terms

- Quasi-static two-phase flow theory + inertia terms

Example: impact of phase configuration!



Example : comparison with experiments



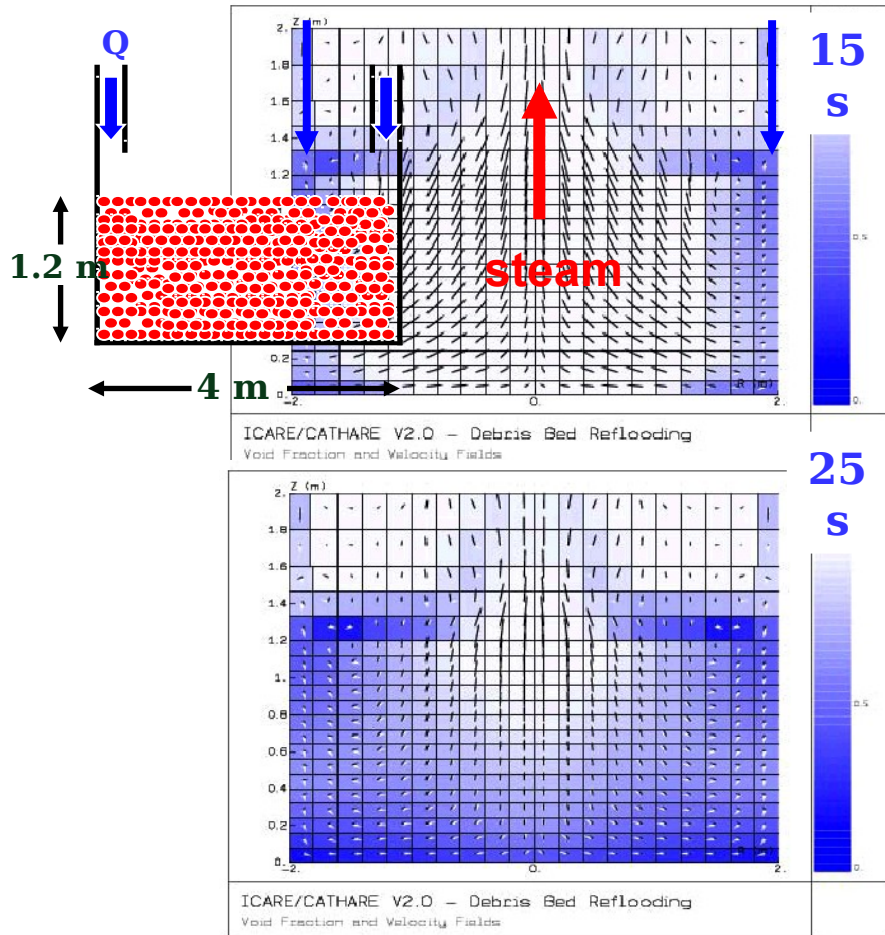
IRSN Experiments:
PRELUDE, SYLPHIDE, ...

Work confirm main required features (inertia, NLE,...)
 → Macro-scale behavior (heuristic time averaging)
 → Need for adapted correlations

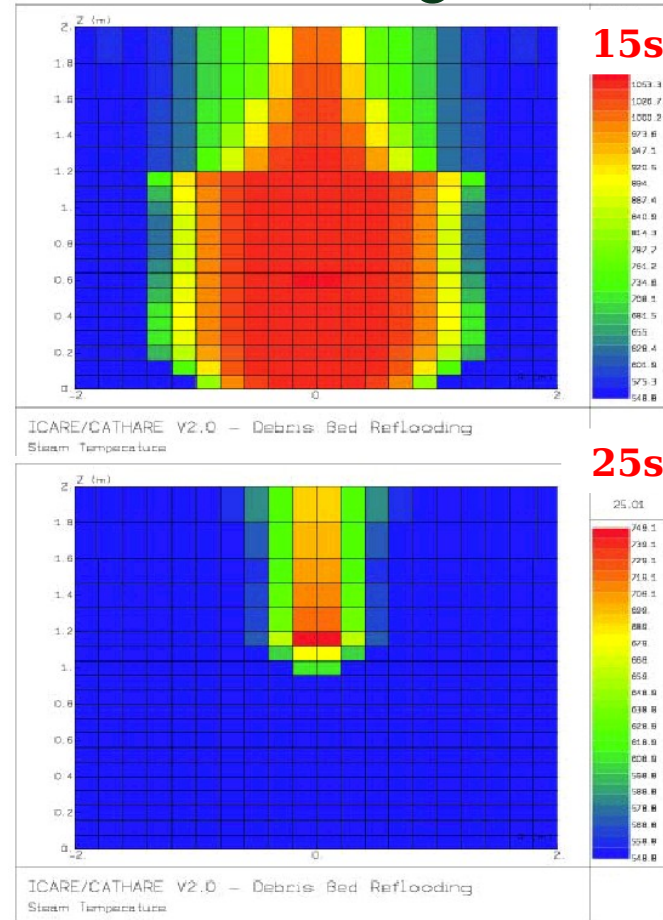


Example of Macro-Scale Simulations (Quenching)

Tregoures et al. (2003)



Water and steam velocities



Temperature field



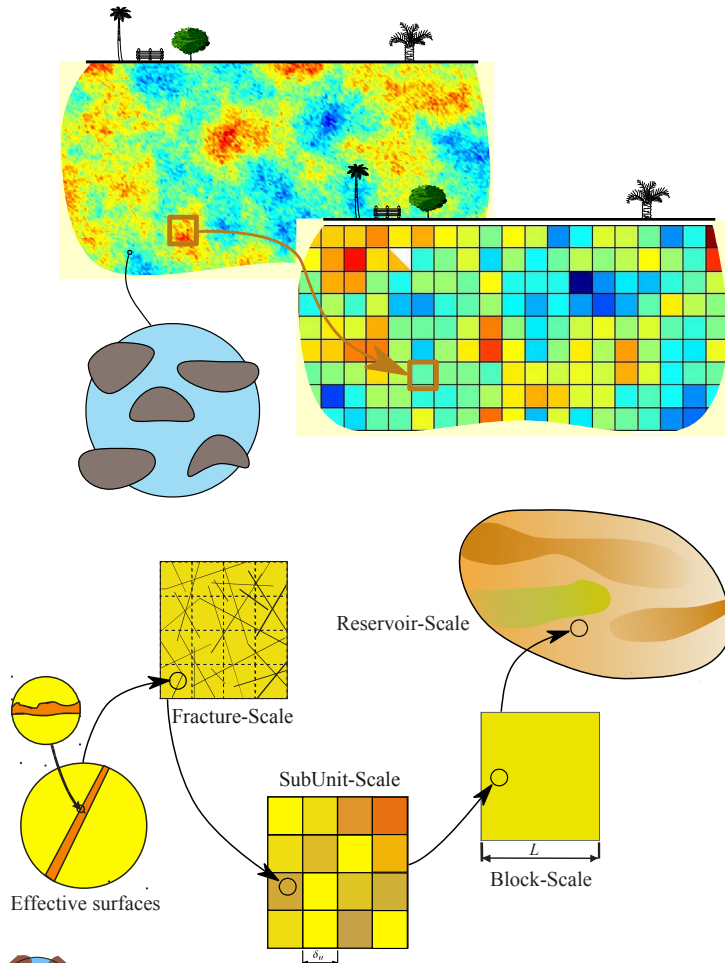
Conclusions on Porous Medium Modelling Approaches

- Various types of models (1-Eq, N-Eq, asymptotic, non-equilibrium, mixed or hybrid models, convolution, etc...)
- Validity conditions may be broken *during the same process!*
 - See Vafai, Nield, Vadasz, Jiang, ... MANY others! → depend on 3D, various Bcs and ICs, heterogeneity, ...
 - Better robustness of non-Equilibrium models
- Effective properties: estimates, bounds, computation from 3D images, measurement, ...
- Couplings and non-linearities: a lot of open problems!
 - Coupled closure problems
 - Role of non-conventional and cross-terms
 - non-linearities, especially reaction rates, radiation, ...
 - time and space averaging (turbulence, boiling, multiphase flow, ...)
- Good modeling practice: keep heterogeneities as much as possible!



A Final Word : Real Life Modeling !

- Use macro-scale equations even if :
 - No clear separation of scale
 - Finite length scale ratios
- Sequential upscaling approximately keeps percolation properties
- Keep heterogeneities in the final scale representation to incorporate the maximum of « abnormal » behavior



Percolation problem

