Transport in Porous Media

Michel Quintard

▶ **To cite this version:**

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
https://hal.science/hal-03656508

Submitted on 2 May 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Open Archive Toulouse Archive Ouverte

OATAO is an open access repository that collects the work of Toulouse researchers and makes it freely available over the web where possible

This presentation is published in : http://oatao.univ-toulouse.fr/20693

To cite this version:

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 (Unpublished)

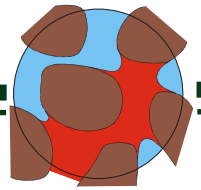
Any correspondence concerning this service should be sent to the repository administrator: tech-oatao@listes-diff.inp-toulouse.fr

Transport in Porous Media

Michel Quintard

D.R. CNRS

Institut de Mécanique des Fluides, Allée Prof. C. Soula
31400 Toulouse cedex – France
quintard@imft.fr

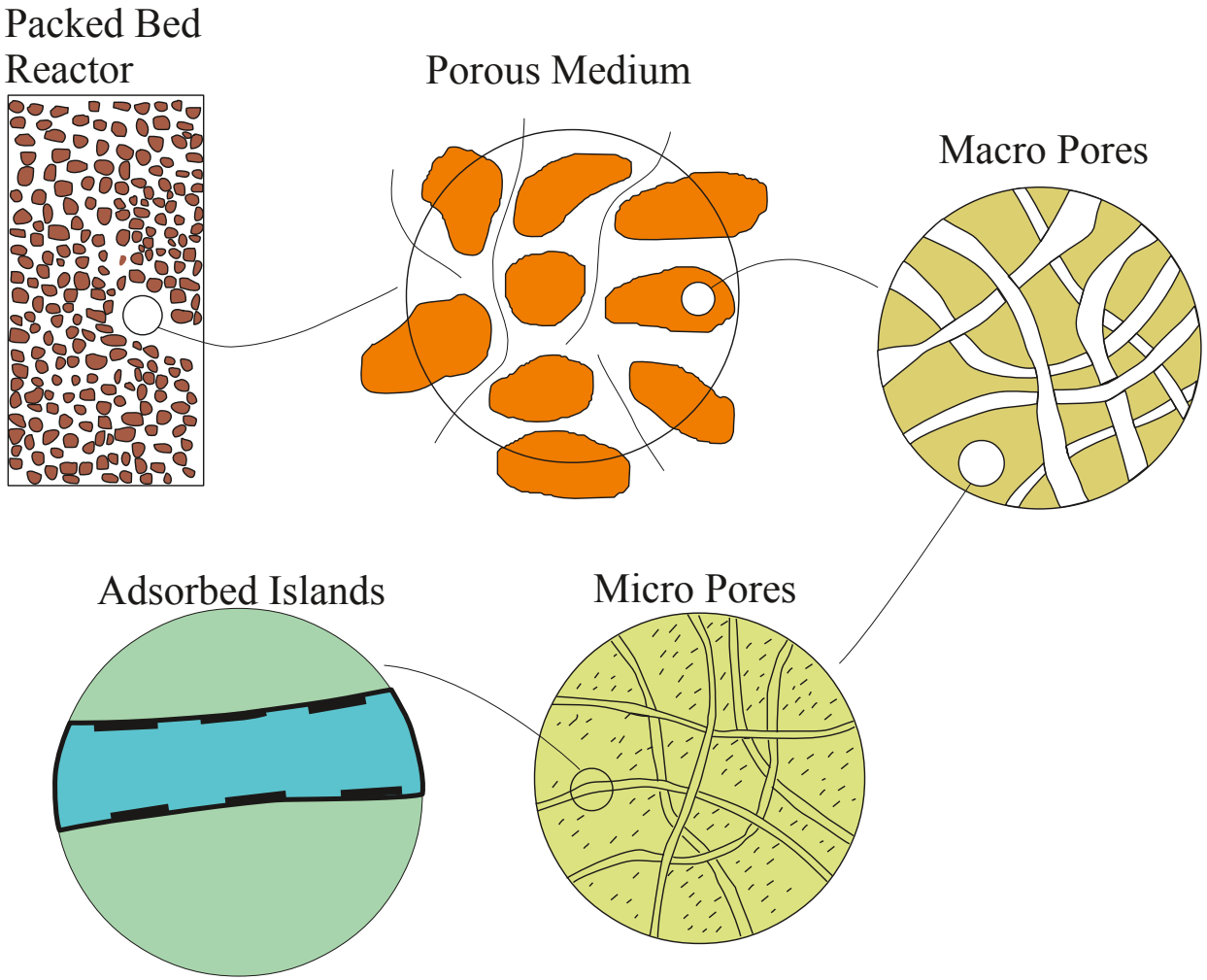


Outline

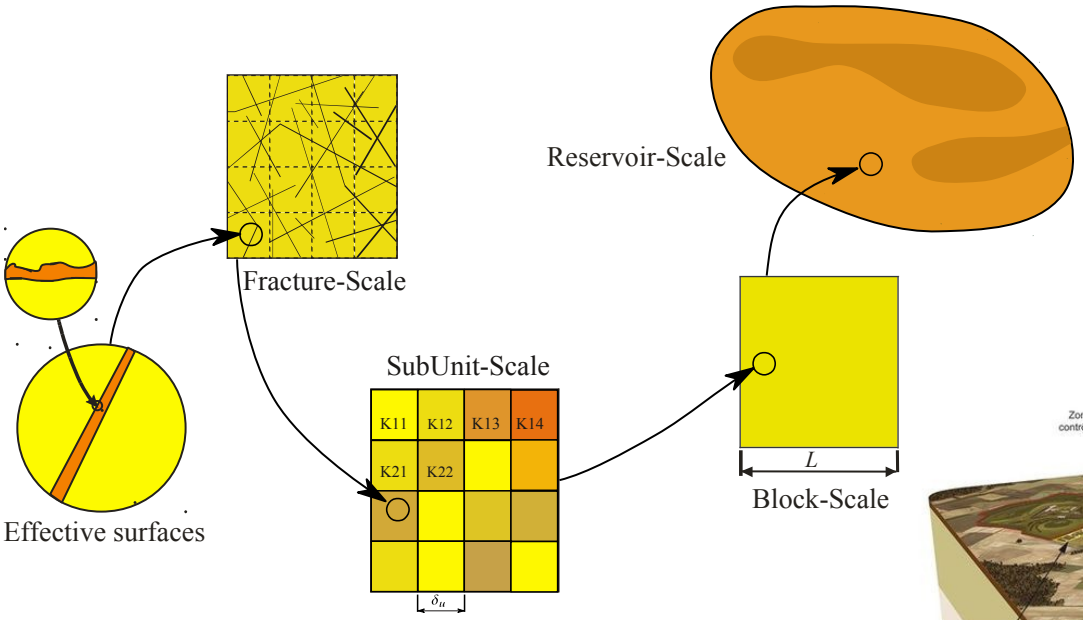
- Introduction
- Multi-scale aspects
- Diffusion/dispersion
- One-Phase flow
- Heat Transfer
- Two-Phase flow
- Coupled transfers: reactive transport, phase change
- Conclusion

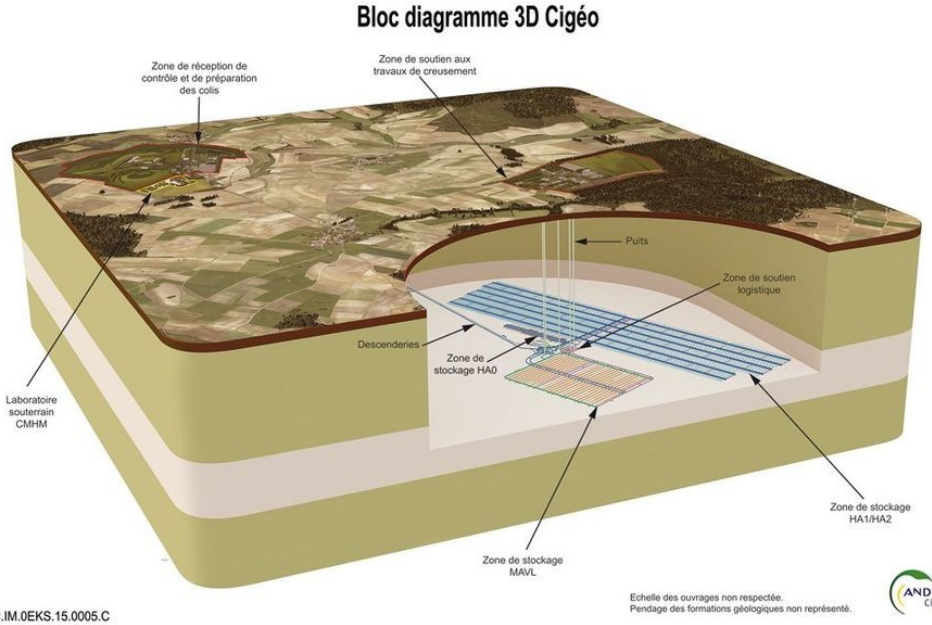
Introduction: multiple-scale analysis

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



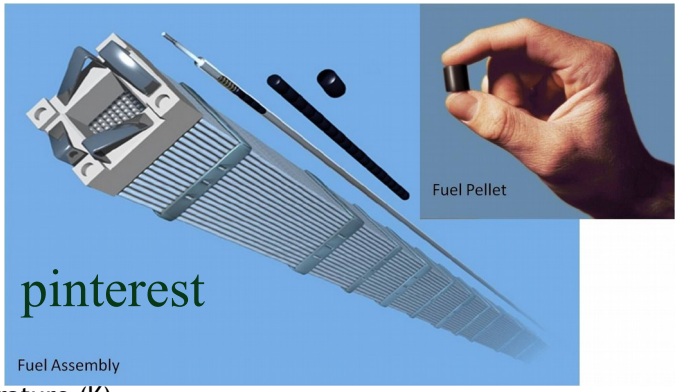
Example: geological formations





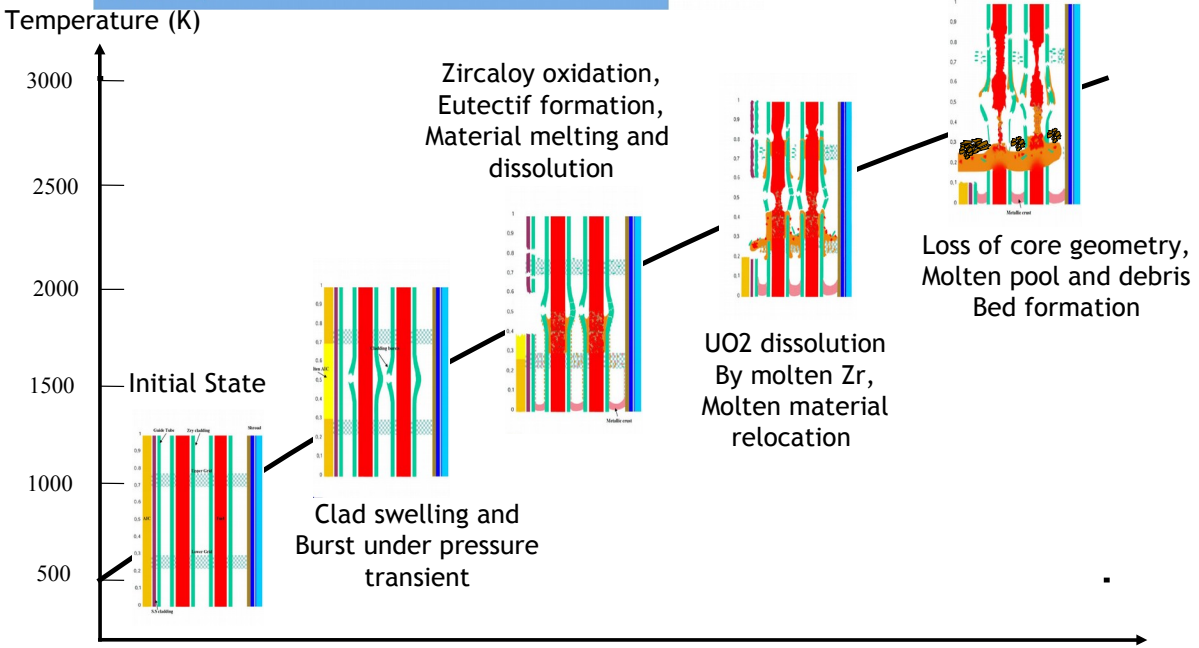
Nuclear Waste storage

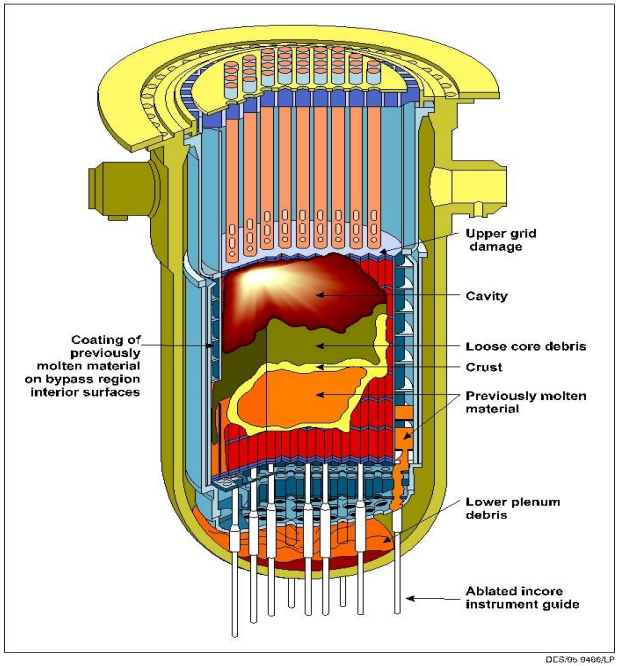
Example : Nuclear Reactor



Undamaged reactor….

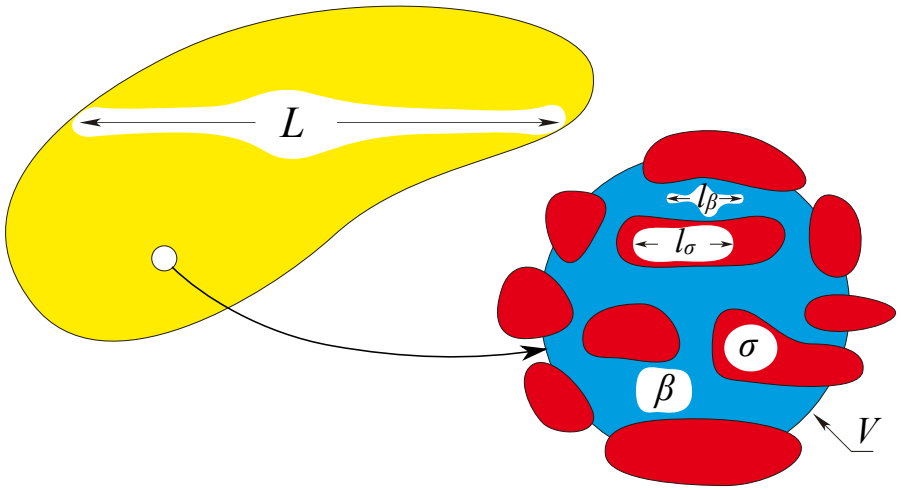
…. and after severe accident

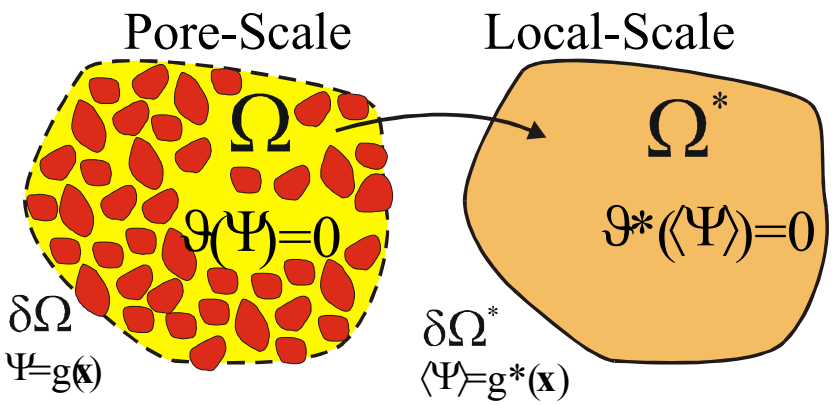




TMI-2 vessel final state

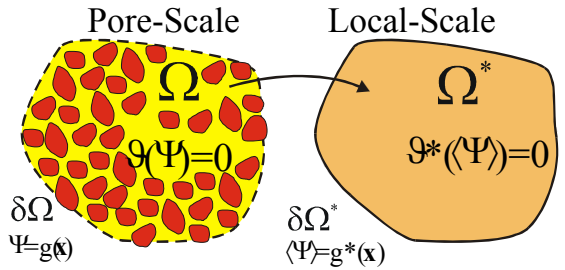
Upscaling





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

Upscaling: different points of view

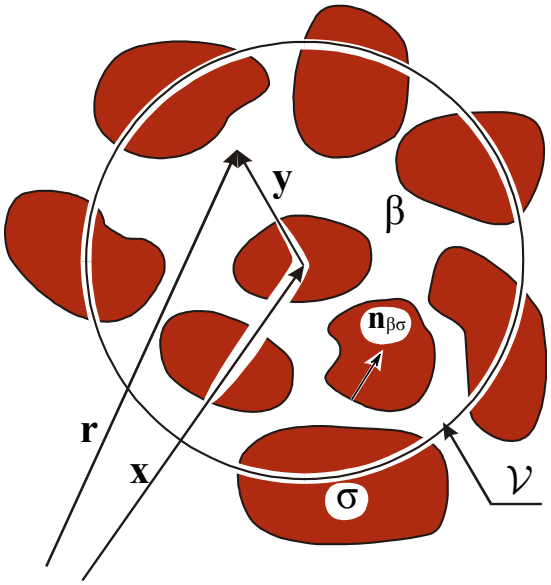


- **Heuristic: Darcy's law (1856)!**
- **Upscaling with *closure*: homogenization theory (*Sanchez-Palencia, Bensoussans et al.,...*), volume averaging (*Whitaker, … and variants*),**

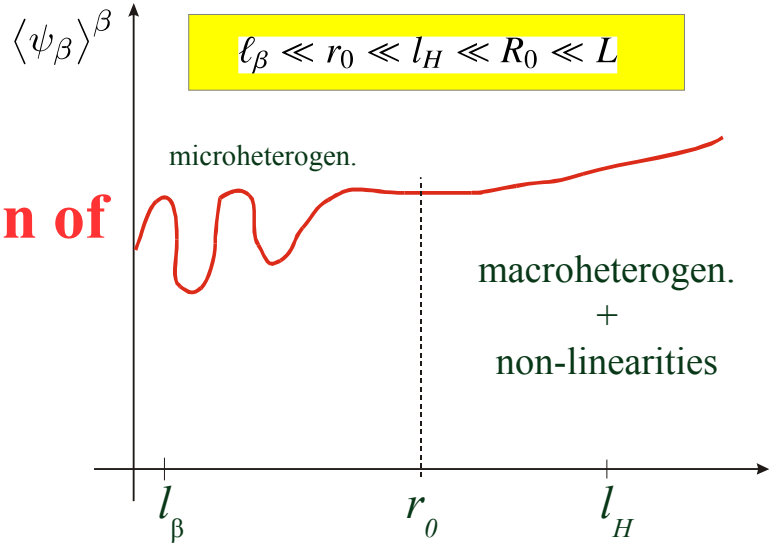
$$p_\beta = P_\beta + \tilde{p}_\beta \qquad \tilde{p}_\beta \stackrel{?}{=} f\left(P_\beta, \nabla P_\beta, \ldots\right)$$

- **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!



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

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

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

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**

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

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

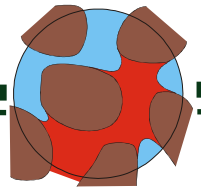
- **Saturation**

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

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

- **Intrinsic phase average**

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



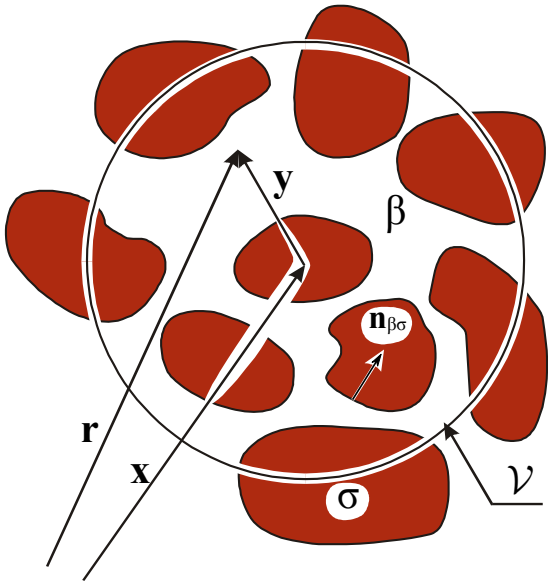
Theorems

Interfacial Effects (tortuosity,...)

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

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

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



Phase change, dissolution , ...

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

Total mass balance (no source/sink)

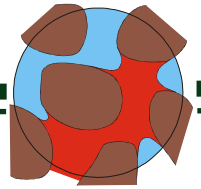
$$\frac{\partial \rho_\beta}{\partial t} + \nabla \cdot \left(\rho_\beta \mathbf{v}_\beta \right) = 0$$ pore-scale

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

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

$$\mathbf{V}_\beta = \left\langle \mathbf{v}_\beta \right\rangle = \varepsilon_\beta \mathbf{U}_\beta \qquad \frac{\partial \varepsilon_\beta \rho_\beta}{\partial t} + \nabla \cdot \left(\rho_\beta \mathbf{V}_\beta \right) = 0$$

  - **Constant density** $\quad \dfrac{\partial \varepsilon_\beta}{\partial t} + \nabla \cdot \mathbf{V}_\beta = 0$
  - **Constant porosity** $\quad \nabla \cdot \mathbf{V}_\beta = 0$



General Structure of a macro-scale transport equation

- **Pore-scale**

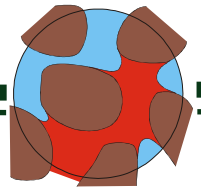
$$\frac{\partial \rho_\beta \omega_\beta}{\partial t} + \nabla . \left(\rho_\beta \omega_\beta \mathbf{v}_\beta \right) = \nabla . \left(\rho_\beta D_\beta \nabla \omega_\beta \right) - \underbrace{r_\beta \left(\omega_\beta \right)}_{\text{homogeneous reaction}}$$

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

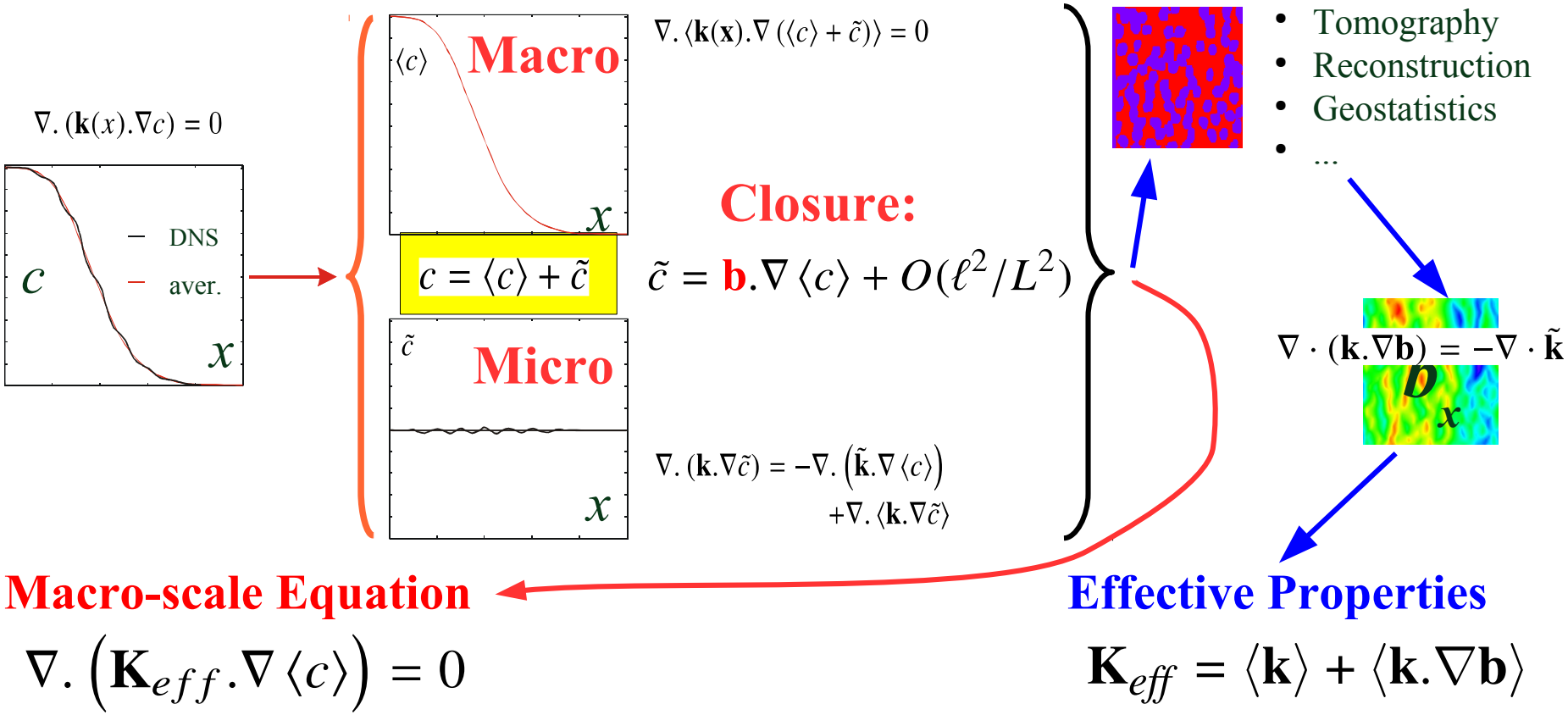
- **Macro-scale**

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

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



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



Note: high performance computing → up to 2048^3 voxels

Diffusion: coupled micro-macro eqs

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

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

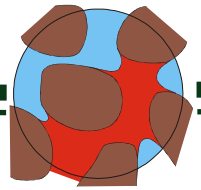
$$\frac{\partial c_\beta}{\partial t} = \nabla.\left(D_\beta \nabla c_\beta\right) \rightarrow \cancel{\frac{\partial \tilde{c}_\beta}{\partial t}} = \nabla.\left(D_\beta \nabla \tilde{c}_\beta\right) - \underbrace{\cancel{\nabla.\left(\frac{D_\beta}{\mathcal{V}_\beta}\int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma}\tilde{c}_\beta\,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

simplification with $\ell_\beta \ll L$

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

- **Averaged Equation**

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



Closure and Macro-scale equation

$$\tilde{c}_\beta = \mathbf{b}_\beta . \nabla C_\beta + \ldots \qquad C_\beta = \langle c_\beta \rangle^\beta$$

- **Local problem over representative UC**

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

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

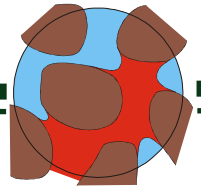
$$\frac{\partial \varepsilon_\beta C_\beta}{\partial t} = \nabla . \left(\varepsilon_\beta \mathbf{D}^*_\beta \cdot \nabla C_\beta \right)$$

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

macro-scale flux density

- **Effective diffusion tensor**

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

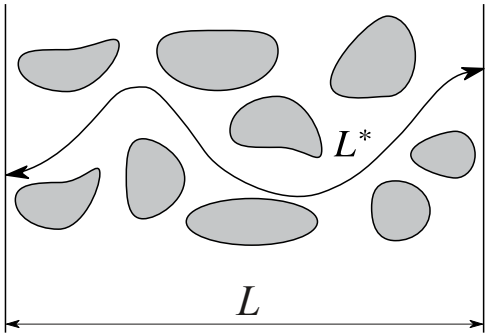


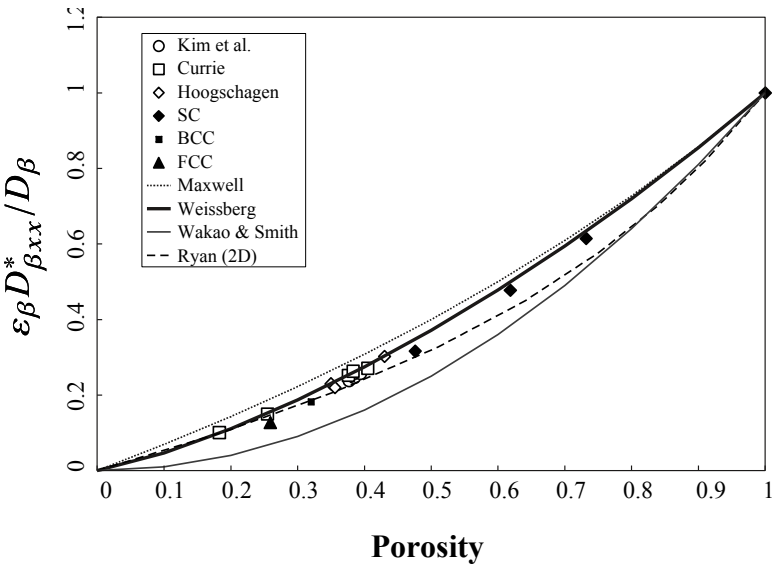
Tortuosity

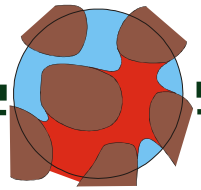
$$\mathbf{D}_\beta^* = D_\beta \left(\mathbf{I} + \frac{1}{\mathcal{V}_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_\beta \, dA \right)$$

- **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**

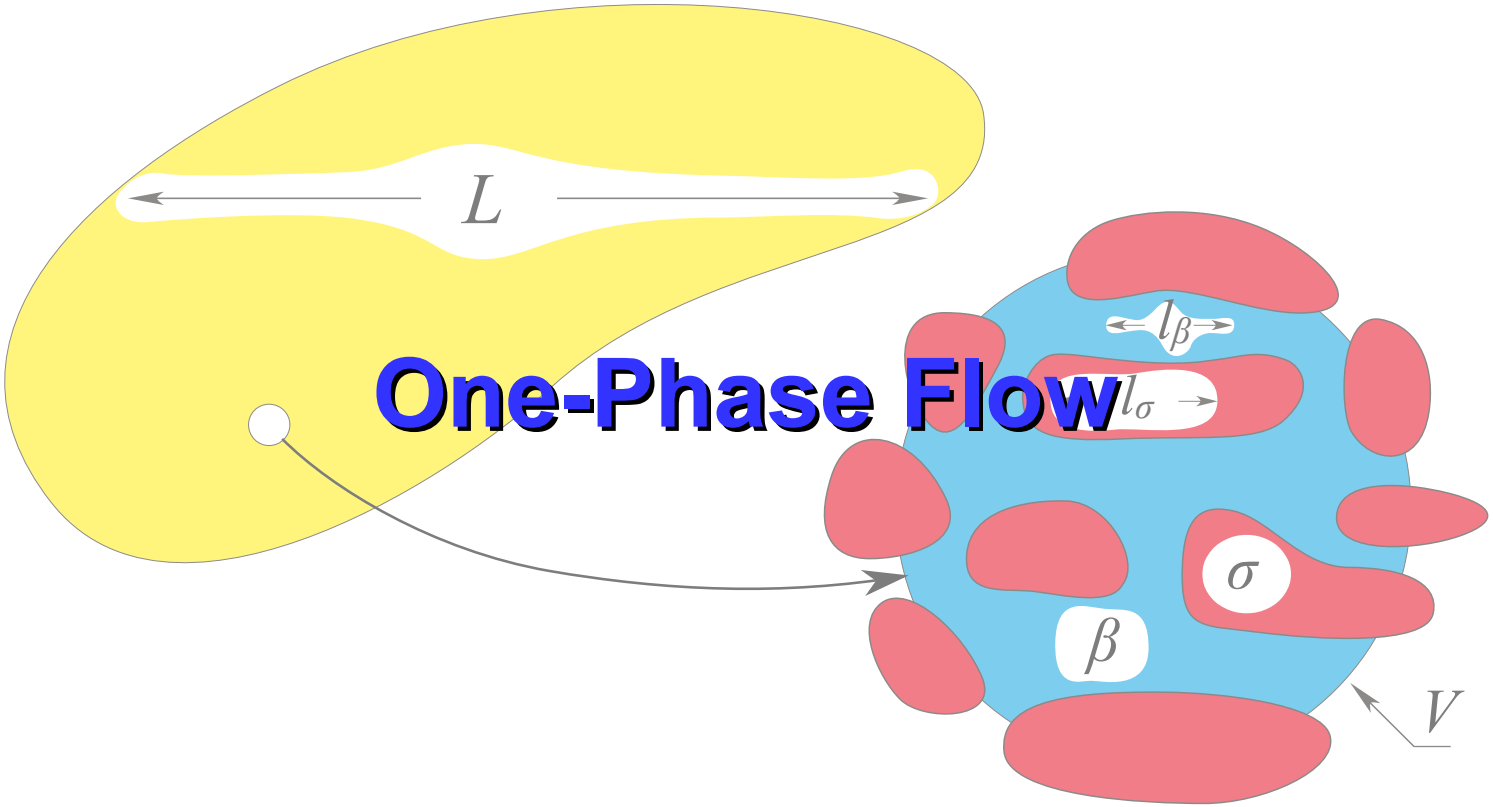
: $\tau_\beta \neq \frac{L^*}{L}$







One-Phase Flow



One-Phase Flow: Phenomenolgy

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

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

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

- **Pore-Scale regimes**
  - **Creeping (Re→ 0): leads to Darcy's law**
  - **Laminar**
  - **Turbulent**

} Various regimes and transitions

Upscaling One-Phase Flow

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

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

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

$$\rho_\beta \frac{\partial \langle \mathbf{v}_\beta \rangle}{\partial t} + \rho_\beta \langle \mathbf{v}_\beta \rangle \cdot \nabla \langle \mathbf{v}_\beta \rangle^\beta + \nabla \cdot \left(\rho_\beta \langle \tilde{\mathbf{v}}_\beta \tilde{\mathbf{v}}_\beta \rangle \right) =$$

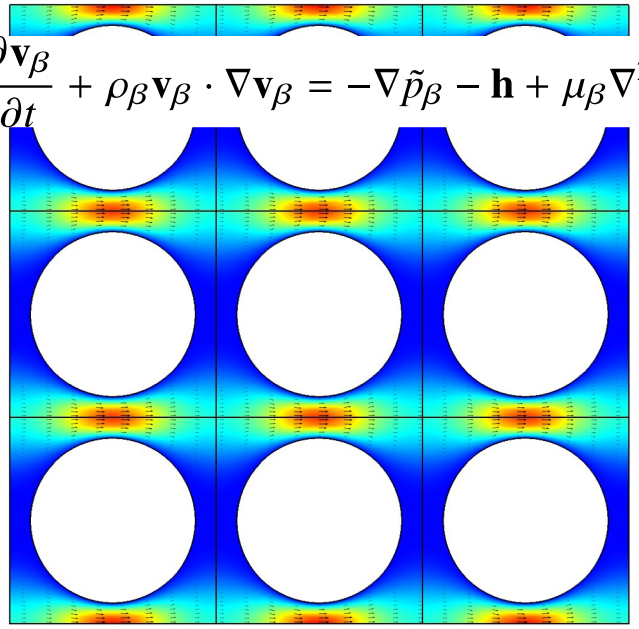
$$-\varepsilon_\beta \nabla \langle p_\beta \rangle^\beta + \varepsilon_\beta \rho_\beta \mathbf{g} + \underbrace{\mu_\beta \nabla^2 \langle \mathbf{v}_\beta \rangle - \mu_\beta \nabla \varepsilon_\beta . \nabla \langle \mathbf{v}_\beta \rangle^\beta}_{\text{Brinkman terms}} + \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\tilde{p}_\beta \mathbf{I} + \mu_\beta \nabla \tilde{\mathbf{v}}_\beta \right) dA$$

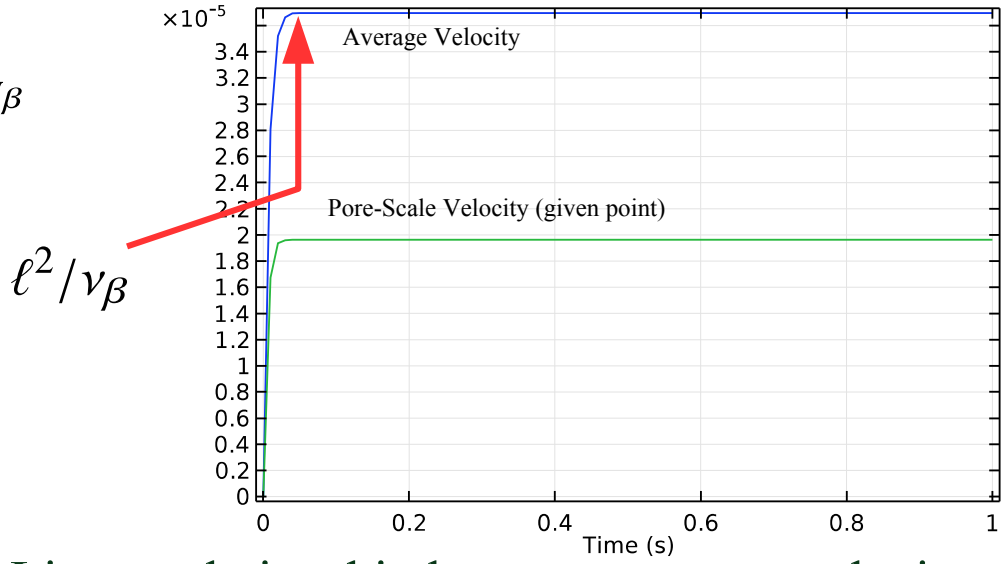
Remark: $\tilde{\mathbf{v}}_\beta \sim \langle \mathbf{v}_\beta \rangle^\beta$

Various Regimes: Creeping

Re~0

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





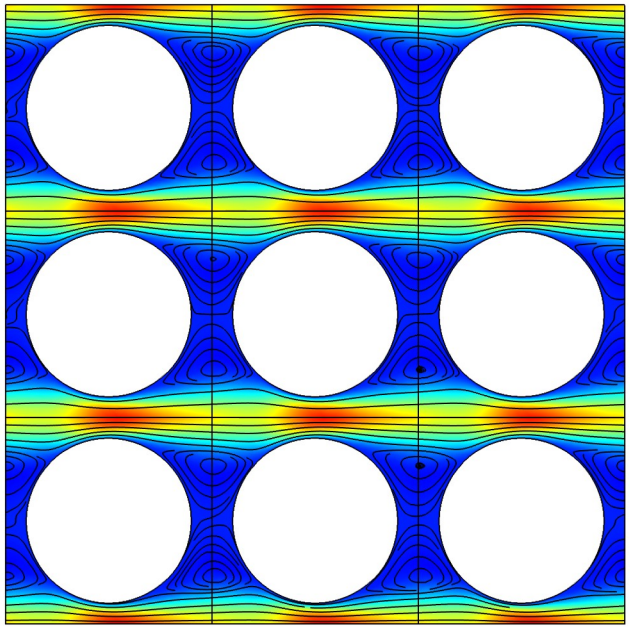
ℓ^2 / ν_β

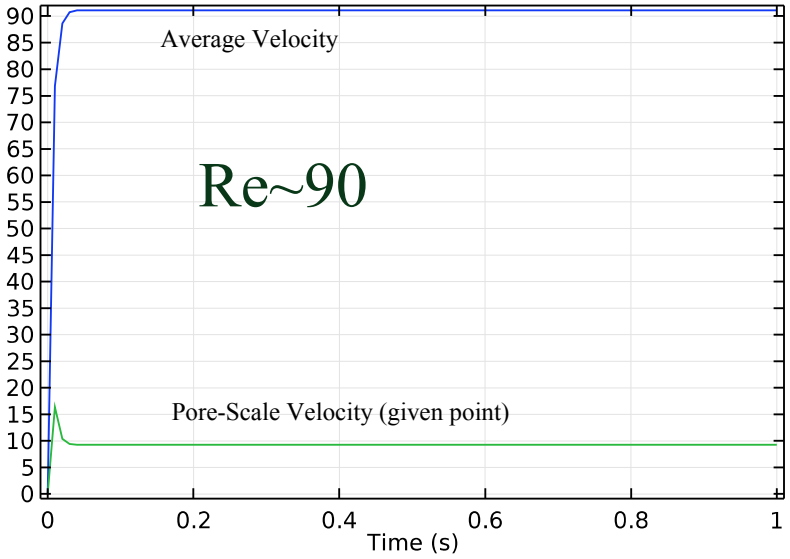
Linear relationship between average velocity and pressure drop!

$$0 = -\varepsilon_\beta \nabla \left\langle p_\beta \right\rangle^\beta + \varepsilon_\beta \rho_\beta \mathbf{g} + \mu_\beta \nabla^2 \left\langle \mathbf{v}_\beta \right\rangle - \mu_\beta \nabla \varepsilon_\beta \nabla \left\langle \mathbf{v}_\beta \right\rangle^\beta + \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\tilde{p}_\beta \mathbf{I} + \mu_\beta \nabla \tilde{\mathbf{v}}_\beta \right) dA$$

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

Various Regimes: Laminar Inertial



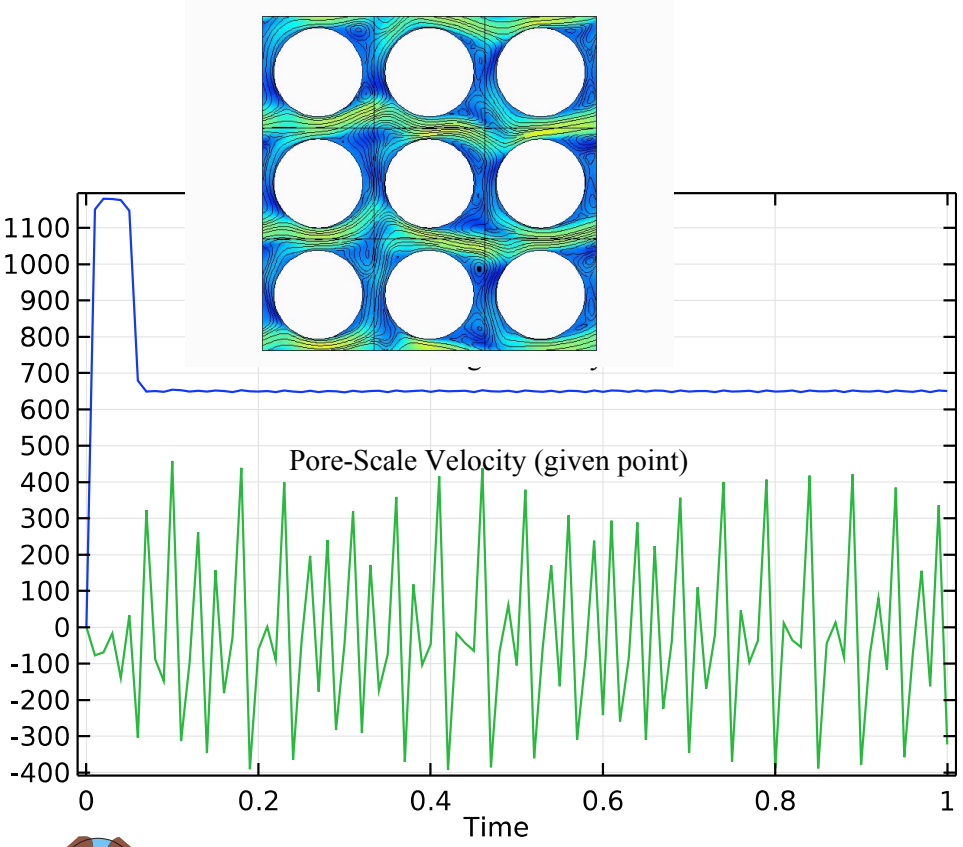


Still $$0 = -\varepsilon_\beta \nabla \left\langle p_\beta \right\rangle^\beta + \varepsilon_\beta \rho_\beta \mathbf{g} + \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-\tilde{p}_\beta \mathbf{I} + \mu_\beta \nabla \tilde{\mathbf{v}}_\beta \right) dA$$

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

Various Regimes: towards turbulence

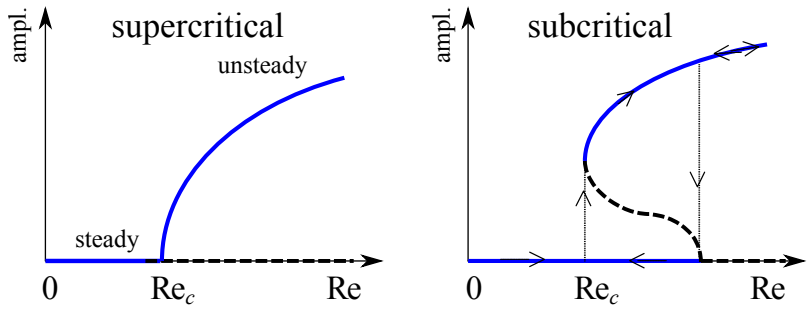
- ⟨v⟩=steady-state



- Macro-Scale Turbulence? (see Jin et al., 2015, DNS)
  - Localized turbulence (nearly periodic over *N*-UC) need $\overline{\langle \mathbf{v}_\beta \rangle}$
  - 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 ⊥ to axis

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

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

and up to localized turbulence one has

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

Closure: Darcy regime (Stokes problem=creeping flow)

Re~0

- **PDEs for deviations**

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

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

- **Closure in the linear case (3 elementary solutions for e_i)**

$$\tilde{p}_\beta = \mu_\beta\mathbf{b}.\left\langle\mathbf{v}_\beta\right\rangle^\beta + .. \; ; \; \tilde{\mathbf{v}} = \mathbf{B}.\left\langle\mathbf{v}_\beta\right\rangle^\beta + ..$$

Closure and Macro-Scale Equation (Darcy regime)

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

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

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

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

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

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

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...)

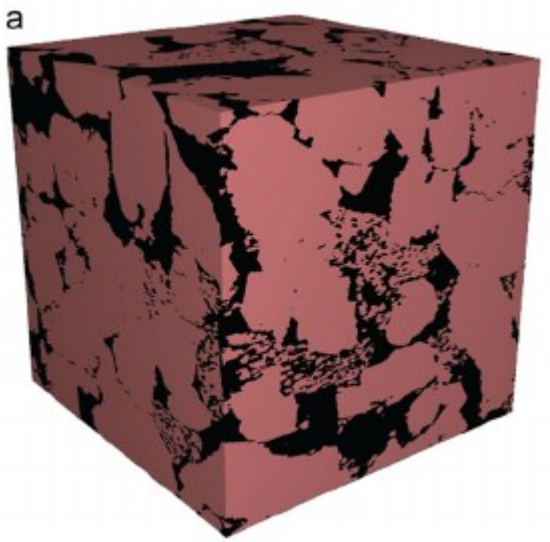
$$\rho_\beta \mathbf{v}_\beta \cdot \nabla \tilde{\mathbf{v}}_\beta = -\nabla \tilde{p}_\beta + \nabla \cdot \left(\mu_\beta \left(\nabla \tilde{\mathbf{v}}_\beta + \nabla \tilde{\mathbf{v}}_\beta^T \right) \right) - \left(\nabla \left\langle p_\beta \right\rangle^\beta - \rho_\beta \mathbf{g} \right)$$

=0, Darcy regime

$$\nabla . (\tilde{\mathbf{v}}_\beta) = 0 \qquad \tilde{\mathbf{v}} = -\left\langle \mathbf{v}_\beta \right\rangle^\beta \text{ at } A_{\beta\sigma}$$

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, ...

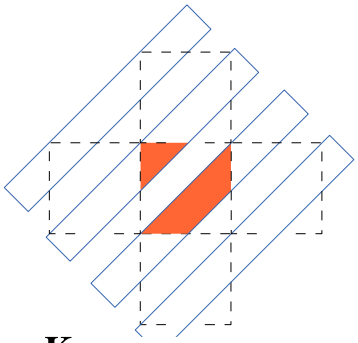


Calculation of the permeability

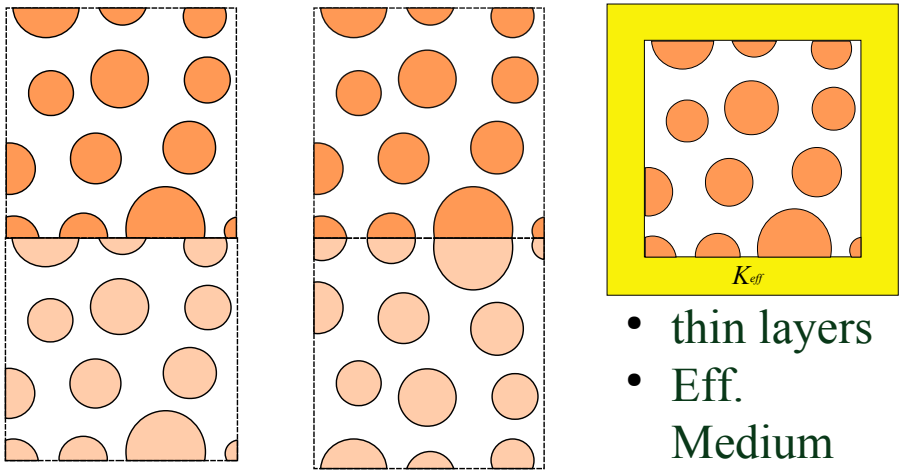
Case of "diffusion" problem: e.g., permeability, effective diffusion

- **Periodicity : good for anisotropy**
- **Making image periodic?**
  - **I: Percolation problem**
  - **II: Loss of anisotropy**
  - **III: potentially various bias**

See discussion in Guibert et al., 2015



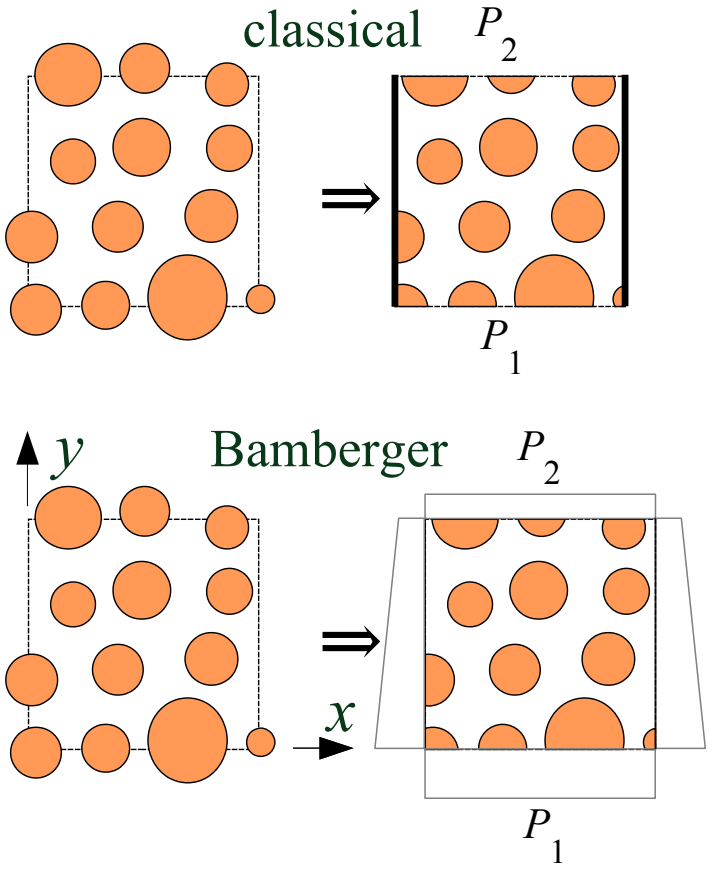
$$\mathbf{K}_{eff} = \varepsilon_\beta \mathbf{K}_\beta + \varepsilon_\sigma \mathbf{K}_\sigma + \frac{\varepsilon_\beta \varepsilon_\sigma \left(\mathbf{K}_\beta - \mathbf{K}_\sigma\right) \cdot \mathbf{ii} \cdot \left(\mathbf{K}_\sigma - \mathbf{K}_\beta\right)}{\mathbf{i} \cdot \left(\varepsilon_\beta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



- thin layers
- Eff. Medium

Calculations over non-periodic images (cont.)

- "permeameters"
  - All methods have bias
  - $\langle v_x \rangle^{\beta} \neq 0$
  - $K_{xy} \neq K_{yx}$



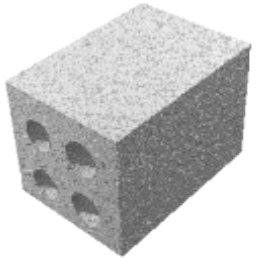
Note: minimal bias if large sample and anisotropy along the axis

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

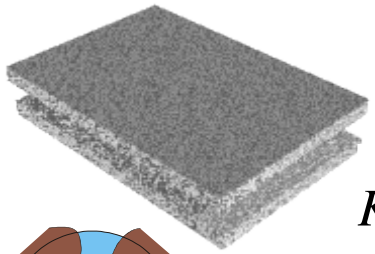
Permeability : $K \sim d_p^2$, 1 Darcy $= 10^{-12}$ m^2

Rocks : shale sandstone

Soils: clay silt sand gravel



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



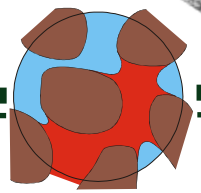
$$K = \varepsilon \frac{b^2}{12} \quad \text{Hele Shaw}$$

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

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

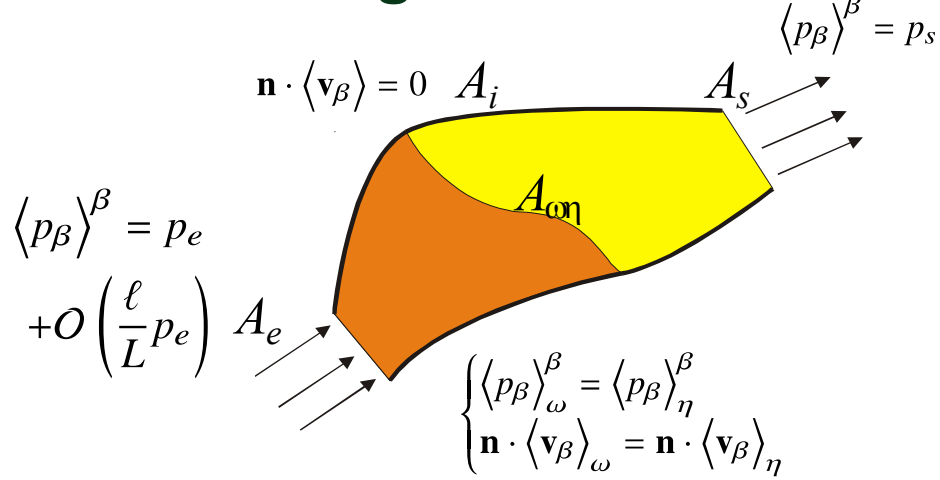
$$K = \frac{\varepsilon^3 d_K^2}{h_K (1-\varepsilon)^2} \qquad a_{vs} = \frac{a_v}{1-\varepsilon}$$

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

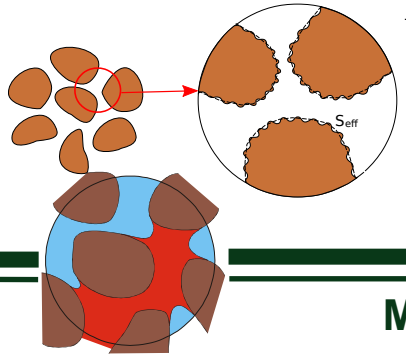


Boundary Conditions

- **Heterogeneous media**



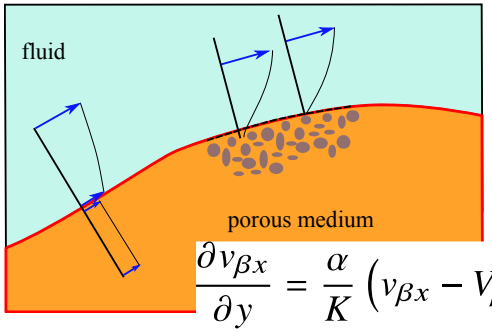
- **Rough surfaces**



$$\mathbf{U}_0 = \mathbf{M} \cdot \left[\mathbf{n} \cdot \left(\nabla \mathbf{U}_0 + (\nabla \mathbf{U}_0)^T\right) \cdot (\mathbf{I} - \mathbf{nn})\right]$$

General Navier BC

- **fluid/porous medium**



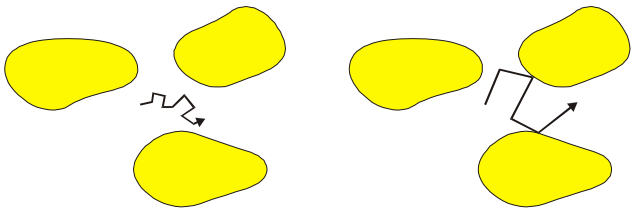
$$\mathbf{n} \cdot \mathbf{v}_\beta = \mathbf{n} \cdot \mathbf{V}_\beta \quad ; \quad p_\beta = P_\beta$$

$$\mathbf{n} \cdot \left(-p_\beta \mathbf{I} + \mu_\beta \left(\nabla \mathbf{v}_\beta + \left(\nabla \mathbf{v}_\beta\right)^T\right)\right) \cdot (\mathbf{I} - \mathbf{nn}) = \left(\alpha \mu_\beta \sqrt{3} / \sqrt{tr(\mathbf{K})}\right)\left(\mathbf{v}_\beta - \mathbf{V}_\beta\right) \cdot (\mathbf{I} - \mathbf{nn})$$

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

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

Klinkenberg Effect (1941)



p *p≈0*

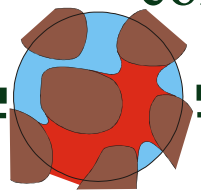
$$K = K_\infty \left(1 + \frac{b}{P_\beta}\right)$$

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



Non Darcean regimes (Re>1)

- **Heuristic: Forchheimer, Ergun, …**

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

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

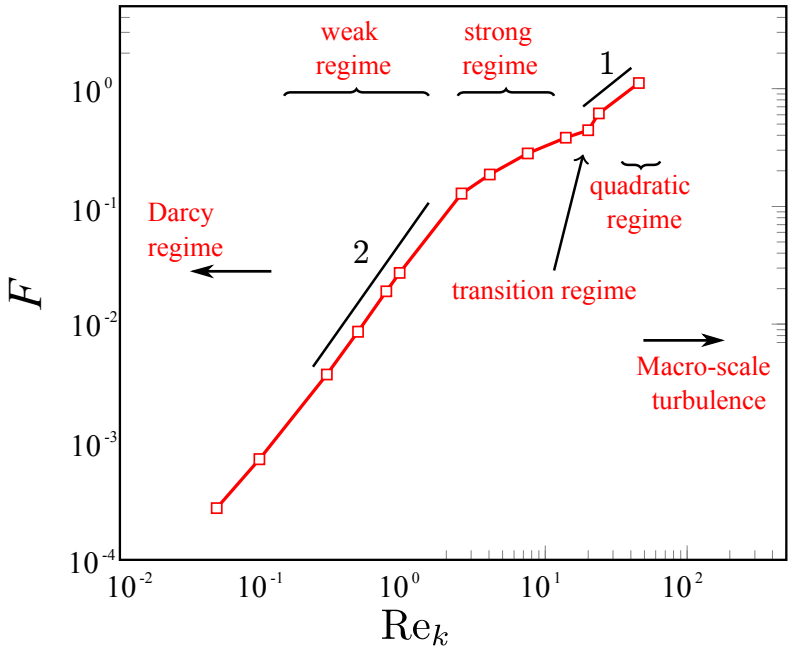
(passability)

- **Upscaling?**

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

$$\Downarrow$$

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



Non Darcean regimes (Re>1)

- laminar inertia effects: theory → generalized Forchheimer equation

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

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

Weak Inertia

- **Solution following asymptotic expansions in Re**

$$\delta = \frac{\ell}{\nu_\beta} v = \mathrm{Re}$$

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

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

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

- **1st correction?**
  - **Periodic media:** $F_{\parallel} \sim v^2$
  - **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** $\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \Rightarrow \left(\tilde{p}_\beta, \mathbf{v}_\beta\right) \Rightarrow \langle \mathbf{v}_\beta \rangle^\beta = v\boldsymbol{\lambda}$

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

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

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

P: rotation

F: non-linear scaling

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

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

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

Transition to inertia regimes: which Re number?

$$\mathrm{Re} = \frac{\langle \mathbf{v}_\beta \rangle^\beta \ell}{\nu_\beta}$$

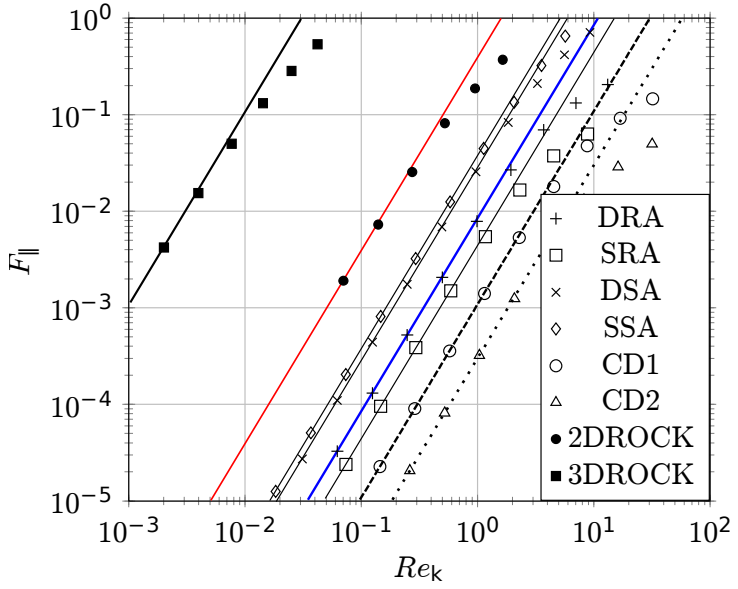
- Literature discussion (see polemic in Lage et Antohe, 2000; etc...)
- $\ell = \sqrt{K}$?
  - $K = \varepsilon d^2/32$ for a bundle of tubes (transition would change with porosity! → better

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

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

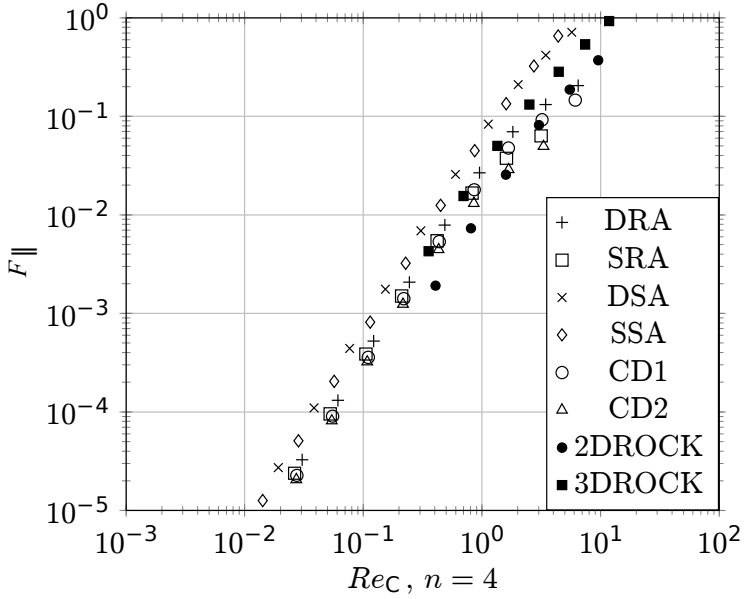
Transition to inertia effect: effect of topology (Pauthenet et al., 2017)

- If Re_k



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

- Re_C



$$\mathrm{Re}_C = \frac{v}{\nu_\beta}\sqrt{\frac{K_\lambda}{\varepsilon_\beta}C_\lambda}$$

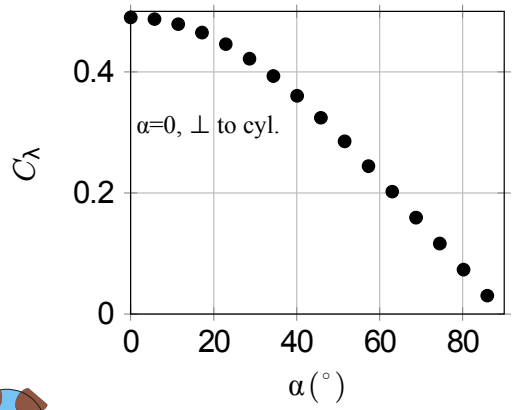
Topology effect (Ex.: array of Cylinder)

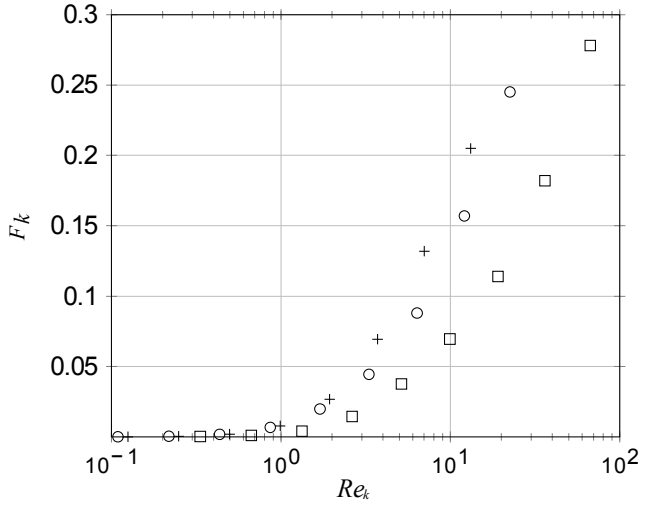
- **Tentative (open question)**

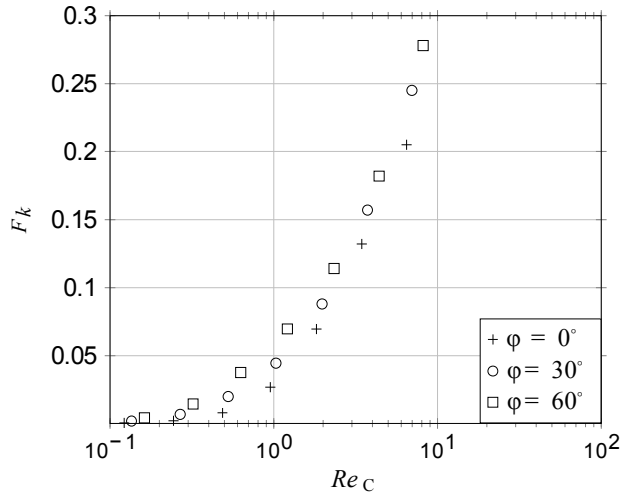
from Darcy closure

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

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



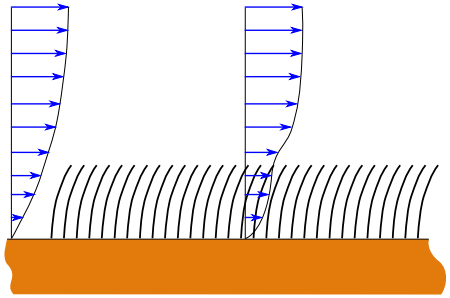


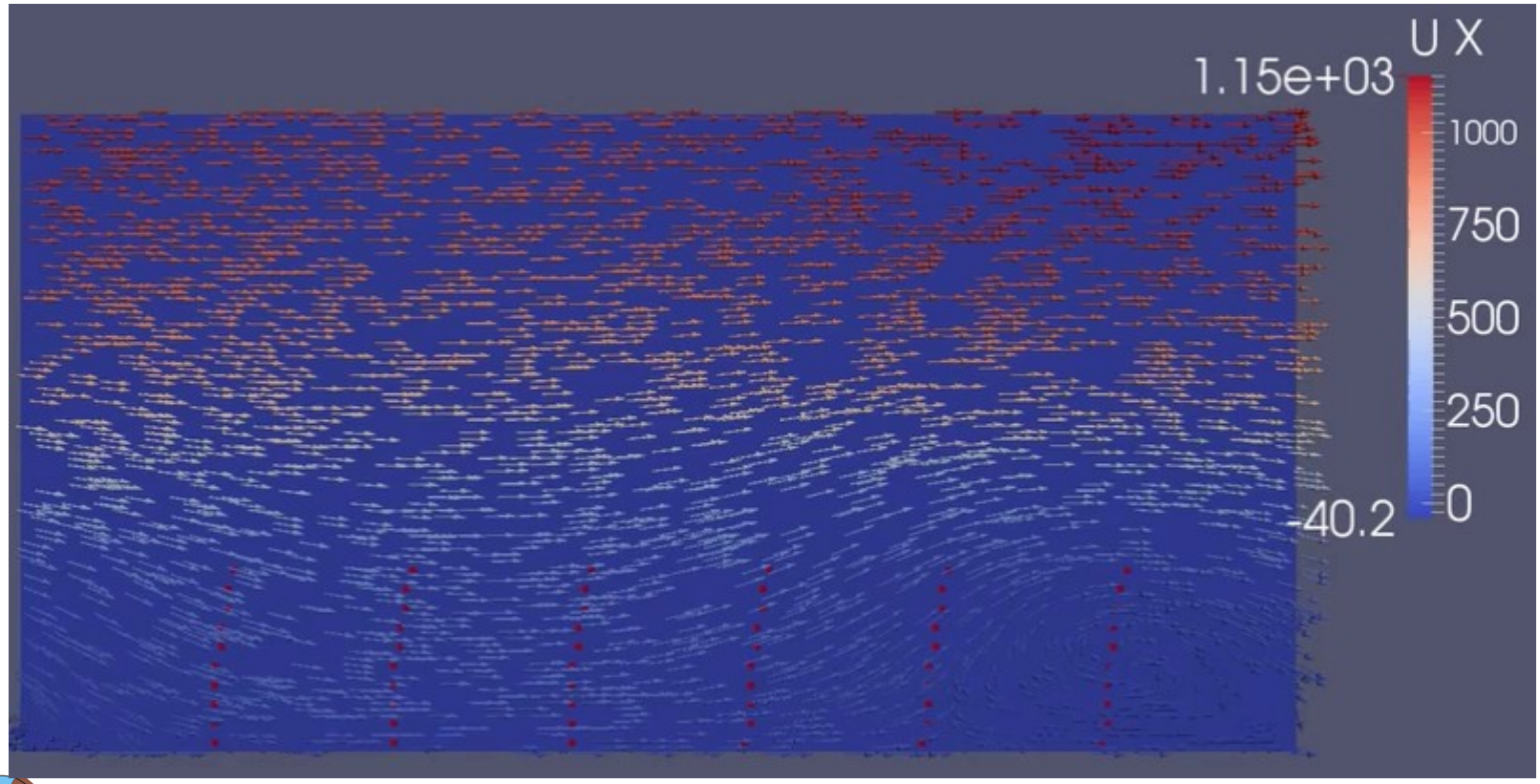


Example: canopy flow

Honami generation (Pauthenet, 2017)

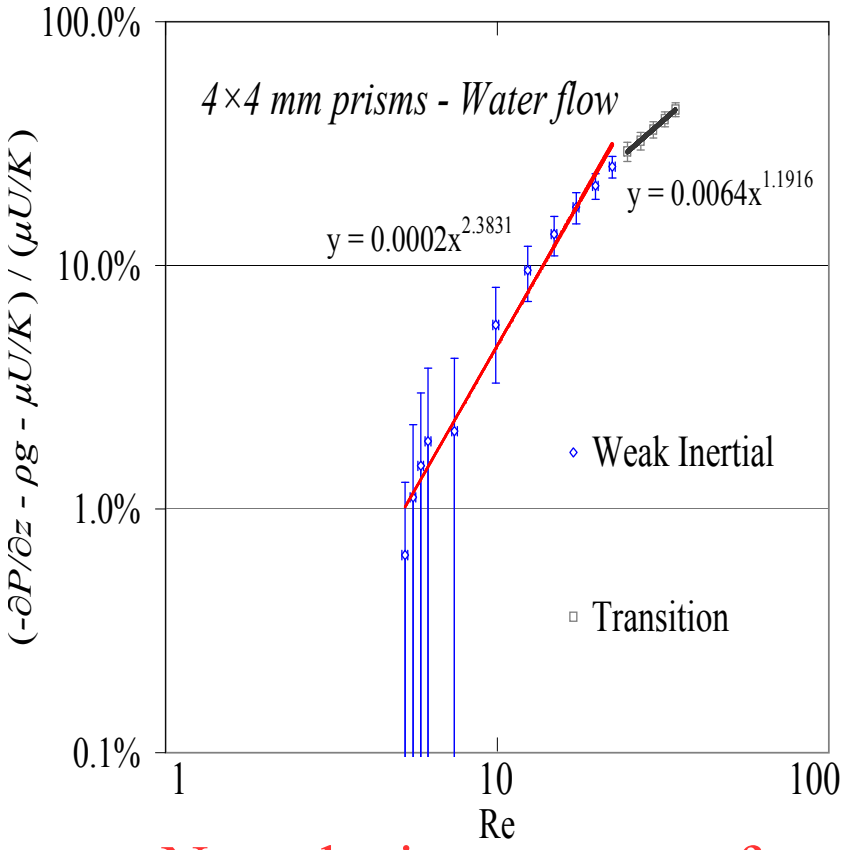
...need $\mathbf{K}_{app}$ for all fiber directions and $\mathbf{V}_{\beta}$



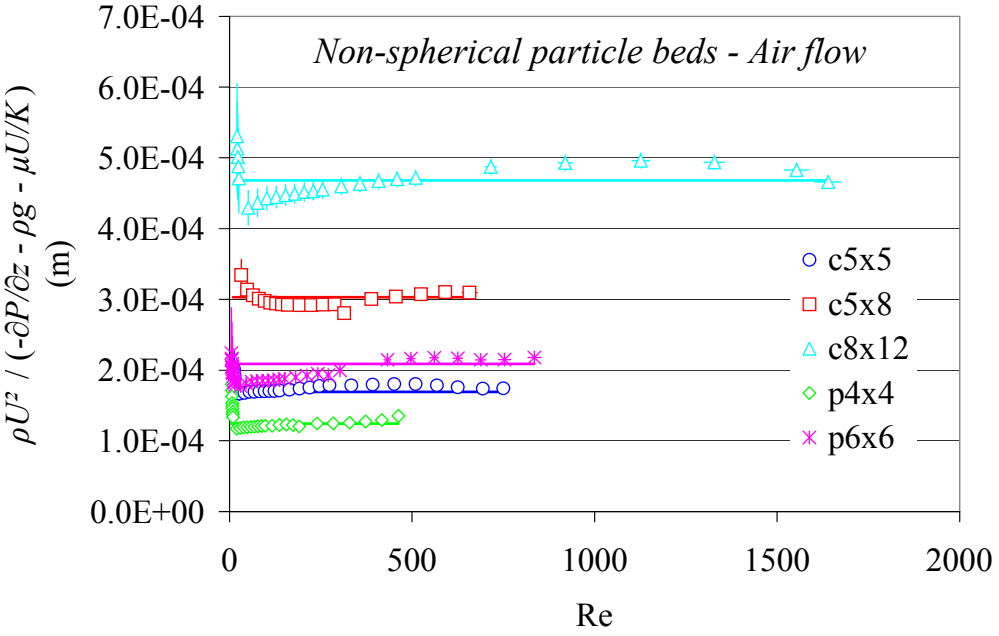


Experimental Evidence: inertia regime

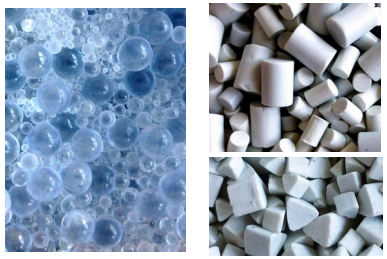
Weak inertia



Strong inertia



Clavier et al., 2014



Note the importance of transition regimes!

Turbulent flows in porous media (Re>>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!?

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

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

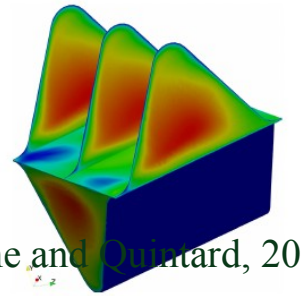
  - For one-phase flow: scheme "II" seems preferable: contrary to Antohe & Lage (1997), Getachew et al. (2000), see discussion in Nakayama & Kuwahara (1999), Pedras and de Lemos (2001), etc...
- Open: Simultaneous closure over $[R^3 \times R^t]$? More complex sequential closures ($t \rightarrow x \rightarrow t \rightarrow \ldots$) 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** $\langle \overline{\mathbf{v}_\beta} \rangle$ 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

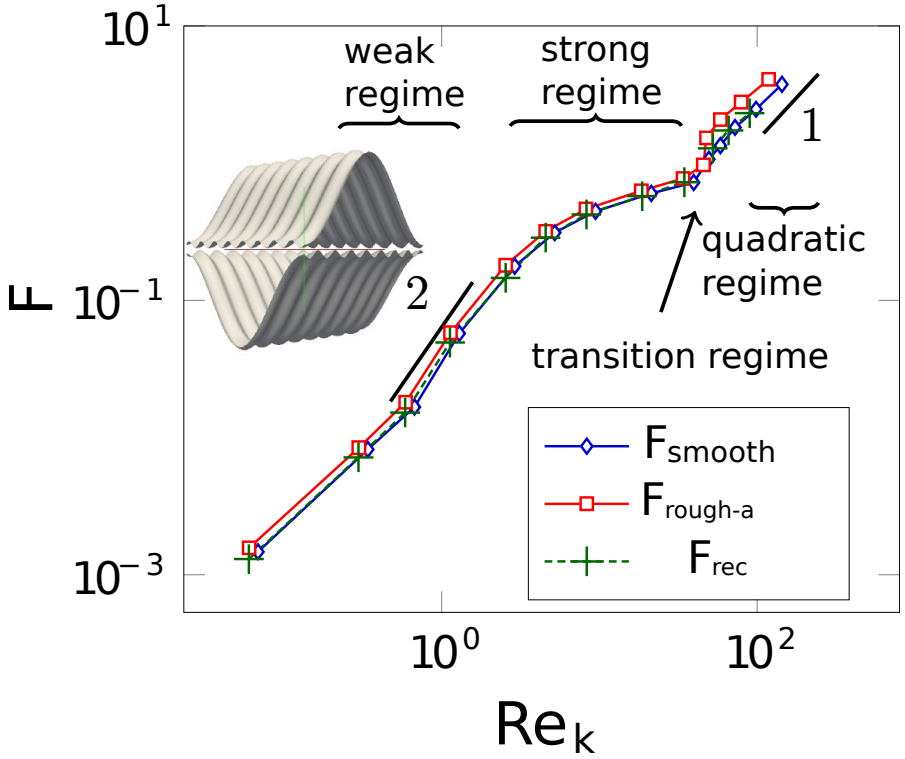
$$K^*_{yy} = \frac{K_0}{1 + \gamma_l \sqrt{Re}} \text{ (laminar)} \quad ; \quad K^*_{yy} = \frac{K_1}{1 + \beta_t Re} \text{ (turbulent)}$$

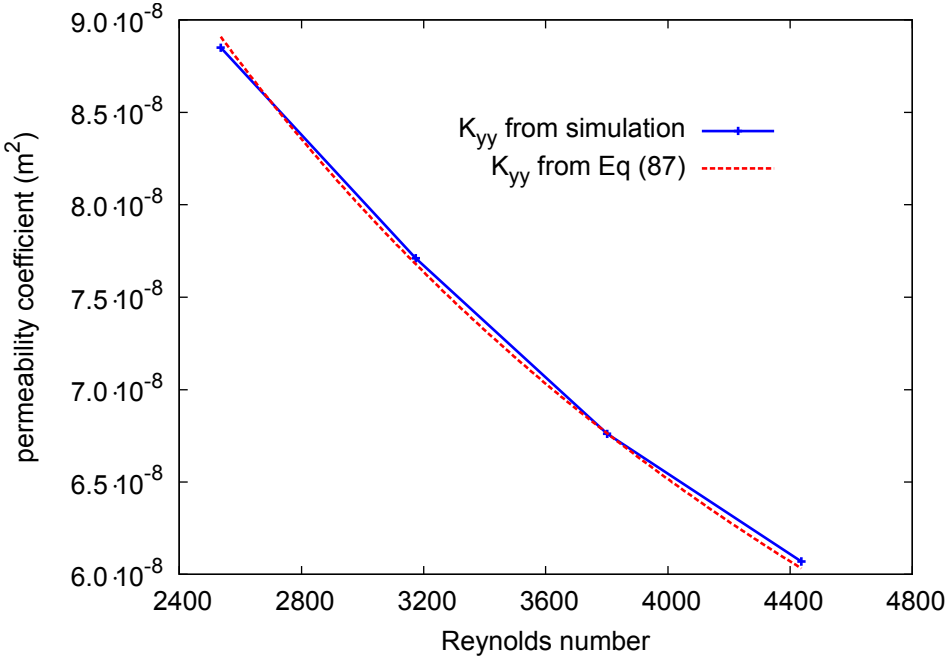


Soulaine and Quintard, 2014

- **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)



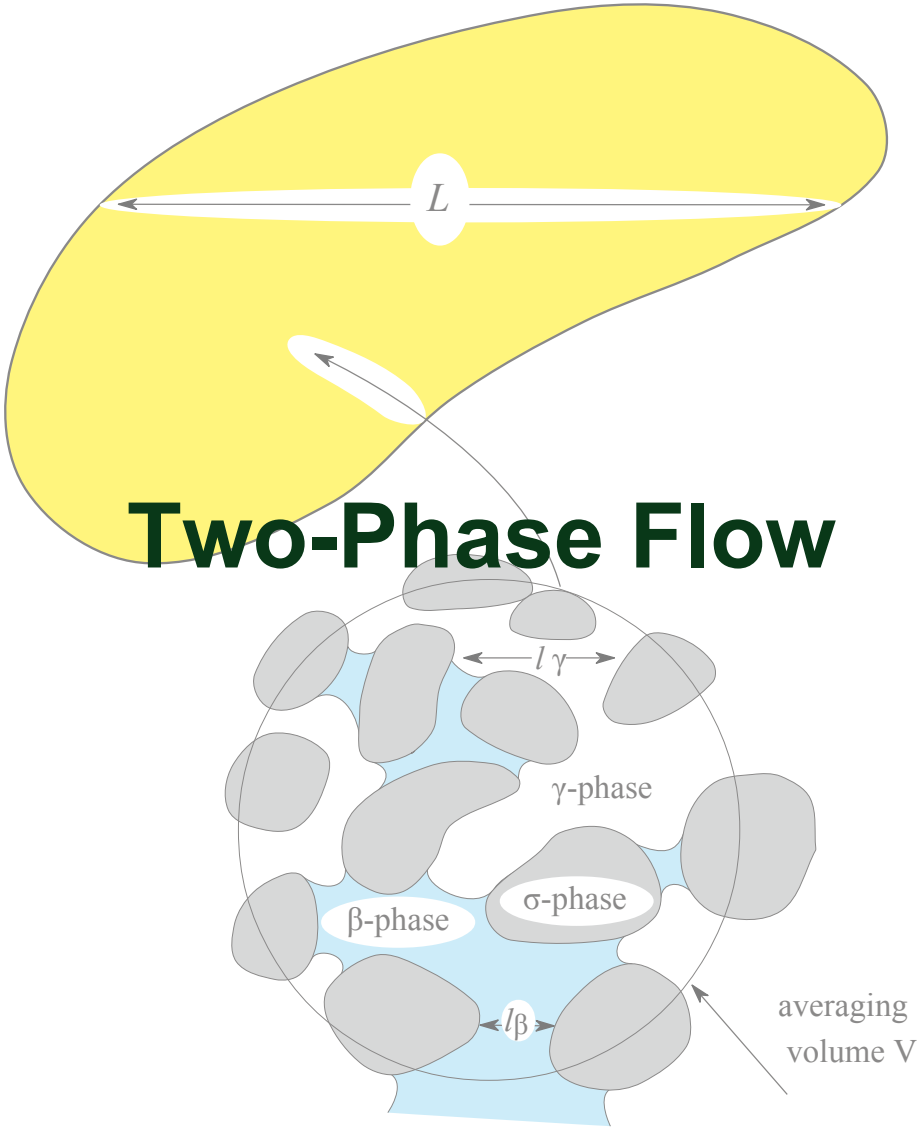


↑ Averaging of NS; Pasquier et al., 2016

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

Averaging of RANS model; Soulaine & Quintard, 2014 ↗

Two-Phase Flow



Two-Phase Flow

- **Pore-scale**

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

$$\frac{\partial \rho_\alpha \mathbf{v}_\alpha}{\partial t} + \nabla . (\rho_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha) =$$

$$-\nabla p_\alpha + \rho_\alpha \mathbf{g} + \mu_\alpha \nabla^2 \mathbf{v}_\alpha \text{ in } V_\alpha \qquad \alpha = \beta, \gamma$$

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

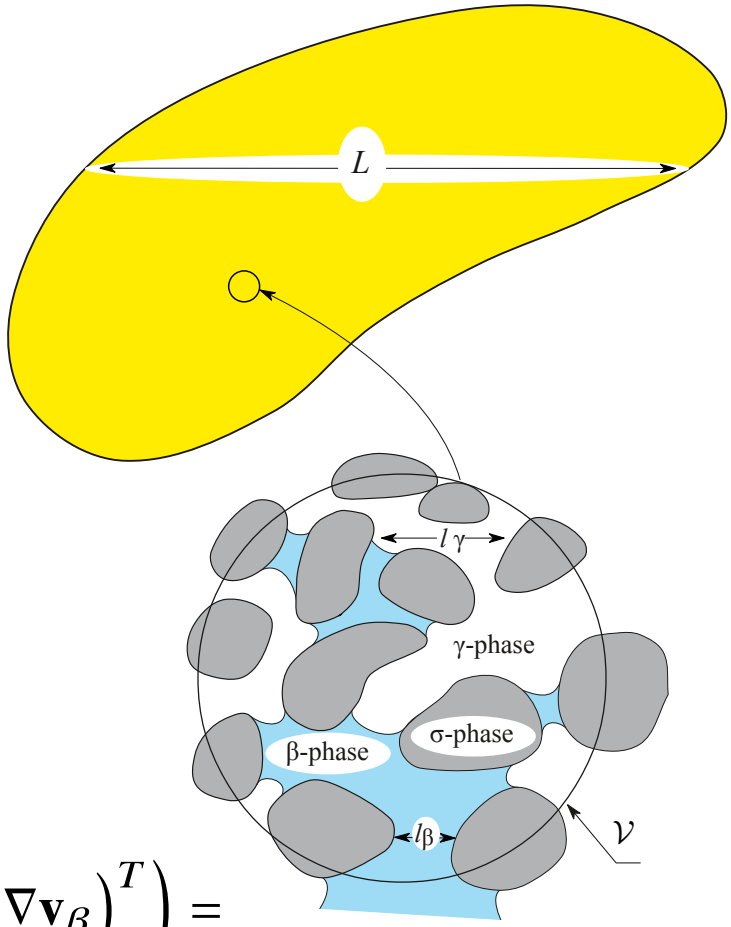
B.C. 2 $\mathbf{v}_\gamma = 0$ at $A_{\gamma\sigma}(t)$

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

B.C. 4

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

$$-\mathbf{n}_{\beta\gamma} p_\gamma + \mu_\gamma \mathbf{n}_{\beta\gamma} \cdot \left(\nabla \mathbf{v}_\gamma + \left(\nabla \mathbf{v}_\gamma \right)^T \right) + 2\sigma H_{\beta\gamma} \mathbf{n}_{\beta\gamma} \text{ at } A_{\beta\gamma}(t)$$



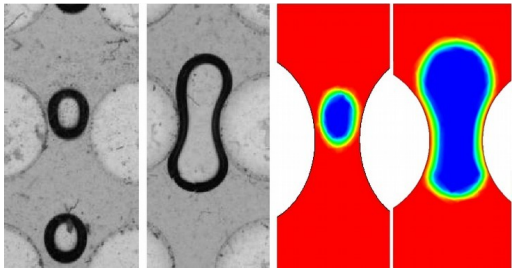
Note: complex and transient pore-scale flows

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

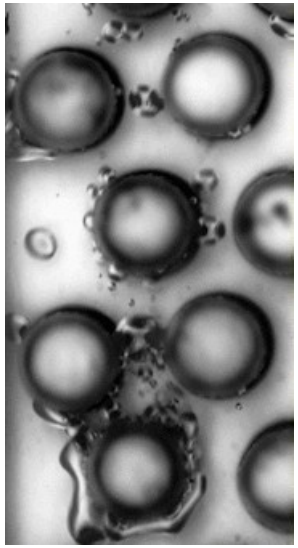
⇓

- 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

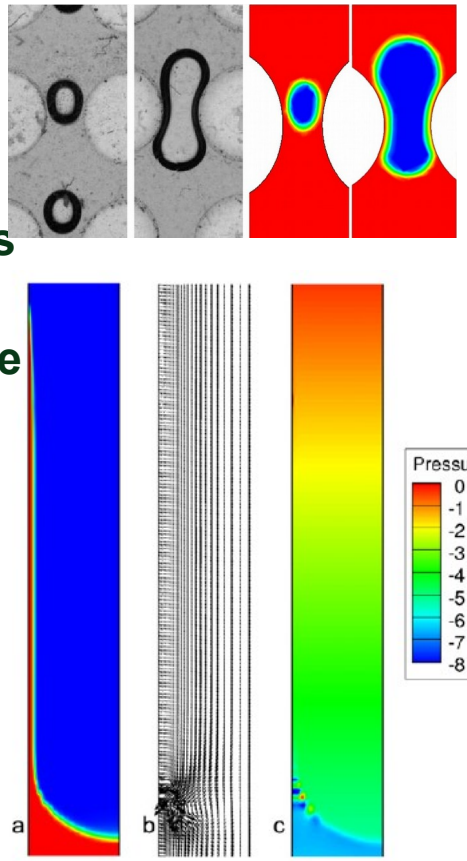


Fig. 6. Simulation of drainage with spurious currents along the meniscus curvature (HRIC, $Co = 1.00$, $Ca = 0.03$), (a) volume fraction, (b) velocity profile, (c) pressure distribution.

Horgue et al., 2012

Upscaling: quasi-static theory

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

- **Example: Case of B.C. 4**

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

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

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

+ Re, (We=Re×Ca) numbers

+ *Dynamic* Bond number

} If $\approx 0 \Rightarrow$

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

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

i.e., the classical capillary pressure theory!

Macro-Scale Models : Quasi-Static

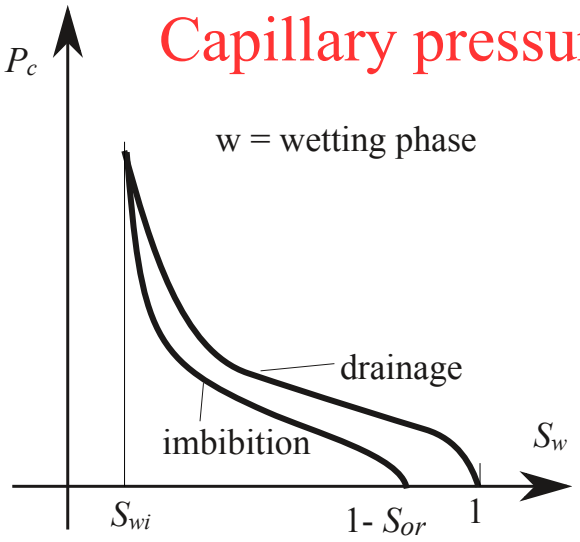
$$\mathbf{V}_\alpha = \langle \mathbf{v}_\alpha \rangle \; ; \; P_\alpha = \langle p_\alpha \rangle^\alpha \; ; \; \varepsilon_\alpha = \varepsilon S_\alpha \qquad \alpha = \beta, \gamma$$

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

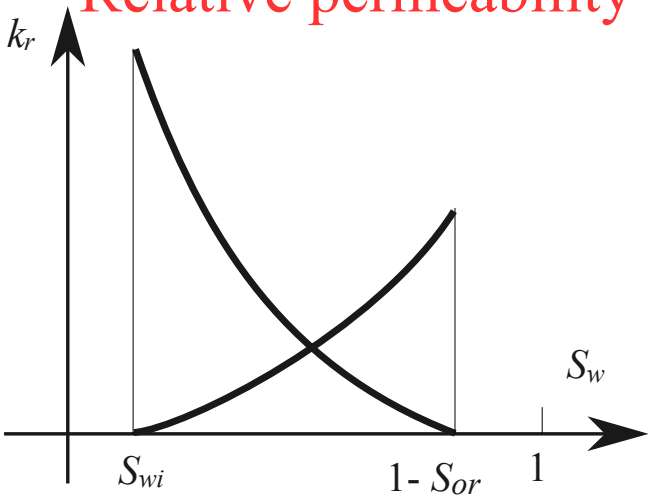
$$\frac{\partial \varepsilon S_\alpha}{\partial t} + \nabla . \mathbf{V}_\alpha = 0 \; ; \; \mathbf{V}_\alpha = -\frac{1}{\mu_\alpha} \mathbf{K}_\alpha . (\nabla P_\alpha - \rho_\alpha \mathbf{g})$$

$$P_\gamma - P_\beta = P_c(S_\beta) \qquad \mathbf{K}_\gamma = \mathbf{K}\, k_{r\gamma}(S_\gamma)$$

Capillary pressure



Relative permeability



Macro-Scale Models : Quasi-Static

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

(Ex. : Whitaker, 1986)

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

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

Phase interaction

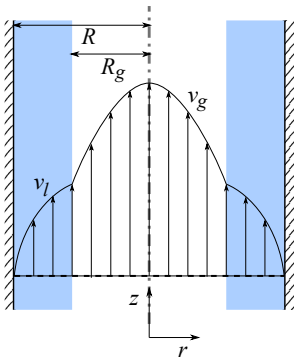
Ex. : Two-Phase Poiseuille Flow

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

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

$$K_{gg} \approx K\alpha^2 \qquad K_{gl} \approx \frac{\alpha}{1-\alpha}$$

$$\alpha = S_\gamma$$



Inertia Effects

- **Ergun (Heuristic): no-phase interaction terms**

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

Ergun, Fourar, Lenormand, ...

- **Schulenberg and Muler (1987) (Heuristic and)**

Similar to theory for fluidized beds

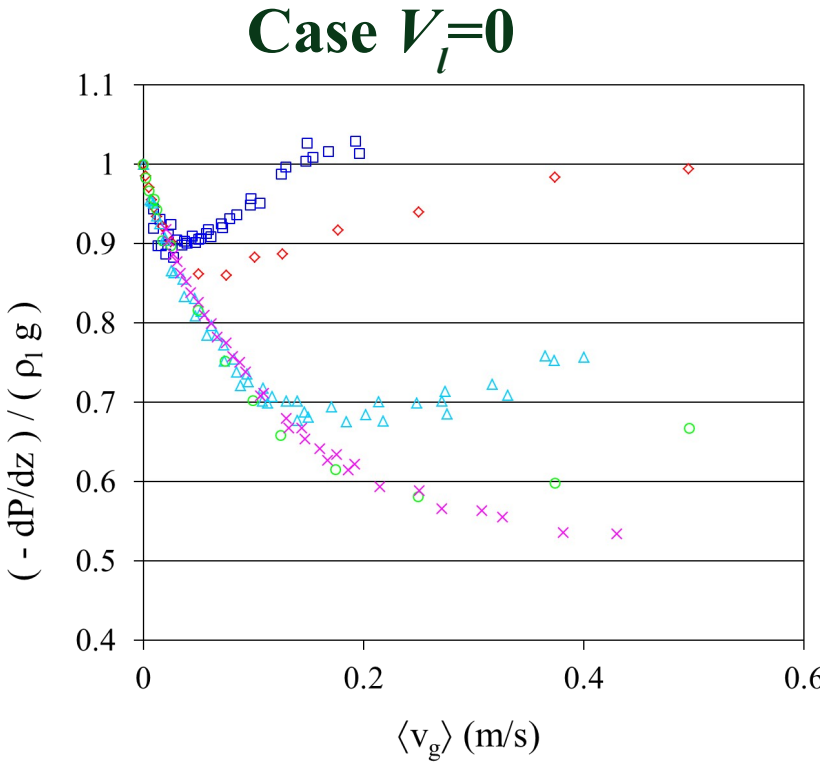
$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta \frac{1}{K\, k_{r\beta}} \mathbf{V}_\beta - \frac{\rho_\beta}{\eta\, \eta_\beta} \left\| \mathbf{V}_\beta \right\| \mathbf{V}_\beta + \frac{\mathbf{F}^S_{\beta\gamma}}{S_\beta}$$

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

$$\mathbf{V}_\alpha = -\frac{1}{\mu_\alpha} \mathbf{K}_\alpha . (\nabla P_\alpha - \rho_\alpha \mathbf{g}) - \mathbf{F}_{\alpha\alpha} \cdot \mathbf{V}_\alpha$$

$$+ \mathbf{K}_{\alpha\kappa} . \mathbf{V}_\kappa - \mathbf{F}_{\alpha\kappa} \cdot \mathbf{V}_\kappa \qquad \alpha, \kappa = \beta, \gamma \qquad \alpha \neq \kappa$$

Importance of Cross-Terms, and Non-Linear Effects



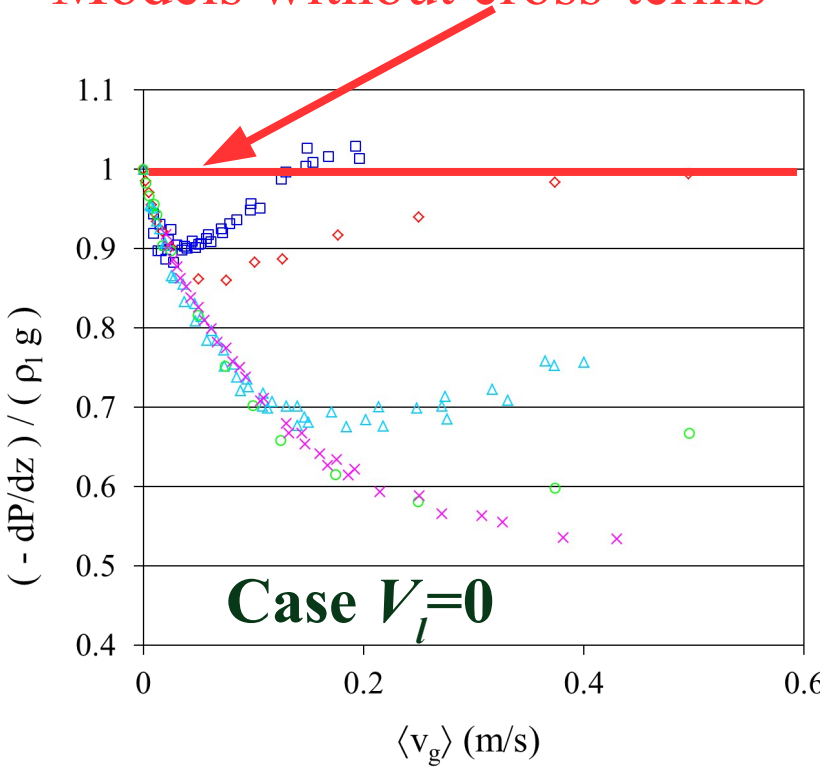
from Clavier et al. (2015)

(IRSN: context of nuclear reactor severe accident)

See also Taherzadeh & Saidi (2015)

Importance of Cross-Terms, and Non-Linear Effects

Models without cross-terms



$$t \to \infty$$

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

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

Case V_β=0 :

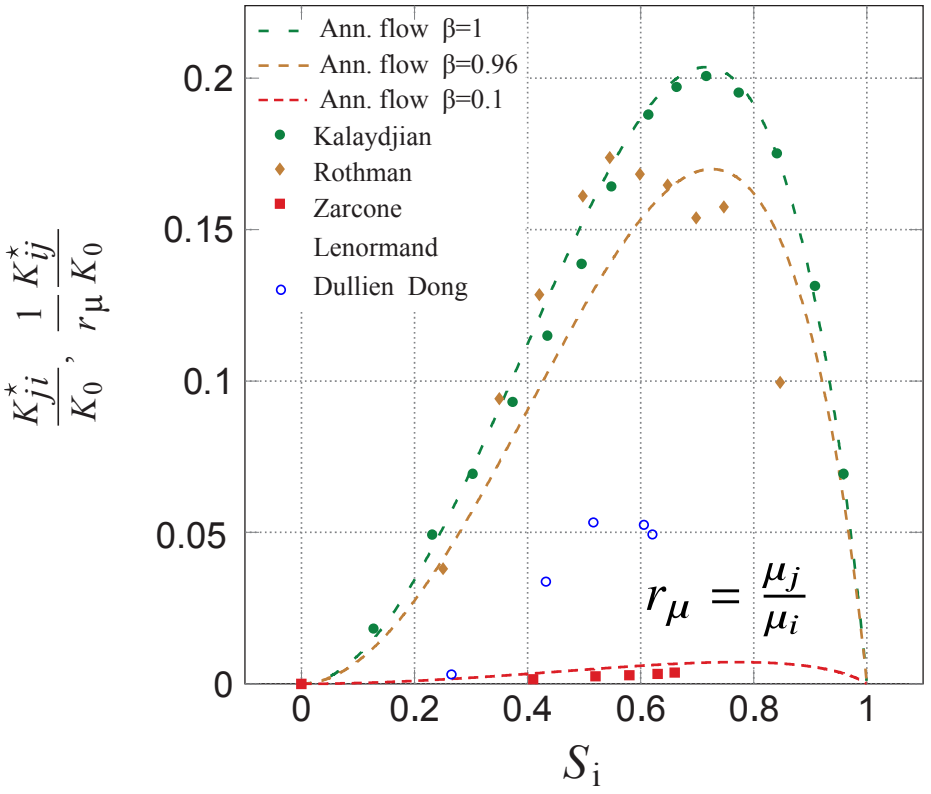
$$\left(\frac{\partial P_\beta}{\partial z} - \rho_\beta \mathbf{g}.\mathbf{e}_z\right) = +\mu_\beta K_\beta^{-1} K_{\beta\gamma}\left(1 - K_{\beta\gamma}^{-1} F_{\beta\gamma}\right) V_\gamma$$

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)

$K_{ij} = \beta K_{ij}$ (annular 2-phase flow) (Pasquier et al., 2017)



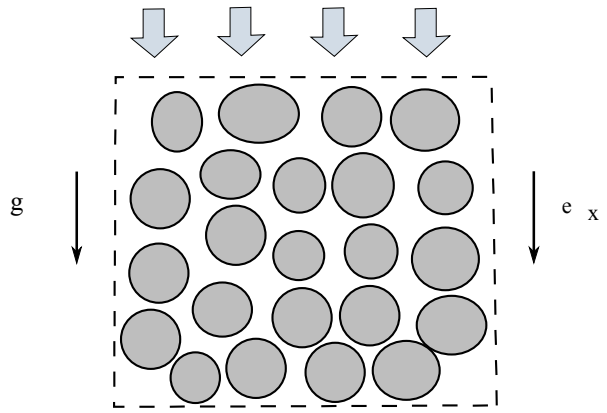
$$\begin{pmatrix} U_i \\ U_j \end{pmatrix} + \mathcal{K}^\star \begin{pmatrix} \frac{\partial P}{\partial x} - \rho_i g \\ \frac{\partial P}{\partial x} - \rho_j g \end{pmatrix} = 0$$

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

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

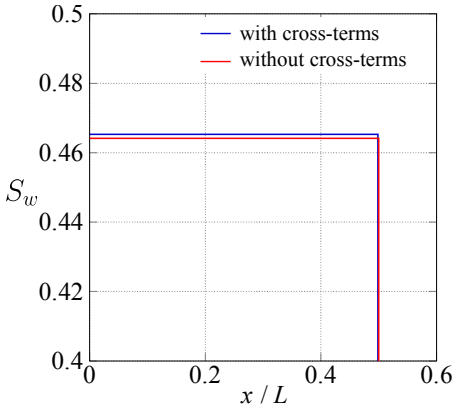
Effect of cross terms on the flow dynamic

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

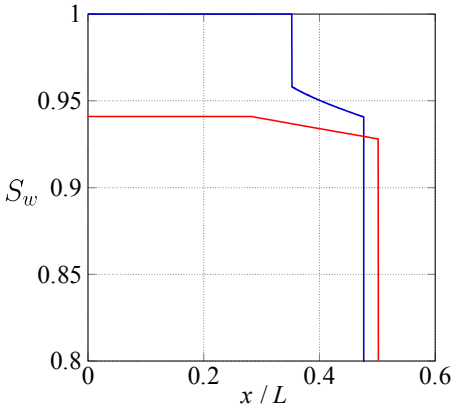


(a) Configuration 1: Imbibition

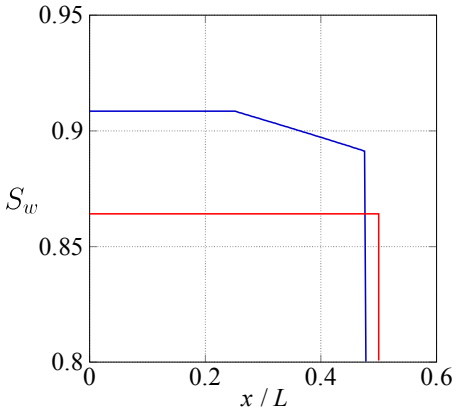
adapted Buckley-Leverett theory (*Pasquier et al., 2017*)



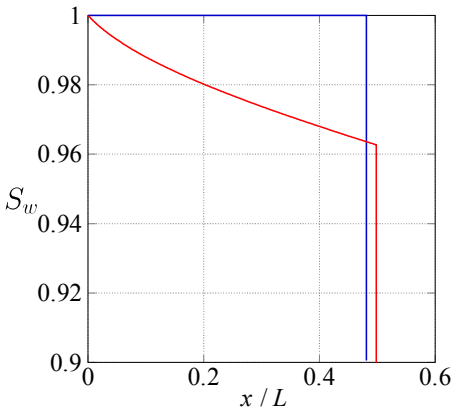
(b) $\frac{1}{N_g} = 0$



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

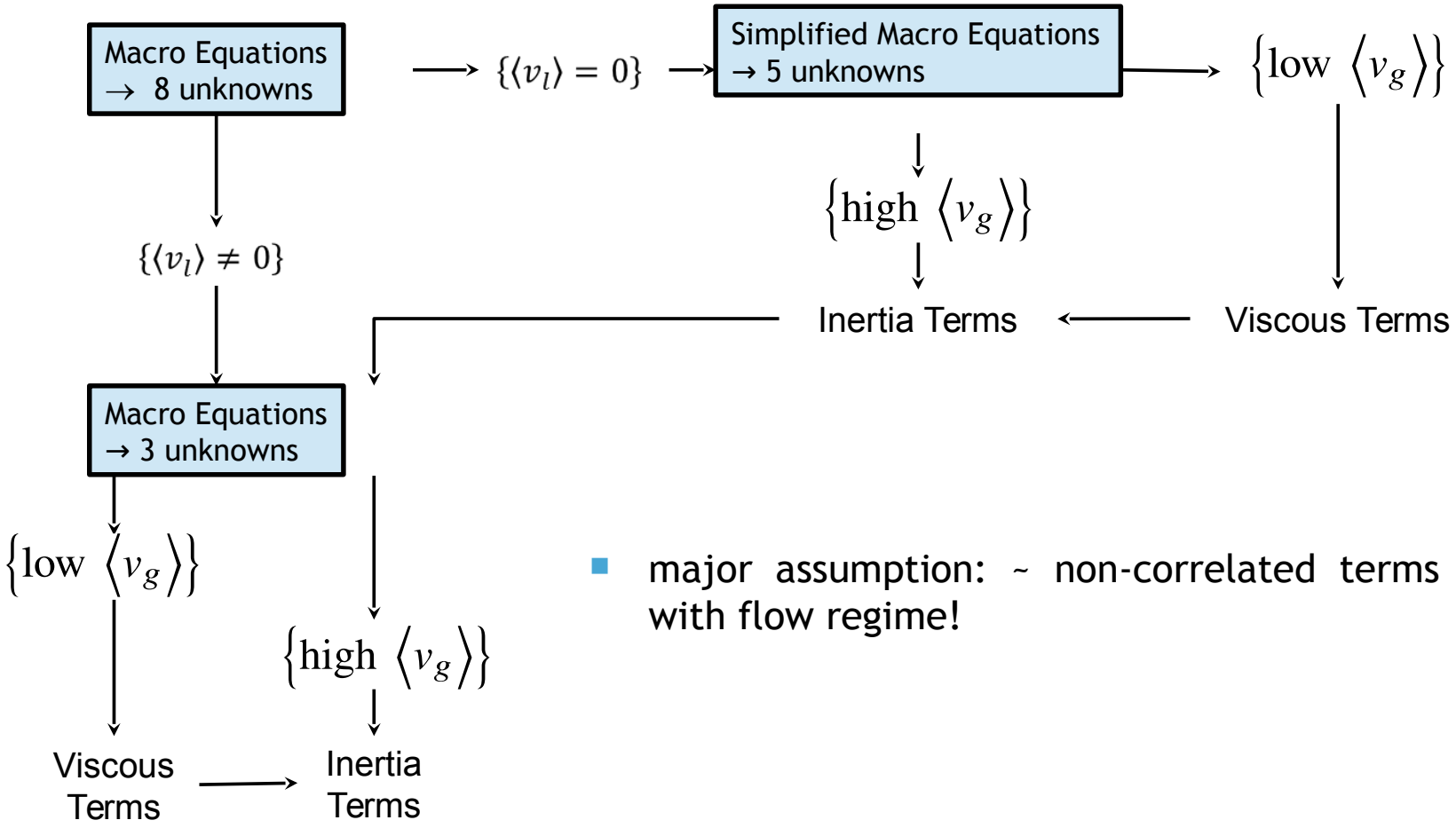


(d) $\frac{1}{N_g} = 0$



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

Estimation of multiphase parameters? Ex. from IRSN experiments



- major assumption: ~ non-correlated terms with flow regime!

Obtained correlations

$$K_{ll} = K(1-\alpha)^3 \qquad K_{lg} = k_{lg}\frac{\mu_g}{\mu_l}\frac{(1-\alpha)^2}{\alpha} \qquad f_{lg} = \frac{\alpha^3}{\alpha^3 + (1-\alpha)^3}$$

$$F_{ll} = \frac{\rho_l}{\mu_l}\frac{K}{\eta}\langle v_l \rangle \qquad F_{lg} = K_{lg} f_{lg}$$

$$K_{gg} = K\alpha^4 \qquad K_{gl} = \frac{\mu_l}{\mu_g}\frac{K_{gg}K_{lg}}{K_{ll}}$$

$$F_{gg} = \frac{\rho_g}{\mu_g}\frac{K}{\eta}\langle v_g \rangle \qquad F_{gl} = f_{lg}\alpha^6$$

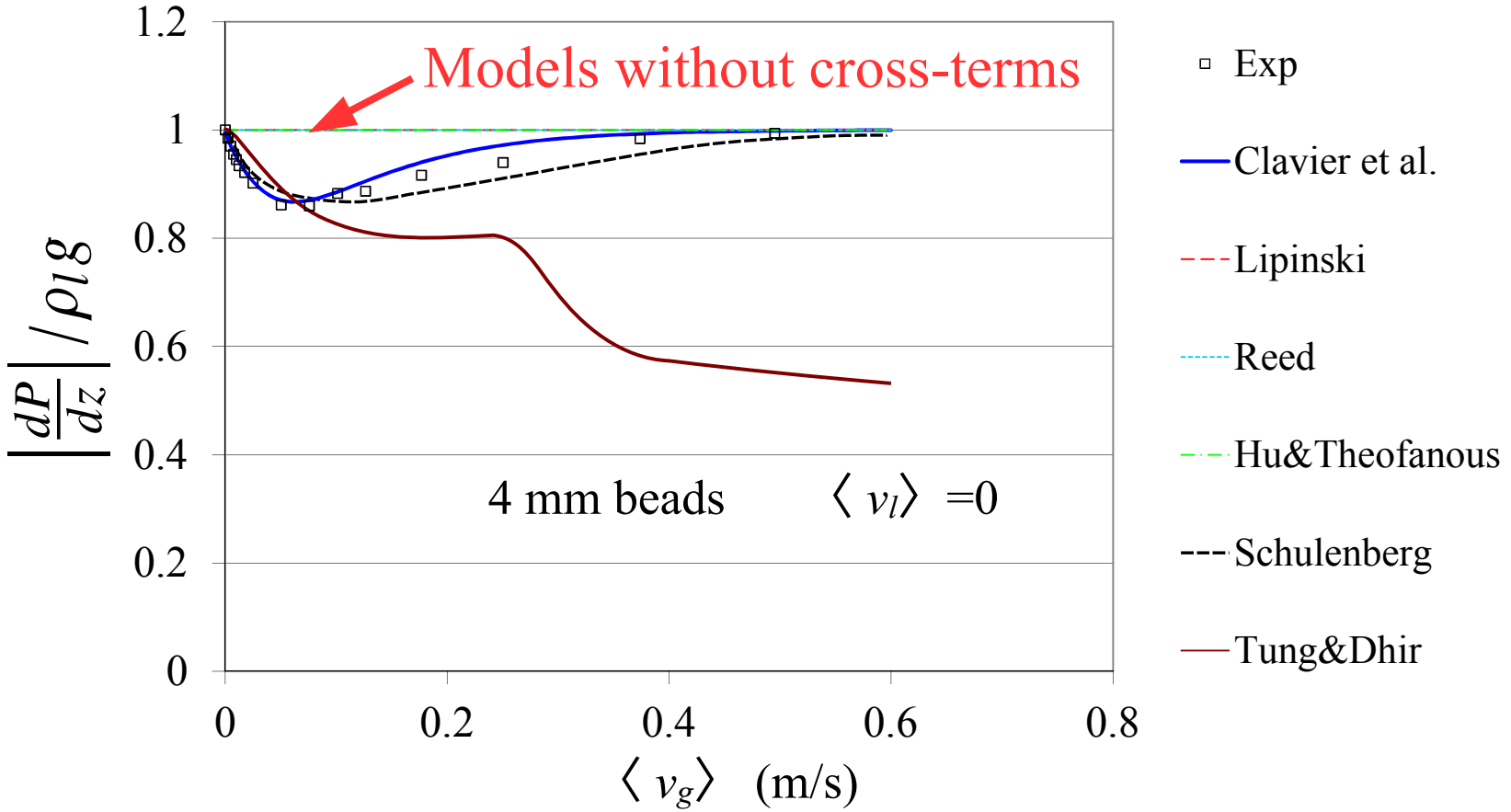
: No-dependence of f_{lg} with velocities?

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}

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

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

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**

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

$$p_c = \mathcal{F}\left(S_\beta, \left(\rho_\gamma - \rho_\beta\right)\mathbf{g}, \nabla P_\beta, \frac{\partial \varepsilon S_\beta}{\partial t}, \ldots\right)$$

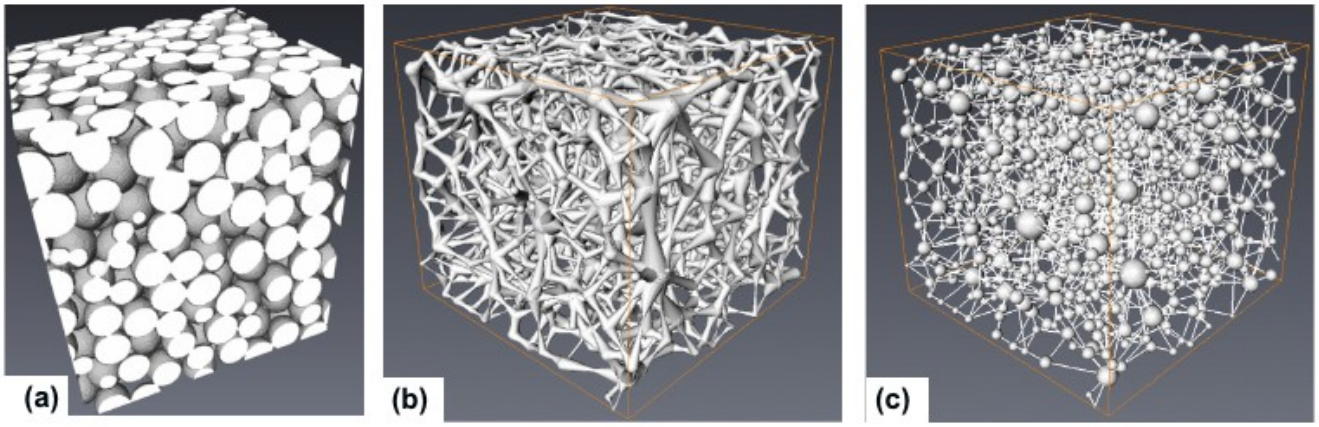
- **Kalaydjian, Hassanizadeh & Gray, …**

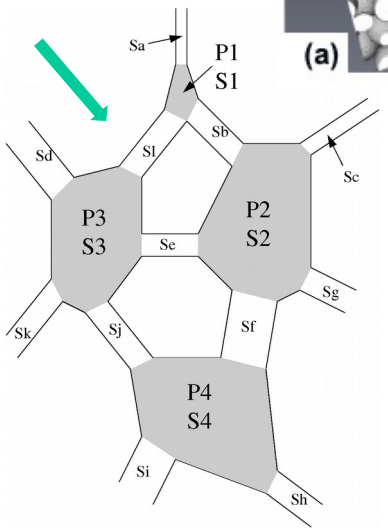
$$P_\gamma - P_\beta = p_c - L_1 \frac{\partial \varepsilon S_\beta}{\partial t}$$

- **…see also Petroleum engng literature on pseudo-functions!**
- **Usefulness for highly prmeable media?**

PNM (Pore Network Model) : quasi-static

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



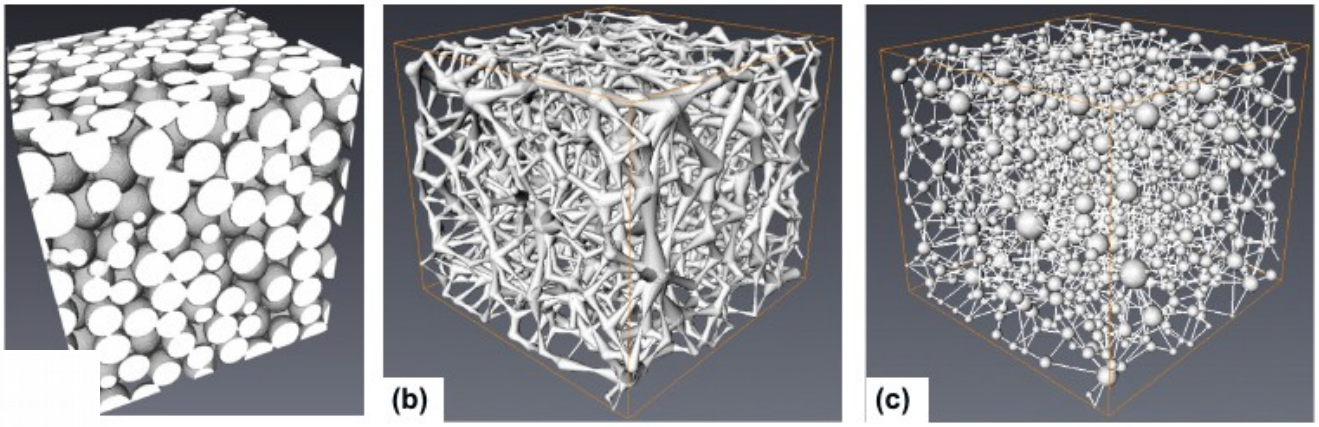


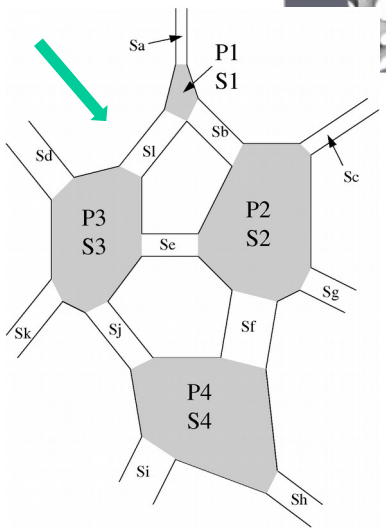
Phase repartition according to capillary equilibrium

- 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)

PNM - Dynamic

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

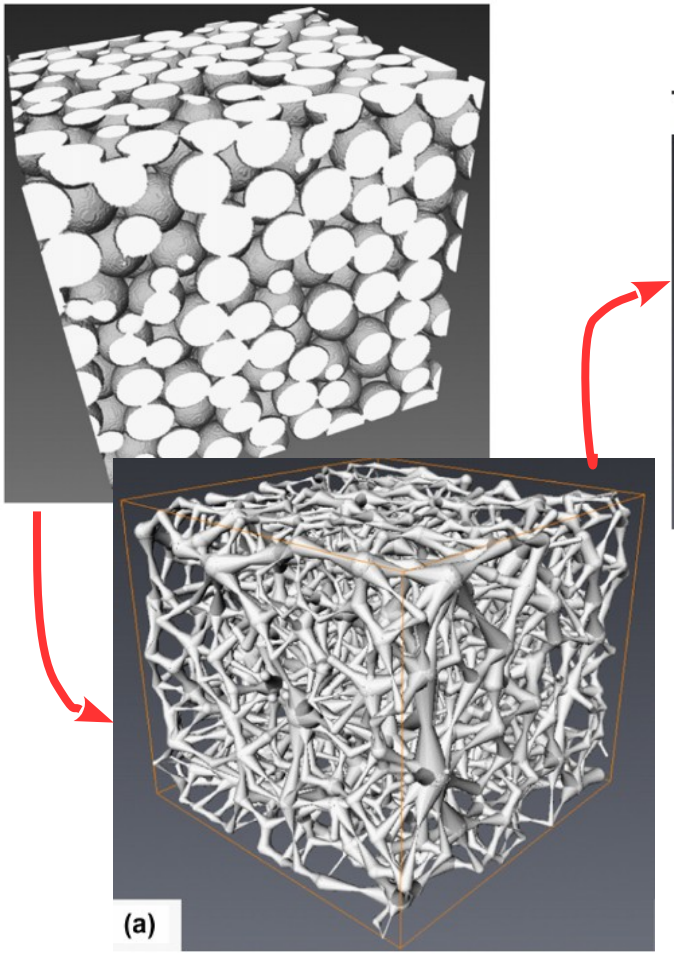




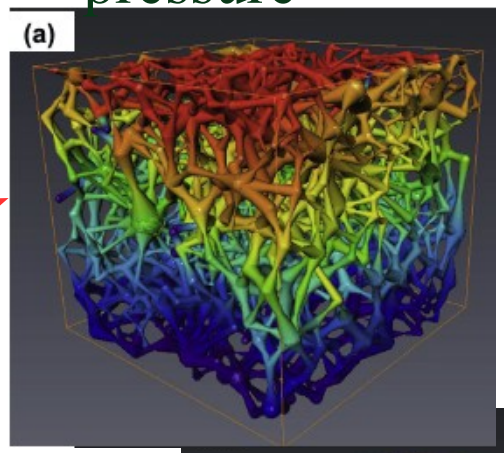
Pore-scale rules
(analytical: e.g. Poiseuille)

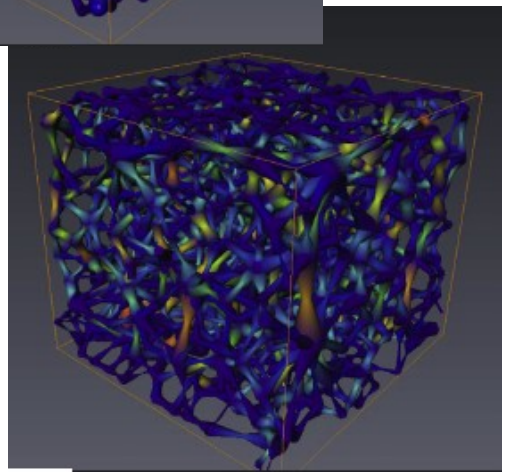
- Time dependent solution, solve for pressure field with approximate solutions for describing flow in connections
- Used to estimate k_r, P_c and other relations (hysteresis)

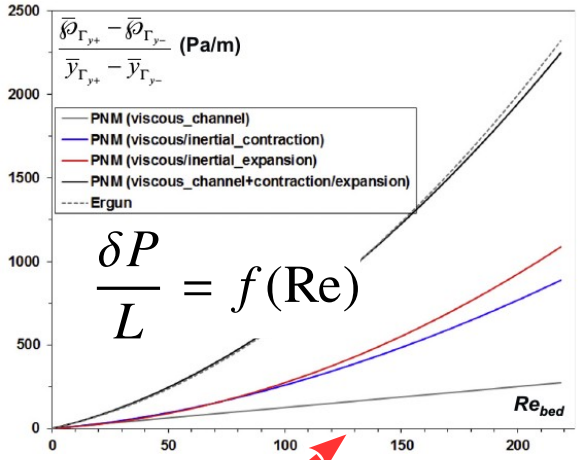
Example: application to the interpretation of tomographic images in the inertia regime



pressure







Larachi et al., 2014

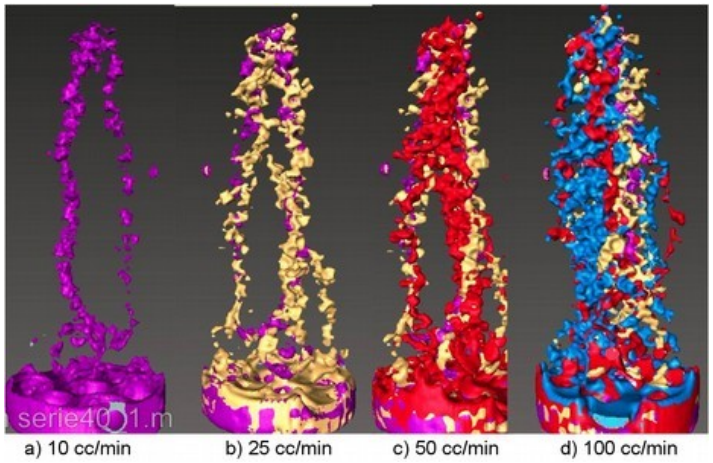
velocity

Mixed or Hybrid Models

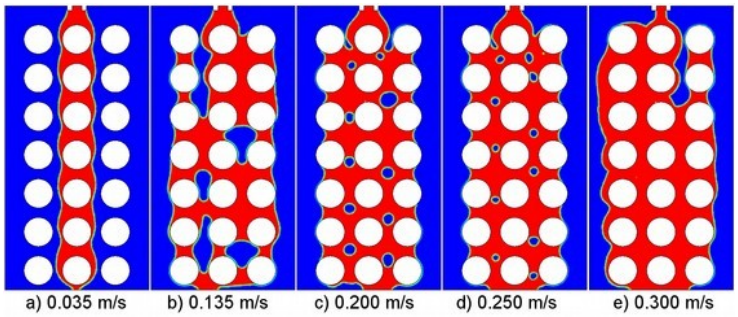
- **Network models → a meso-scale representation!**
- **If low Re, Ca, Bo → percolation theory**
- **Otherwise: Coupling network model and Dynamic rules (which may come from local VOF simulations)**

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

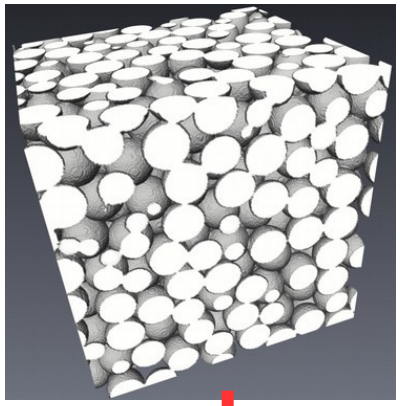
Trickle Bed (X-ray, IFP)

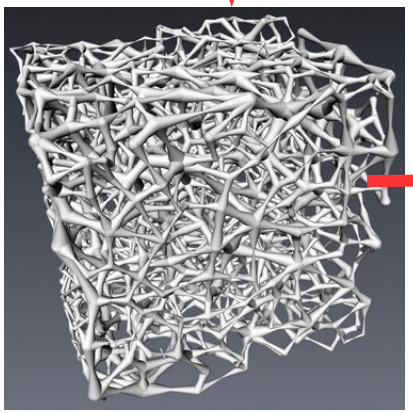


Micromodel experiments

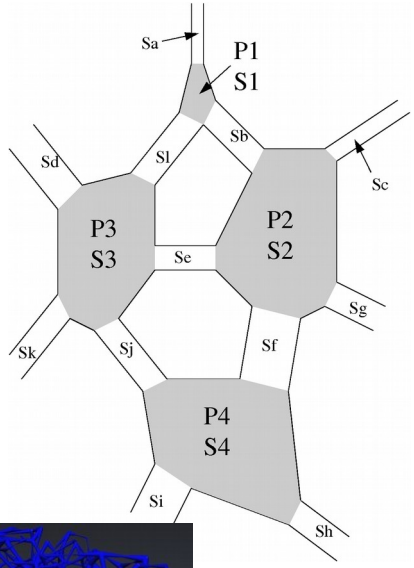


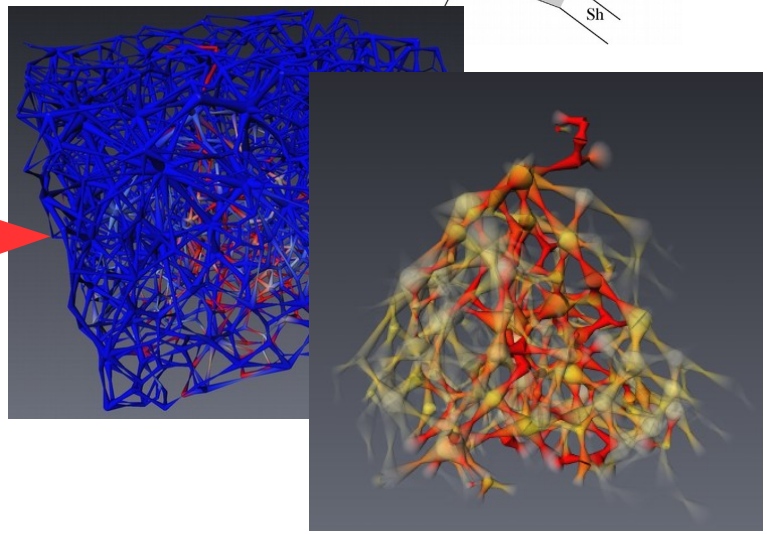
Mixed or Hybrid Models





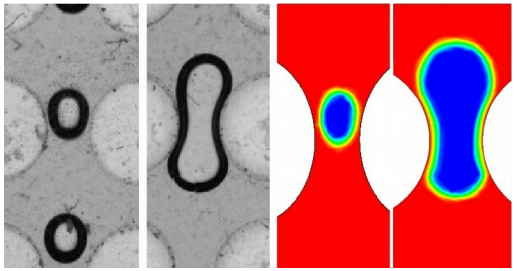
Horgue et al., 2012





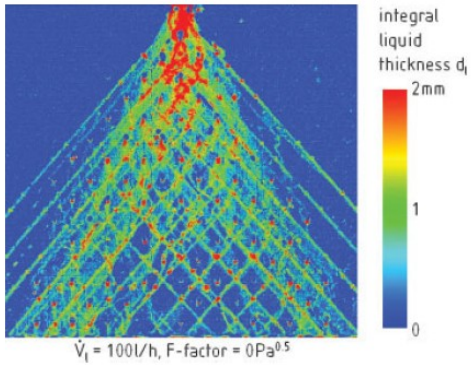
1.) Mass and momentum balance for the network

2.) Dynamic rules coming from local VOF simulations (or from experiments)



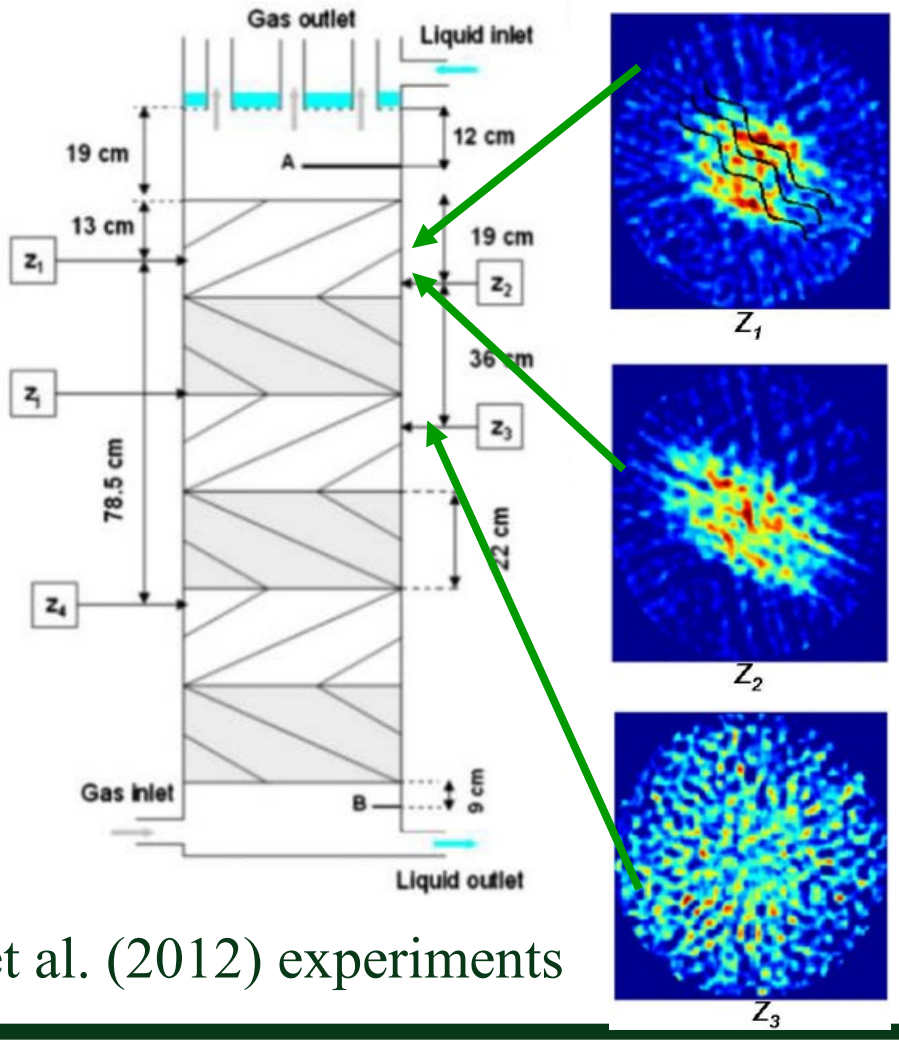
Macro-Scale Models with Phase "Splitting"

- **Example: Flow through Structured Media**



Mahr and Mewes (2007)

MellaPak (Sulzer Chemtech)



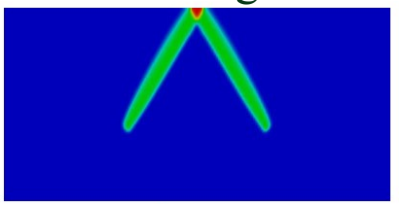
Fourati et al. (2012) experiments

Macro-Scale Models with Phase "Splitting"

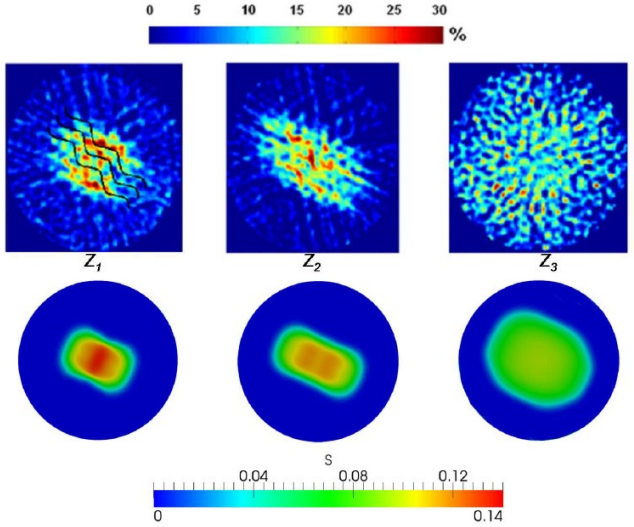
- $$\varepsilon \frac{\partial S_\gamma}{\partial t} + \nabla . \mathbf{U}_\gamma = 0,$$
  $$\varepsilon \frac{\partial S_{\beta_1}}{\partial t} + \nabla . \mathbf{U}_{\beta_1} = \dot{m},$$
  $$\varepsilon \frac{\partial S_{\beta_2}}{\partial t} + \nabla . \mathbf{U}_{\beta_2} = -\dot{m}.$$

+ 3 momentum equations

Model with liquid phase splitting, no-exchange

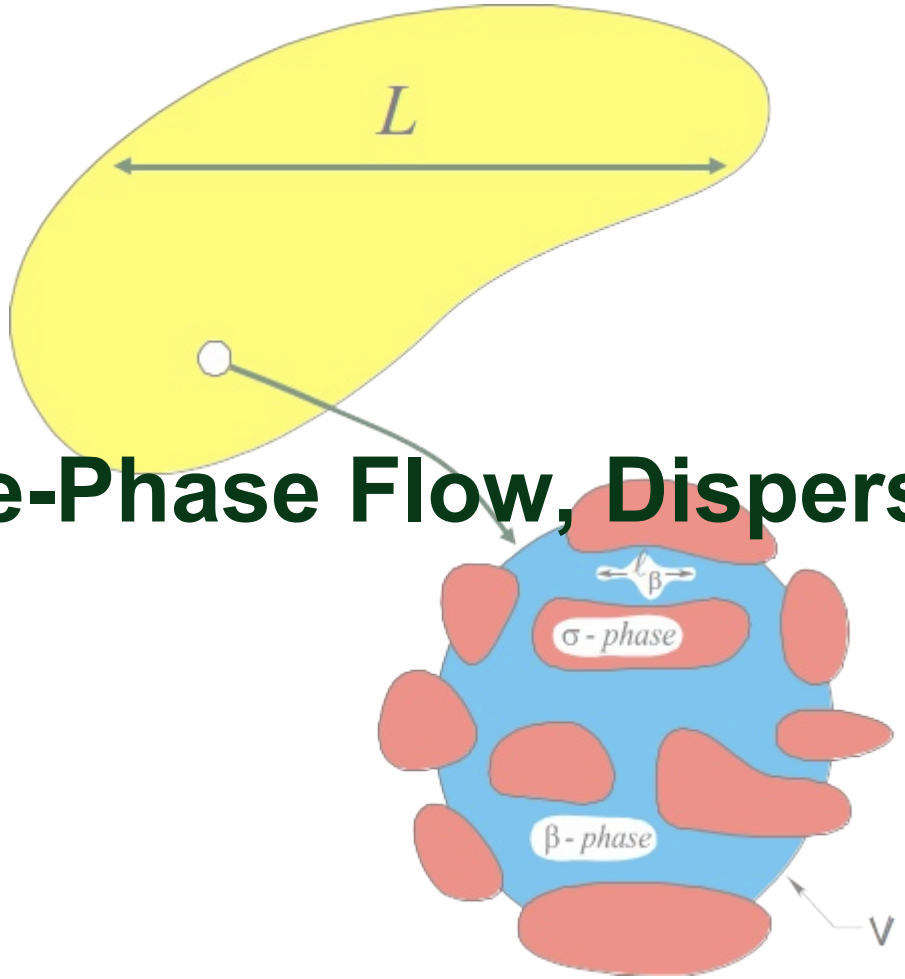


(b) t = 1 s



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

One-Phase Flow, Dispersion



Phenomenolgy

- **Pore-Scale problem**

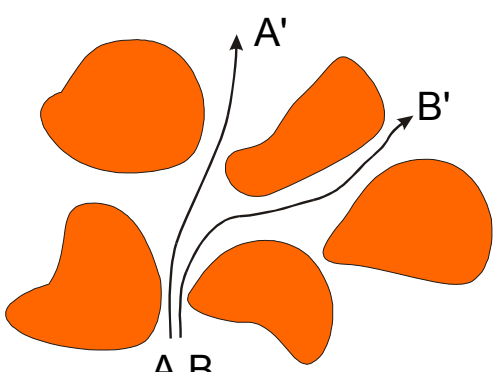
$$\nabla . \mathbf{v}_\beta = 0$$

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

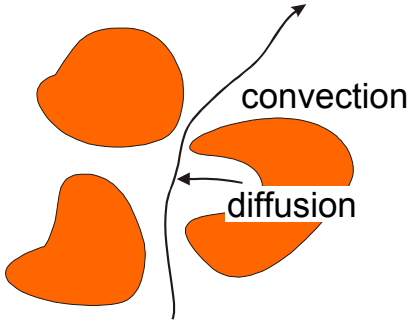
$$\text{B.C.1} \quad \mathbf{n}_{\beta\sigma} \cdot D_\beta \nabla c_\beta = 0 \quad \text{at } A_{\beta\sigma} \qquad \text{passive dispersion}$$

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

Taylor dispersion



Mechanical dispersion



Retardation due to dead-end pores

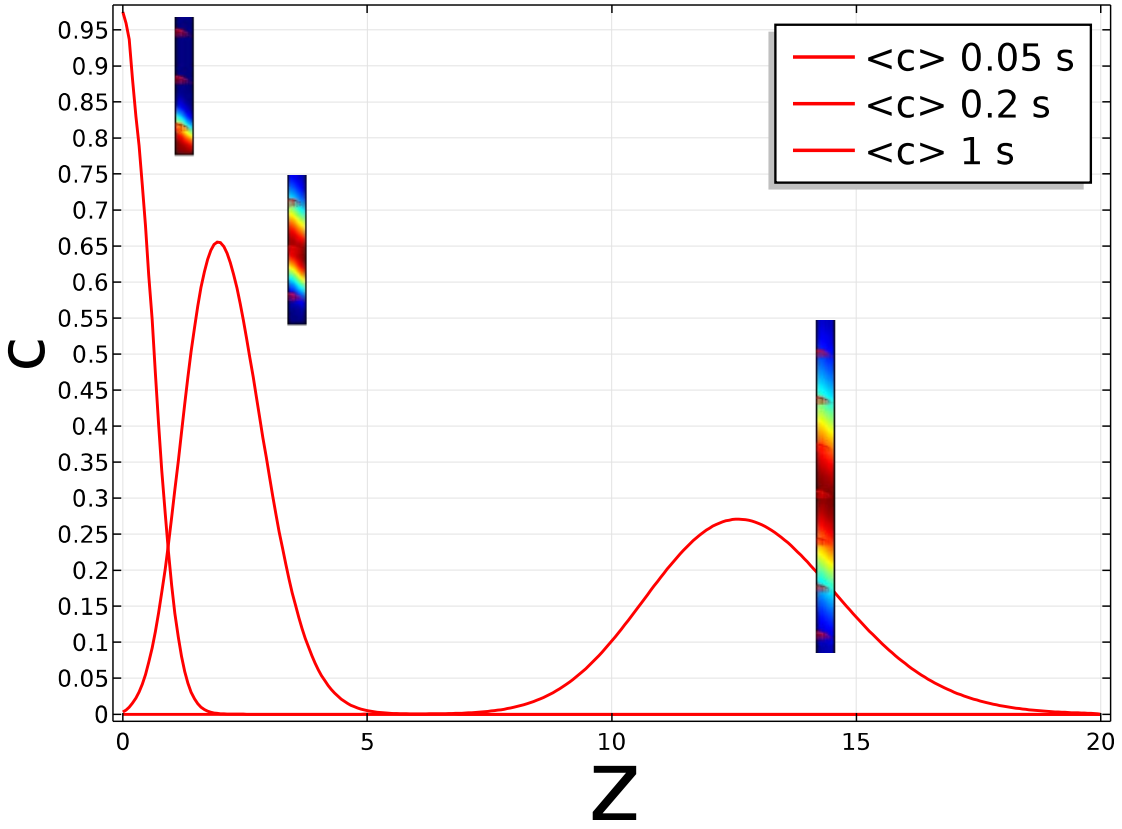
Taylor dispersion

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

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

Which equation for :

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



Macro-Scale Equations (tracer)

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

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

Taylor dispersion :

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

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

Linear dispersion :

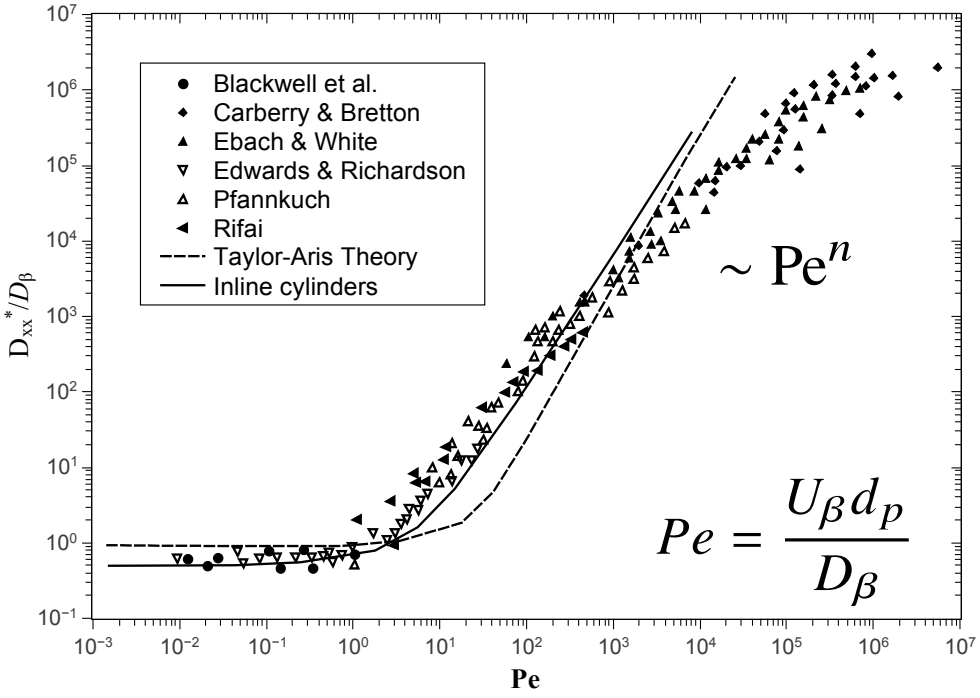
$$\mathbf{D}_\beta^* = \mathbf{D}_0 + \alpha_T \left\| \mathbf{U}_\beta \right\| \mathbf{I} + (\alpha_L - \alpha_T) \frac{\mathbf{U}_\beta \mathbf{U}_\beta}{\left\| \mathbf{U}_\beta \right\|}$$

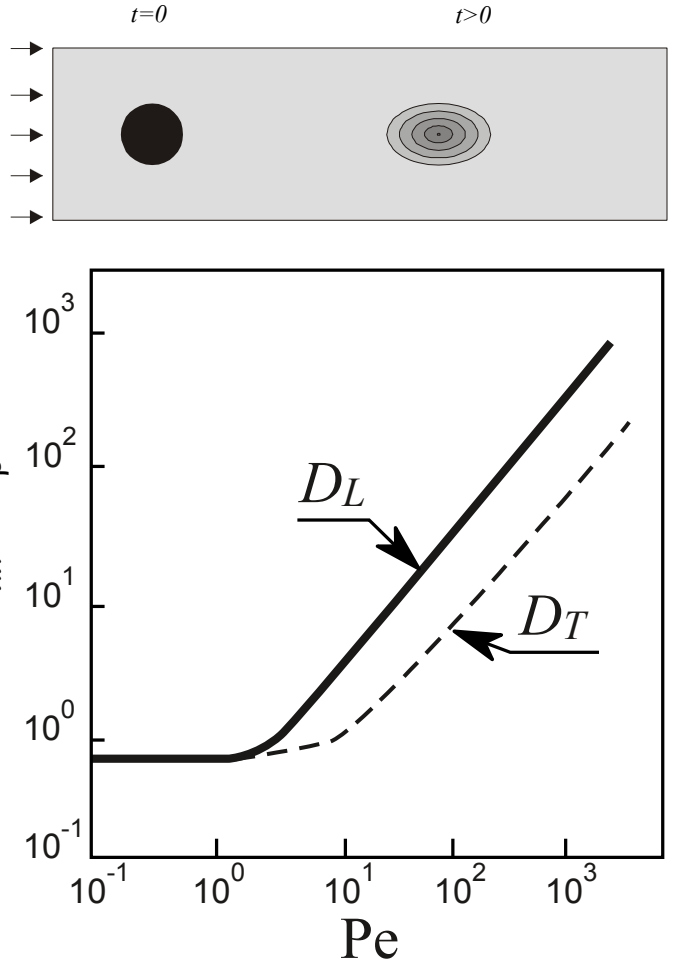
Longitudinal and transversal dispersivity

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





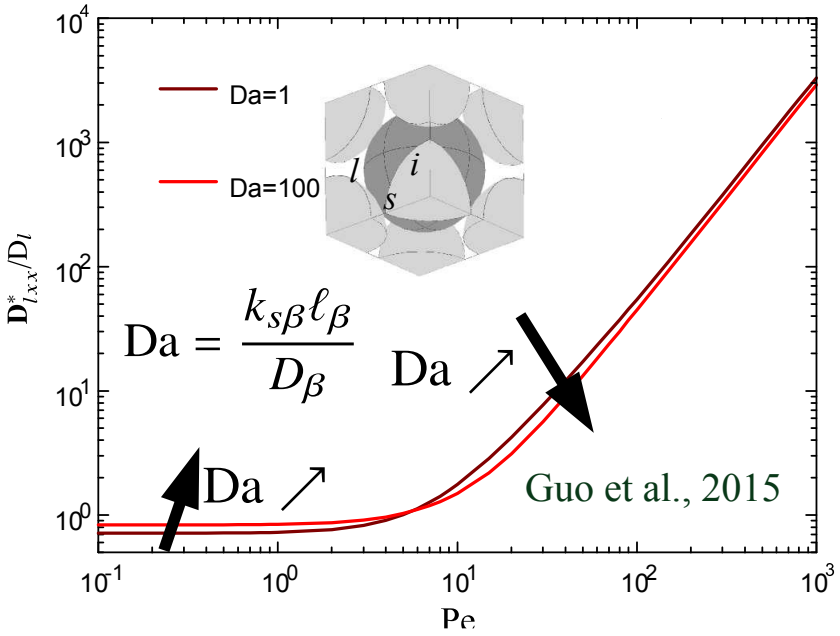
- n=2 : Taylor dispersion
- 2>n>1 : from simple unit cells to highly disordered media

Active dispersion

- **Homogeneous source**

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

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

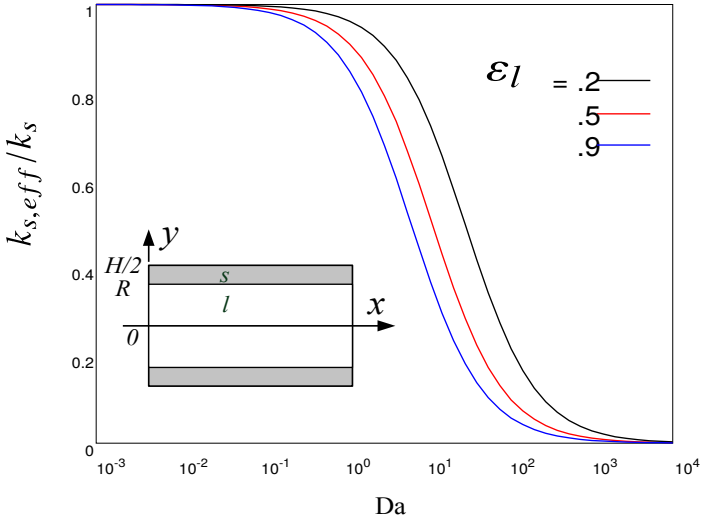


- **Heterogeneous source**

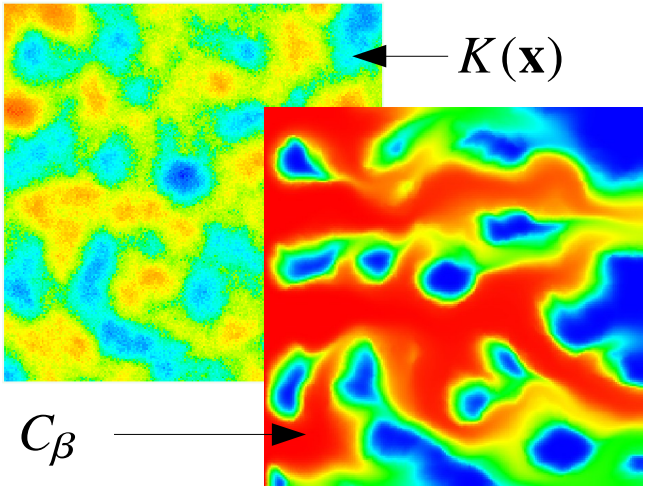
B.C. 1 $\quad \mathbf{n}_{\beta\sigma}.\left(D_\beta \nabla c_\beta\right) = -k_{s\beta} c_\beta$ at $A_{\beta\sigma}$

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

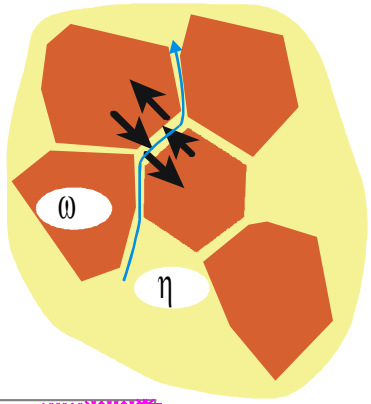
$$K_{\beta\sigma} = \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left(-D_\beta \nabla c_\beta\right) dA = a_v k_{s\beta,eff}$$



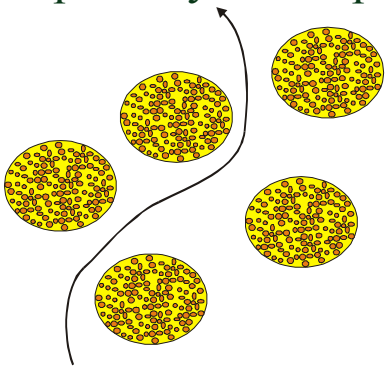
Abnormal dispersion, double-porosity models, ...



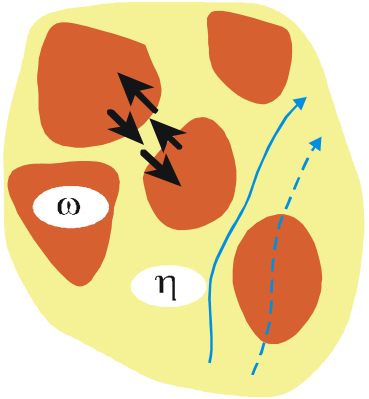
Fractured media

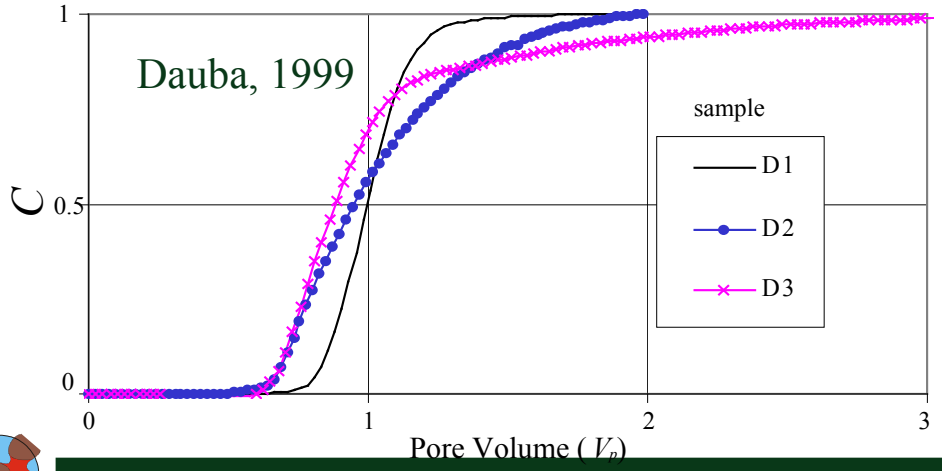


macro-porosity/micro-porosity



mobile/immobile
or
mobile/mobile





Non-Locality: a Simple Example

- **Heterogeneous diffusion: Coupled micro-macro problem**

$$\begin{cases} \dfrac{\partial \widetilde{T}}{\partial t} = \nabla.(k\nabla\widetilde{T}) + \nabla.(\widetilde{k}\nabla\langle T\rangle) - \nabla.\left\langle k\nabla\widetilde{T}\right\rangle & \text{micro} \\ \dfrac{\partial \langle T\rangle}{\partial t} = \nabla.\left(\langle k\rangle\nabla\langle T\rangle + \left\langle k\nabla\widetilde{T}\right\rangle\right) & \text{macro} \end{cases}$$

- **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)**

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

- **Closure**

$$\widetilde{T}_{LT} = p\mathbf{b}_{LT}.\nabla\langle T\rangle_{LT}$$

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

- **Macro-scale Equation**

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

Transient / Steady-State Closure (~asymptotic behavior)

- **Transient Closure**

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

$$\frac{\partial \mathbf{b}}{\partial t} = \nabla \cdot (k \nabla \mathbf{b}) + \nabla \cdot \widetilde{k} \mathbf{I} - \nabla \cdot \langle k \nabla \mathbf{b} \rangle \qquad +\text{period., ...}$$

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

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

- **Steady-State closure**

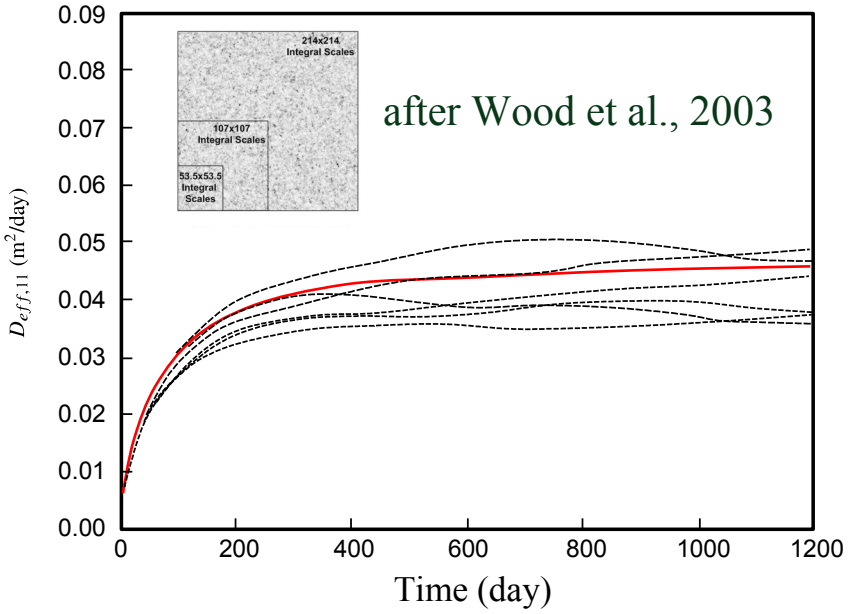
$$\mathbf{b} = const. = \lim_{t \to \infty} \mathbf{b}(t) = \mathbf{b}_\infty$$

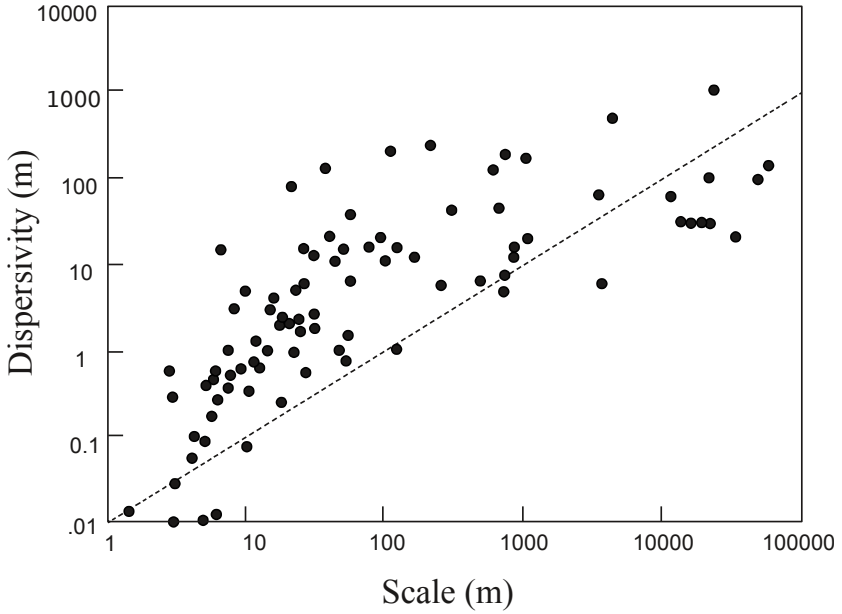
$$\widetilde{T} = \mathbf{b}_\infty \cdot \nabla \langle T \rangle$$

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

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

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

$$\frac{\partial \langle c \rangle}{\partial t} + \mathbf{U}_\beta \cdot \nabla \langle c \rangle = \nabla \cdot \left(\mathbf{K}^*_{eq} \cdot \nabla \langle c \rangle \right)$$

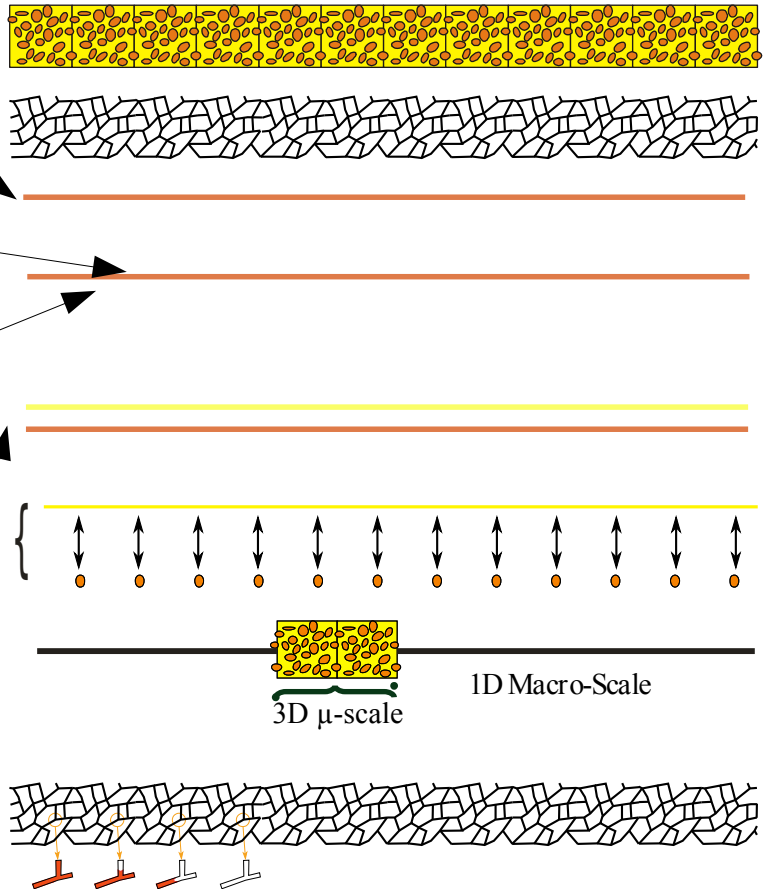
$$\frac{\partial \langle c \rangle^{\beta\sigma}}{\partial t} + \left\langle \mathbf{v}_\beta \right\rangle . \nabla \langle c \rangle^{\beta\sigma} = \nabla . \left(\frac{\partial \mathbf{K}^*}{\partial t} * . \nabla \langle c \rangle^{\beta\sigma} \right) + \ldots$$

$$\frac{\partial \langle c \rangle^{\beta\sigma}}{\partial t} + \left\langle \mathbf{v}_\beta \right\rangle . \nabla \langle c \rangle^{\beta\sigma} = \nabla . \left(\mathbf{K}^*_\infty . \nabla \langle c \rangle^{\beta\sigma} \right)$$

Equations for $\left\langle c_\beta \right\rangle^\beta$, $\langle c_\sigma \rangle^\sigma$

1st order exchange: $-h_{2eq} \left(\langle c_\sigma \rangle^\sigma - \left\langle c_\beta \right\rangle^\beta \right)$

Convolution: $-\frac{\partial h^*}{\partial t} * \left(\langle c_\sigma \rangle^\sigma - \left\langle c_\beta \right\rangle^\beta \right)$



DNS

meso-scale Network model

1-eq local equilibrium

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

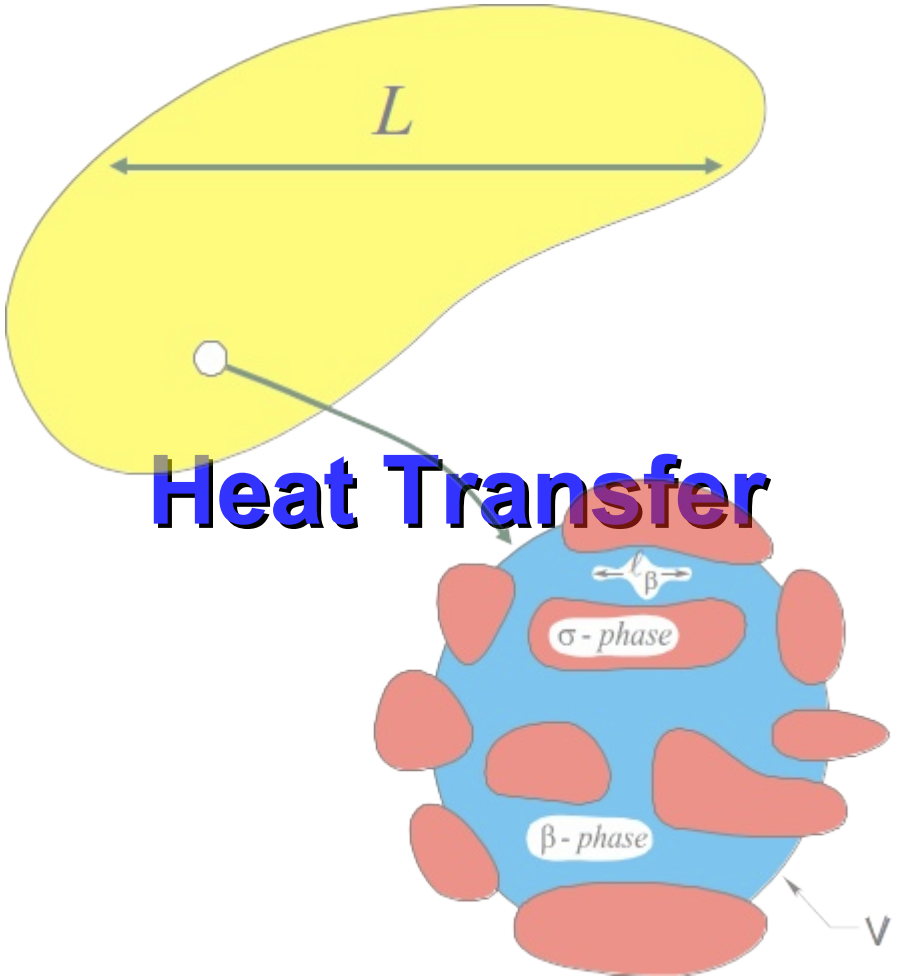
2-equation, N-equation (multi-rate or MRMT, ...

Mixed or Hybrid models

Mixed or Hybrid models for front problems

Mixed or Hybrid Network model (PNM+VOF)

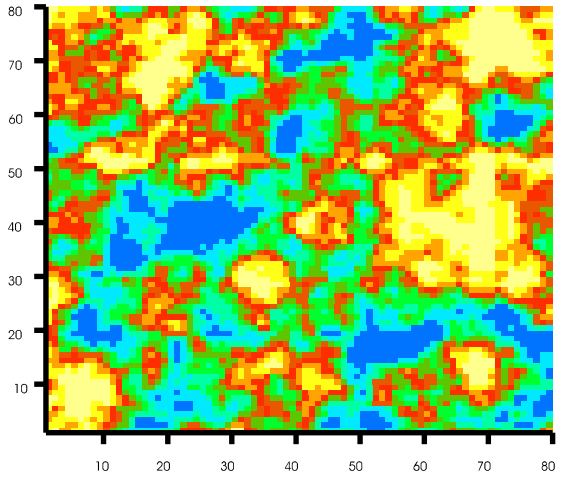
Heat Transfer



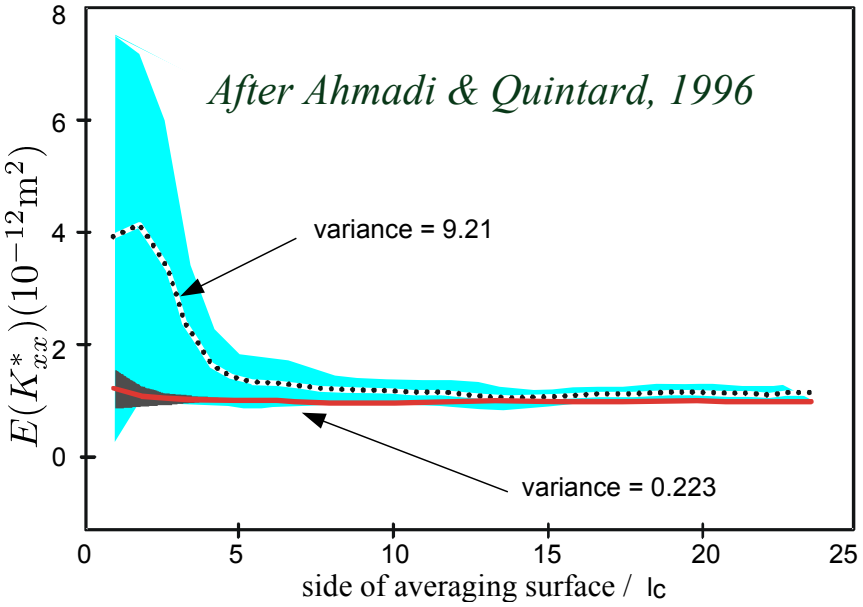
(recall) Diffusion in a heterogenous system : Effective Conductivity

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

$$\nabla \cdot (\mathbf{k} . \nabla \mathbf{b}) = -\nabla \cdot \tilde{\mathbf{k}} + \ldots$$



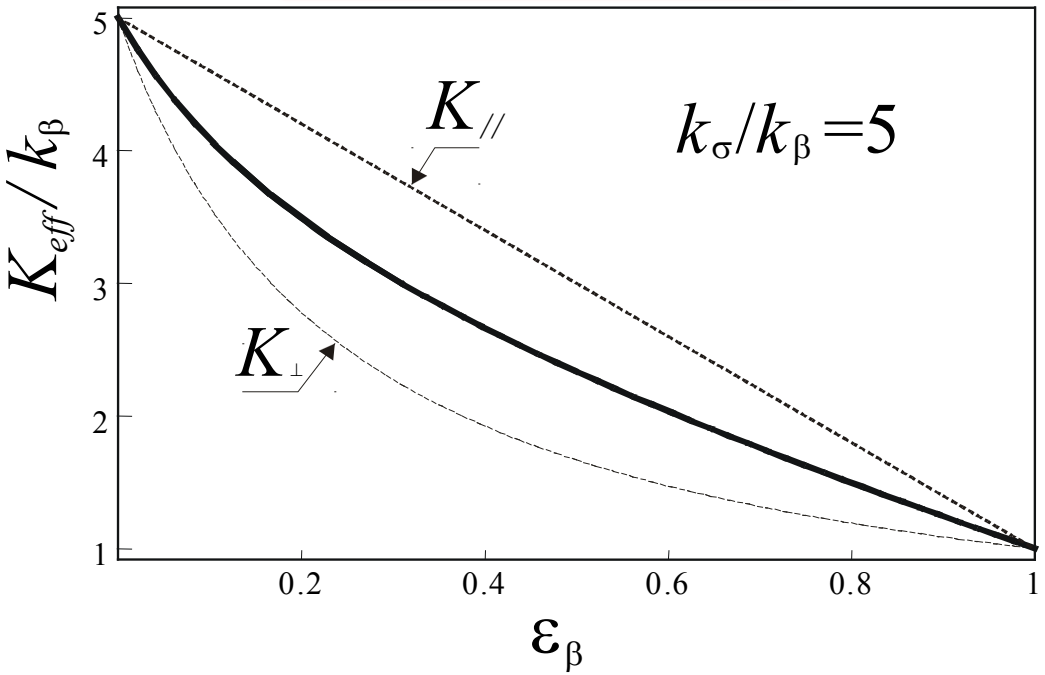
log-normal $k(x)$, spatialy correlated



Bounds

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

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



Maxwell, 1873

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

See also Poisson, Mosotti, Lorenz

Landau and Lifshitz (1960)

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

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: $\mathrm{K}_{eff} = k_\sigma^{\varepsilon_\sigma} k_\beta^{\varepsilon_\beta}$

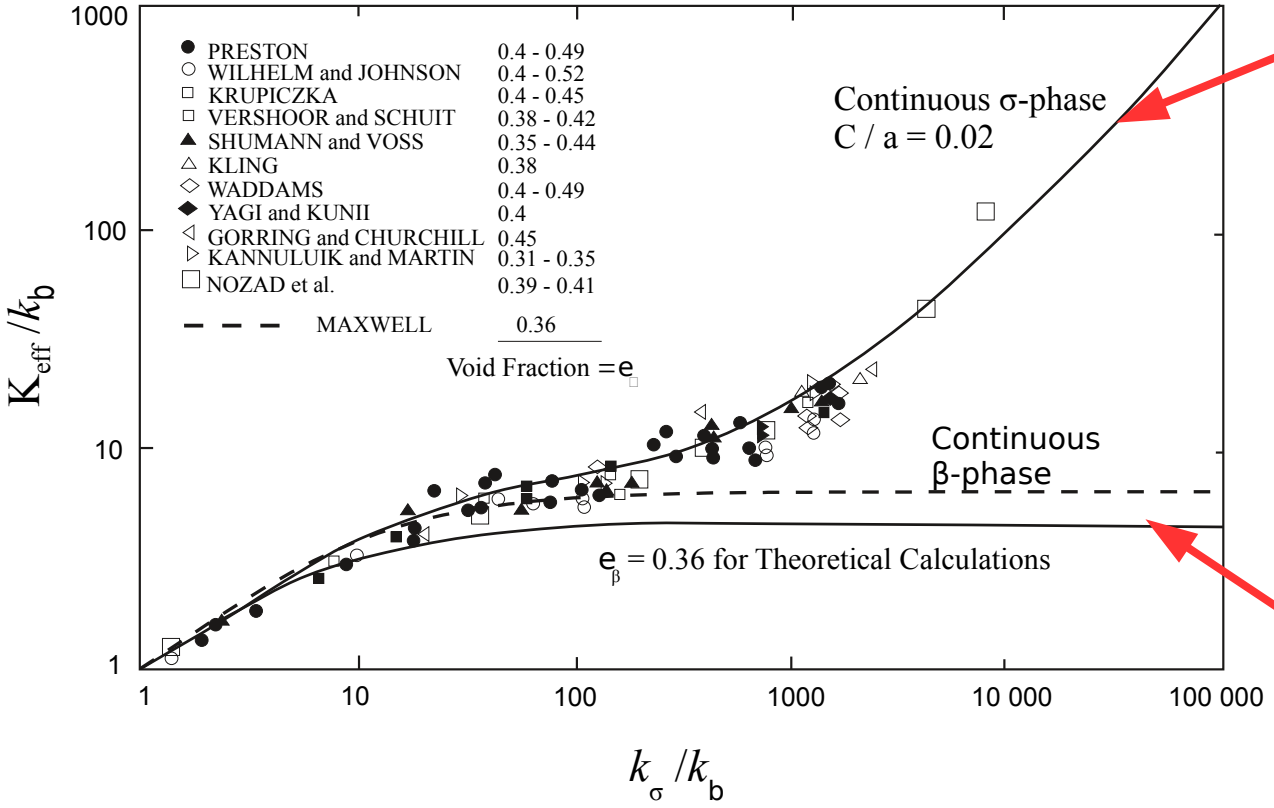
Bruggeman (1935): $\sum_i \varepsilon_i \frac{k_i - k_{eff}}{k_i + (d-1) k_{eff}} = 0$ Spherical inclusions

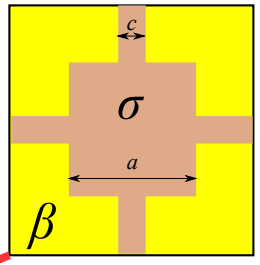
see: *Cellular and Porous Materials: Thermal Properties Simulation and Prediction*, Edited by Andreas Ochsner, Graeme E. Murch, and Marcelo J.S. de Lemos, WILEY, 2008.

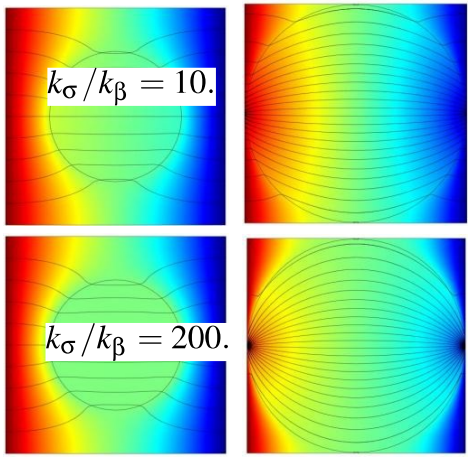
Hashin, Z. & Shtrikman, S. A, Variational approach to the theory of the elastic behaviour of multiphase materials, Journal of the Mechanics and Physics of Solids , 1963, 11, 127 - 140

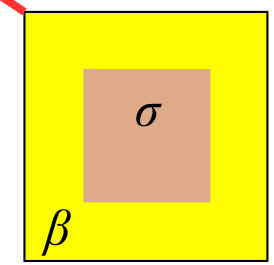
...numerous literature!

Effect of contact points









(Nozad et al., 1985)

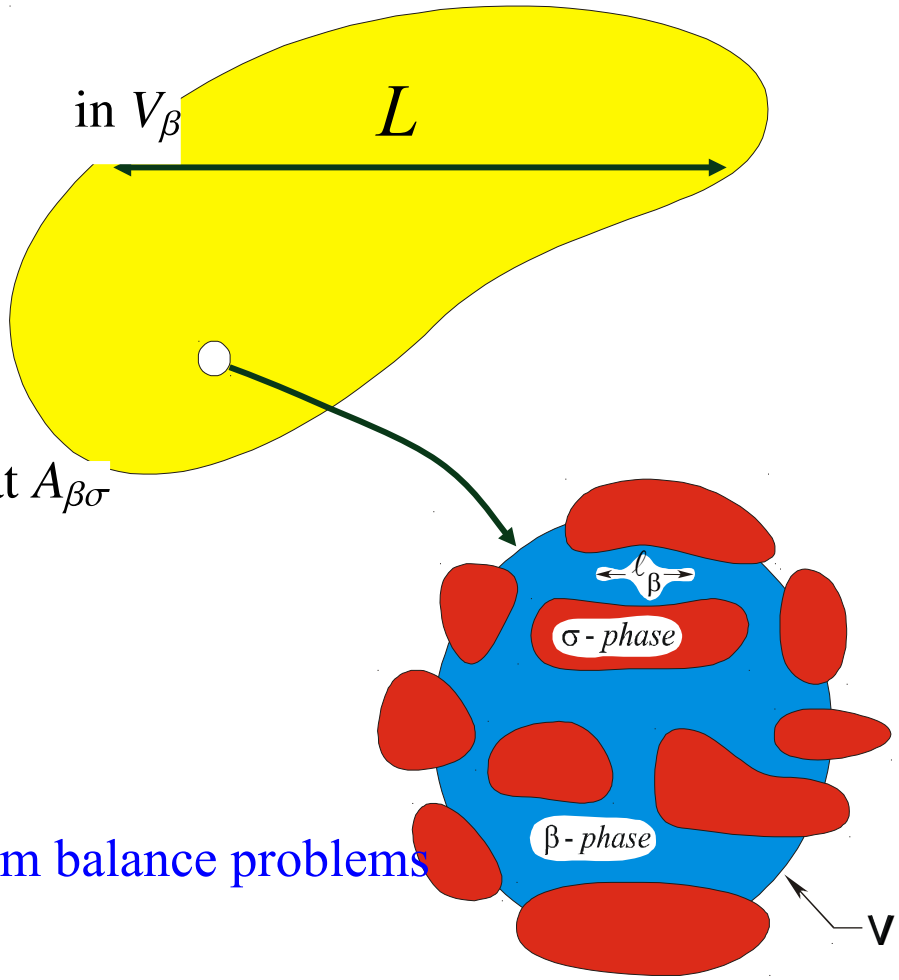
Two-Phase, Unsteady Problem

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

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

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

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



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**

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

- **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)

$$T_\beta = \left\langle T_\beta \right\rangle^\beta + \tilde{T}_\beta \qquad T_\sigma = \langle T_\sigma \rangle^\sigma + \tilde{T}_\sigma$$

Micro:

$$(\rho c_p)_\beta \frac{\partial \tilde{T}_\beta}{\partial t} + (\rho c_p)_\beta \tilde{\mathbf{v}}_\beta . \nabla \left\langle T_\beta \right\rangle^\beta + (\rho c_p)_\beta \mathbf{v}_\beta . \nabla \tilde{T}_\beta =$$

$$\nabla . (k_\beta \nabla \tilde{T}_\beta) - \varepsilon_\beta^{-1} \nabla . \left(k_\beta \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_\beta \, dA \right) - \varepsilon_\beta^{-1} k_\beta \frac{1}{\mathcal{V}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} . \nabla \tilde{T}_\beta \, dA$$

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

B.C.:

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

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

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

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

$\rightarrow$ **local equilibrium**

I - Local Equilibrium → 1-Eq model

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

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

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

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

with:

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

LE Closure Problem

dispersion

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

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

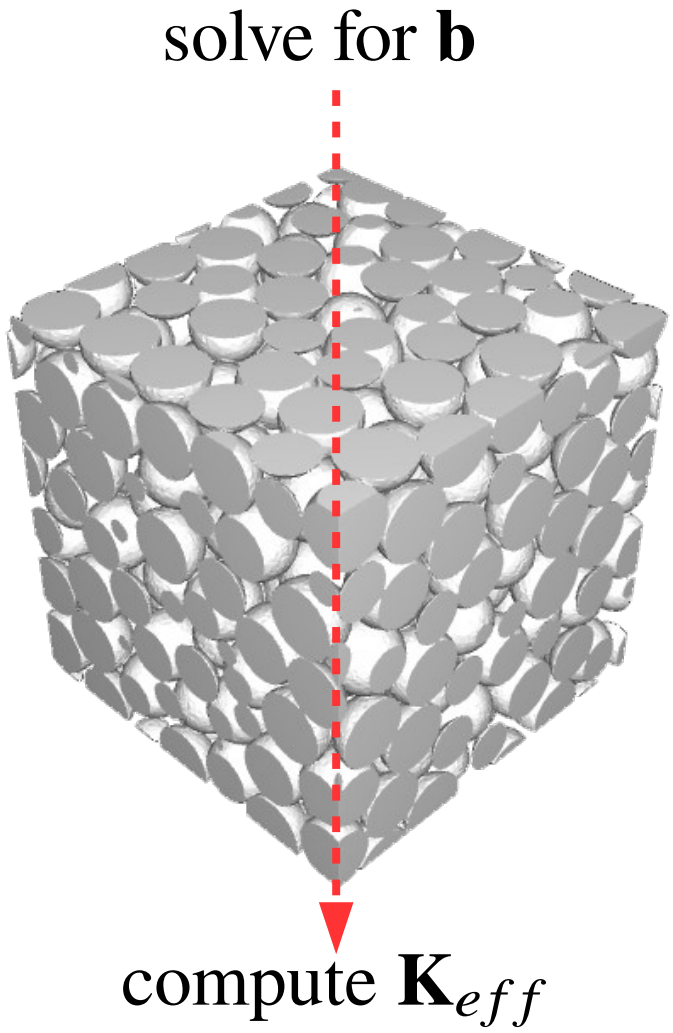
$$\text{B.C.2} \quad \mathbf{b}_\beta = \mathbf{b}_\sigma \quad \text{at } A_{\beta\sigma}$$

tortuosity

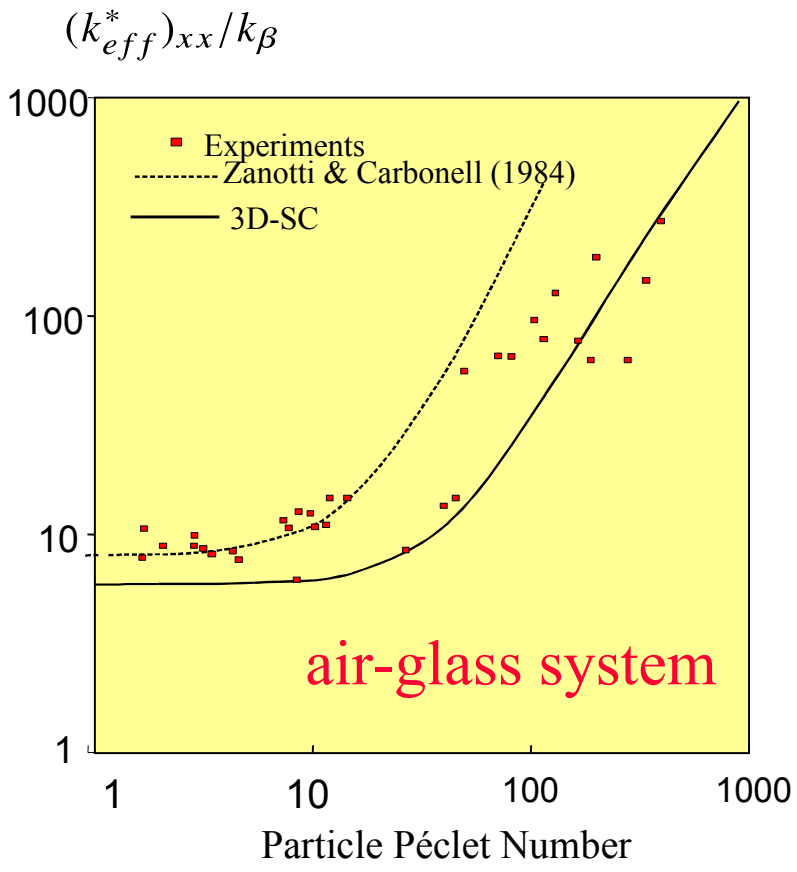
$$0 = k_\sigma \nabla^2 \mathbf{b}_\sigma \quad \text{in } V_\sigma$$

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

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



Application: Thermal Dispersion



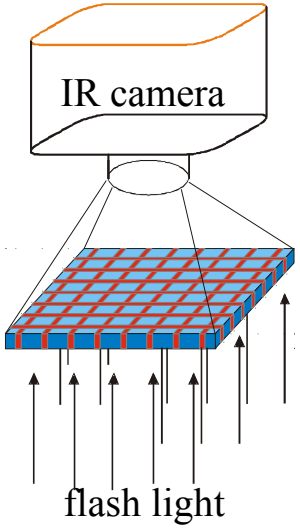
Quintard et al., 1997

- **experiments:** Yagi et al., 1960; Gunn and De Souza, 1974

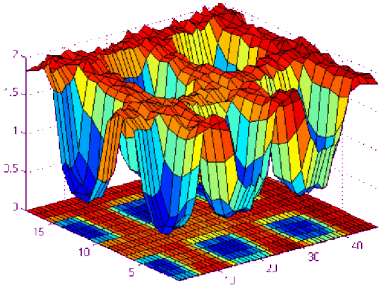
- Zanotti & Carbonell, 1984: fitted at low Pe, square root dependence at large Pe (Taylor's dispersion)

- Quintard & al., 1997: 3D results

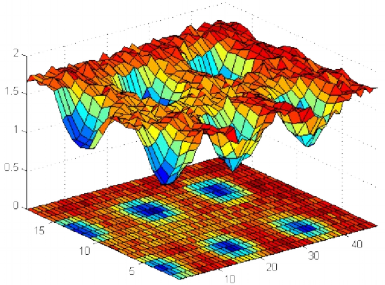
Example of Non-Equilibrium

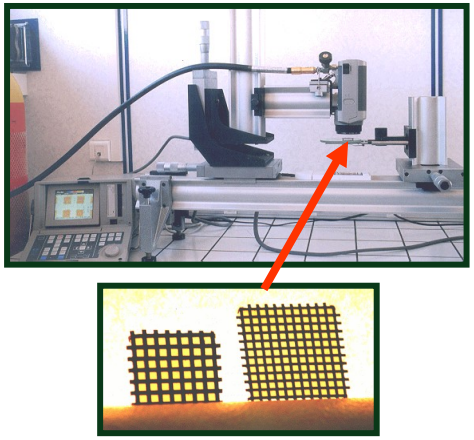


Ramond et al., 98

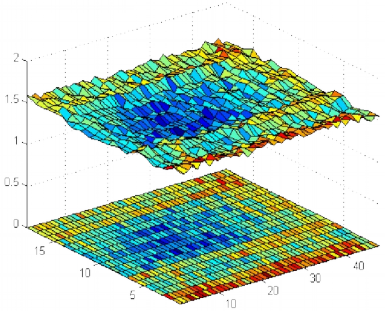


$t = 0$





$t \to \infty$



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

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

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

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

- **quasi-steady closure**

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

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

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

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

- **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; ……)

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

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

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

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 ≠ 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)

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

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

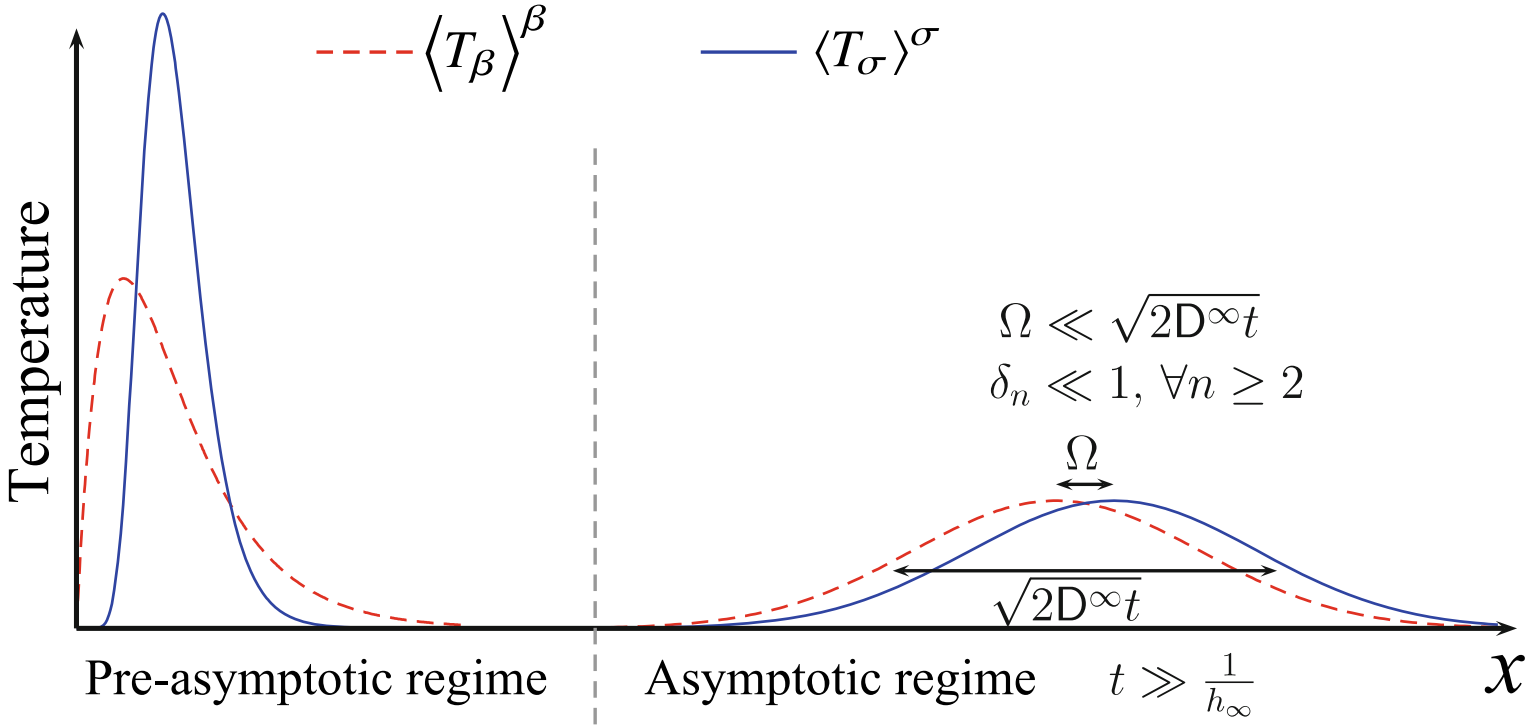
$$\left(\varepsilon_\beta \left(\rho c_p\right)_\beta + \varepsilon_\sigma \left(\rho c_p\right)_\sigma\right) \frac{\partial \left\langle T \right\rangle^{\beta\sigma}}{\partial t} + \varepsilon_\beta \left(\rho c_p\right)_\beta U_\beta \frac{\partial \left\langle T \right\rangle^{\beta\sigma}}{\partial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

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

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

- **$\rightarrow$ 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:**

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

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

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

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

  $\rightarrow$ Direct Estimation of $\mathbf{K}_\infty^*$ (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**

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

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

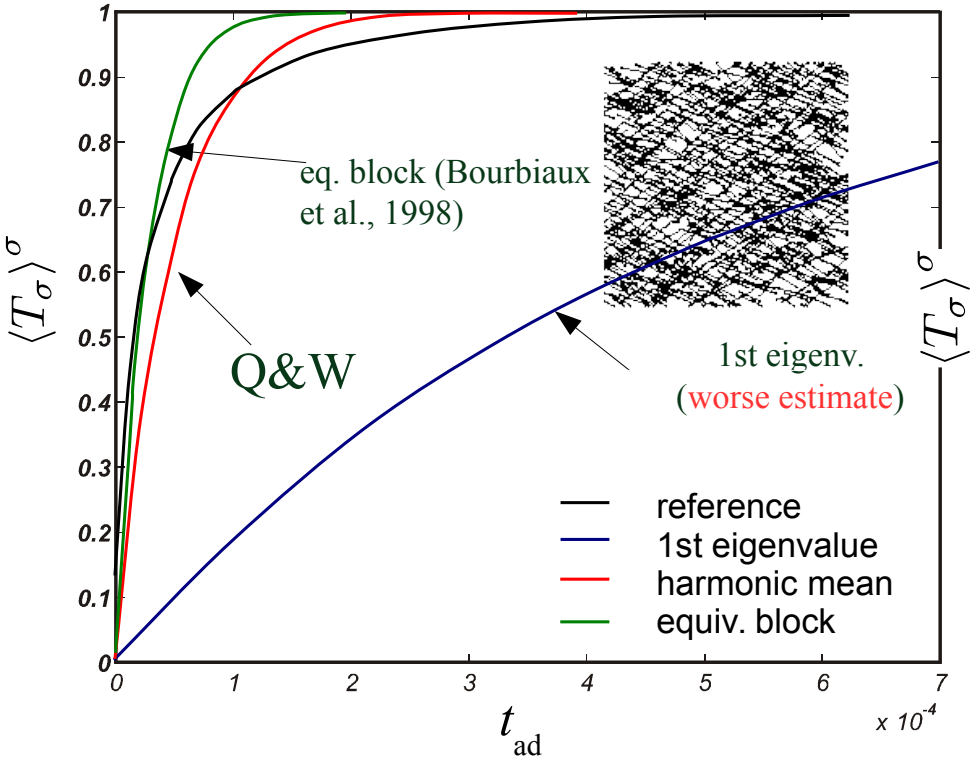
Example: 3-eqs

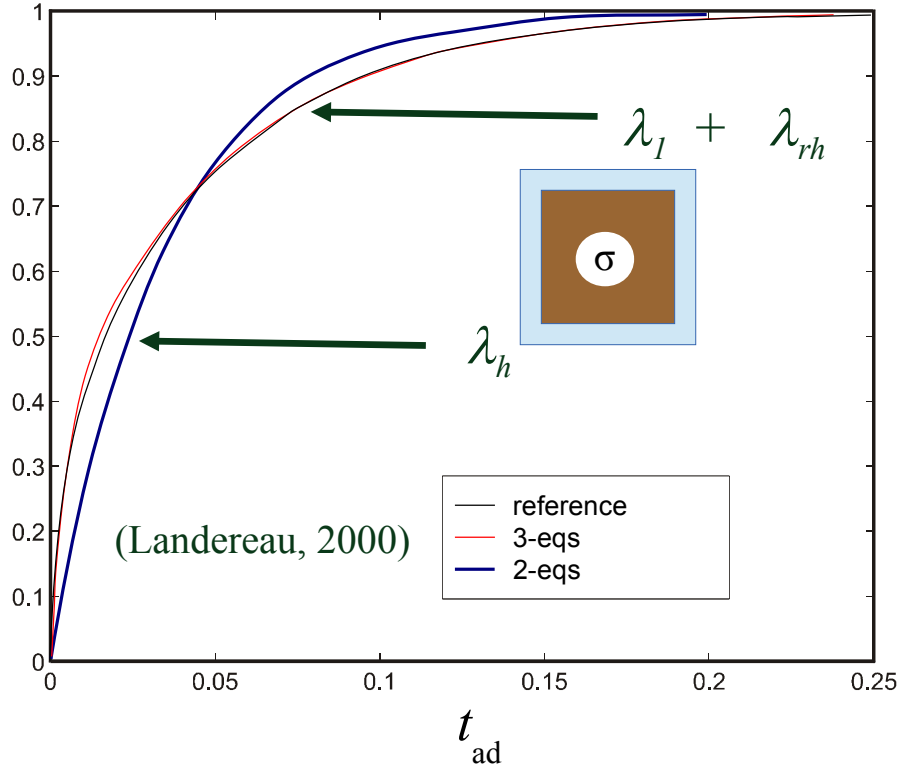
$T_{\sigma 1}$, $T_{\sigma r}$

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, $k_\sigma << k_\beta$, dispersed σ-phase; De Swaan, 1976; .....) (if homogenization theory use $k_\sigma = \varepsilon^2 k_\beta$)

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

Macro-

$$\varepsilon_\beta (\rho C_p)_\sigma \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} = \nabla . \left(\mathbf{K}^*_\beta . \nabla \langle T_\beta \rangle^\beta \right) - \varphi_{\beta\sigma}$$

Micro-

$$(\rho c_p)_\sigma \frac{\partial T_\sigma}{\partial t} = \nabla . (k_\sigma \nabla T_\sigma) \quad \text{in } V_\sigma \qquad T_\sigma = \langle T_\beta \rangle^\beta \text{ , at } A_{\beta\sigma}$$

general solution:

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

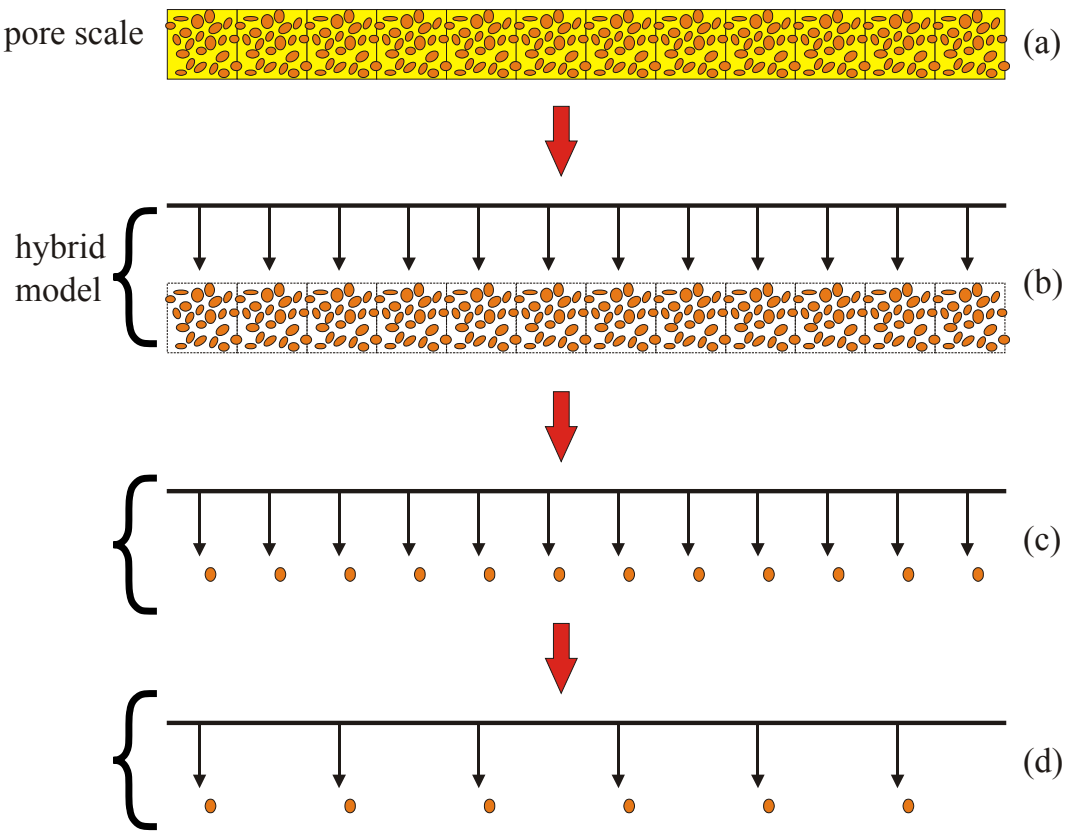
→ involves spectrum of eigenvalues & eigenfunctions → *h*(*t*, *BC*, *IC*)!

Mixed Model: Practical Implementation

-Direct Numerical Simulation (Heavy computations)

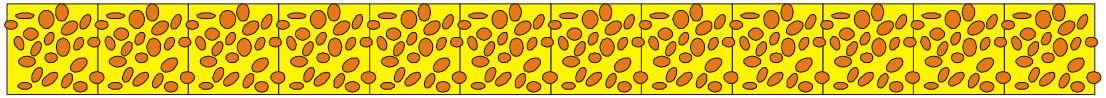
-Mixed Model, Full UC (still Heavy Comp.)

-Mixed Model, Representative Matrix Block,…



…in some cases Analytical Solutions may be available

Summary: a schematic representation of the various models

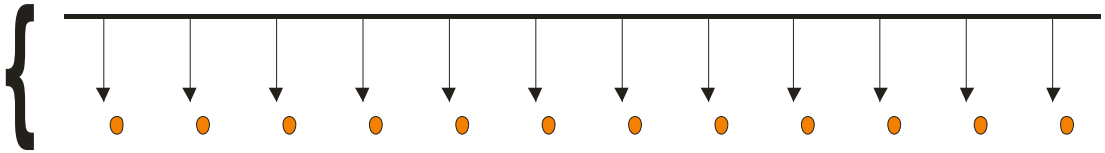


DNS

1-eq local equilibrium

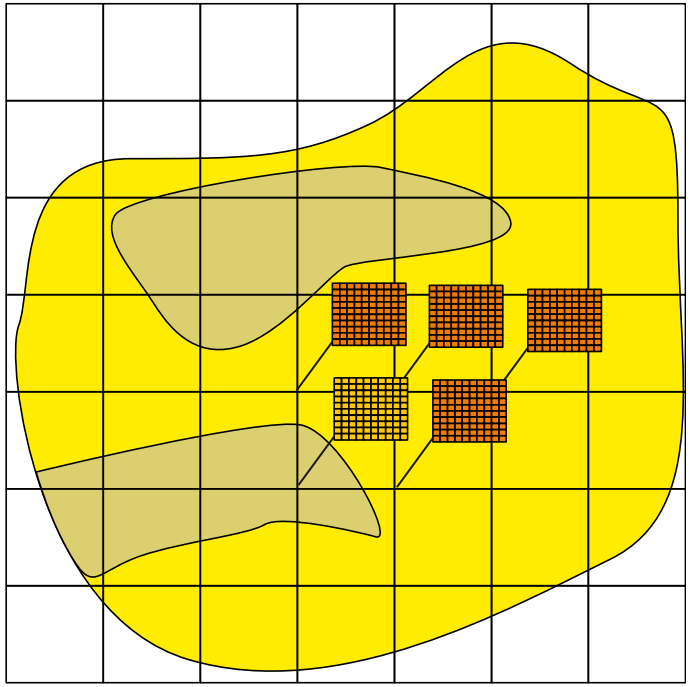
1 equation (convolution, or asymptotic behavior of the 2-eq. model, fractional derivative, Telegraph eq., CTRW ...)

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

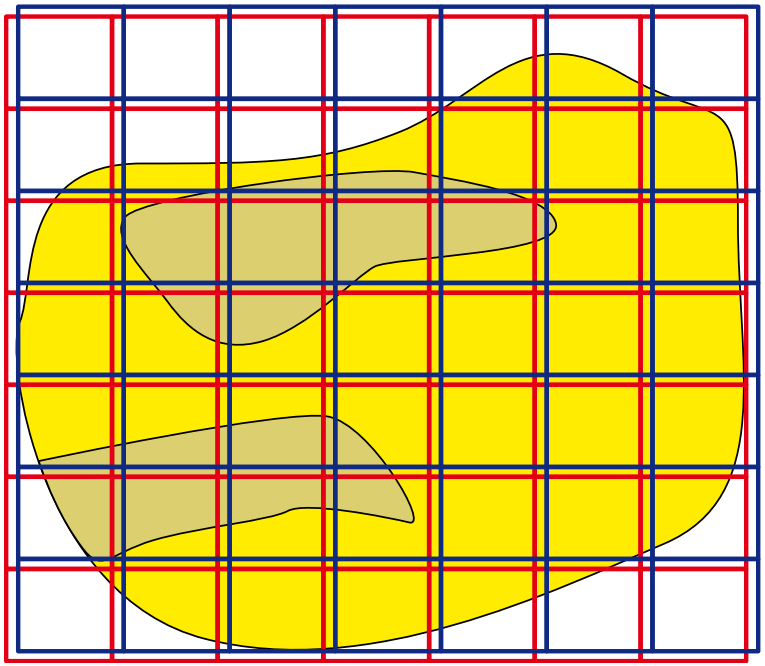


Mixed models

Numerical implementation



Mixed or hybrid models

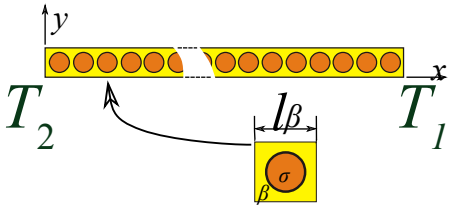


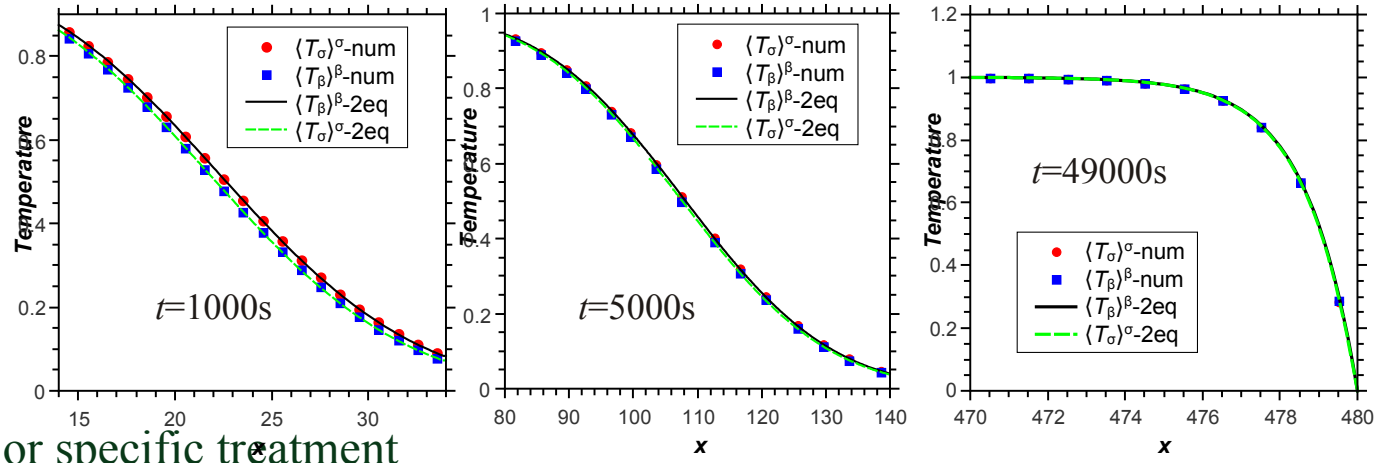
2-eq models

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

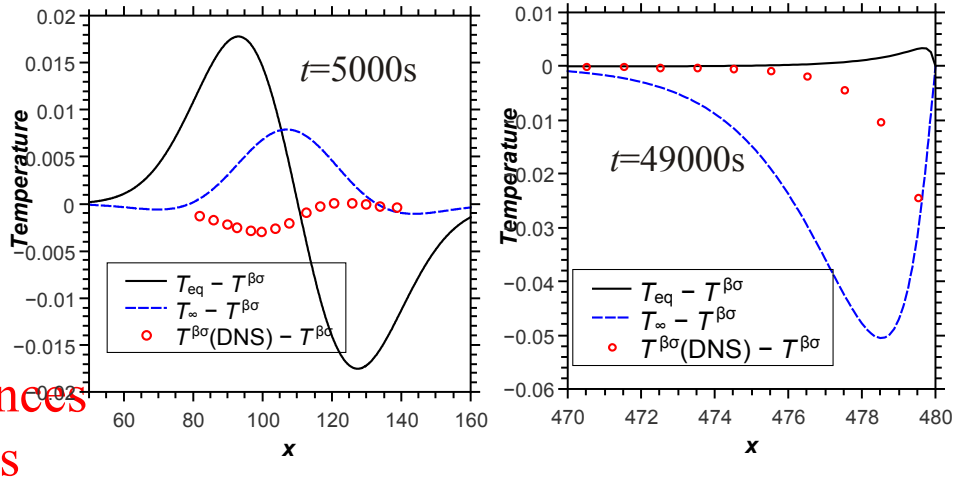
Important: transitions between the various models!

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





- t~0 non-homogenizable or specific treatment
- t>0 LNE models
- t>>0 (if enough length): 1-Eq asymptotic model
- t → ∞ (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:** $-\mathbf{n}_{\beta\sigma}.k_\beta \nabla T_\beta = h\left(T_\beta - T_\sigma\right)$ 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**

$$k_\beta = F\left(T_\beta\right) = F\left(\left\langle T_\beta \right\rangle^\beta\right) + \frac{\partial F}{\partial T_\beta}\left(\left\langle T_\beta \right\rangle^\beta\right)\tilde{T}_\beta + \cdots$$

$$\tilde{T}_\beta = O\left(\frac{l_\beta}{L}\left\langle T_\beta \right\rangle^\beta\right)^*$$

$$\Bigg\} \; k_\beta = F\left(T_\beta\right) \approx F\left(\left\langle T_\beta \right\rangle^\beta\right)$$

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

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

Coupled problems, a simple example: transport with Soret effect

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

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

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

- ***Closure (Lacabanne et al., 2002; Davarzani et al., 2010, 2011, ext. for Pe≠0):***

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

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

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

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

etc... ☺!

Coupled problems, a simple example: transport with Soret effect

- **macro-equation:**

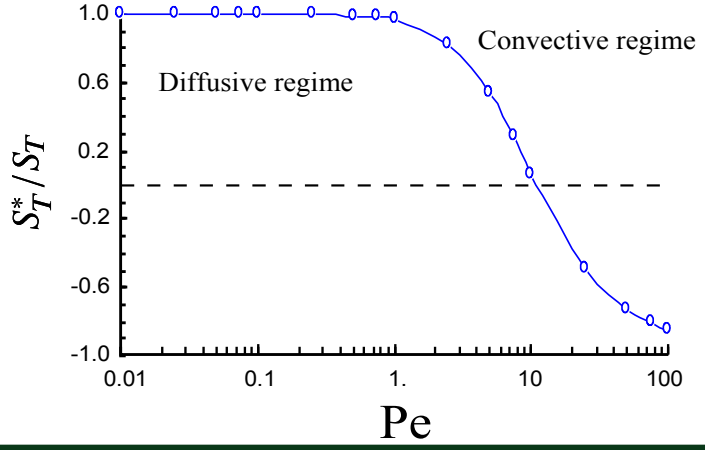
$$\frac{\partial \varepsilon_\beta \left\langle c_\beta \right\rangle^\beta}{\partial t} + \nabla . \left(\varepsilon_\beta \left\langle \mathbf{v}_\beta \right\rangle^\beta \left\langle c_\beta \right\rangle^\beta \right) = \nabla . \left(\varepsilon_\beta \mathbf{D}_\beta^* . \nabla \left\langle c_\beta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

- **Results for Soret Coefficient:**

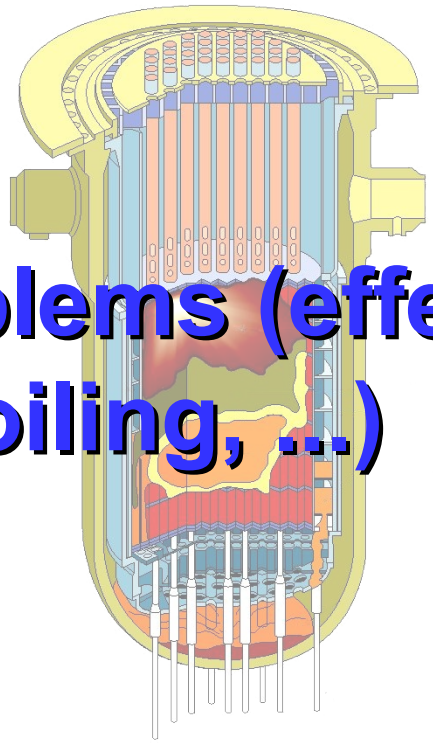
$$S_T = D_{T\beta} / D_\beta$$
$$S_T^* = D_{T\beta}^* / D_\beta^*$$

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

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



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



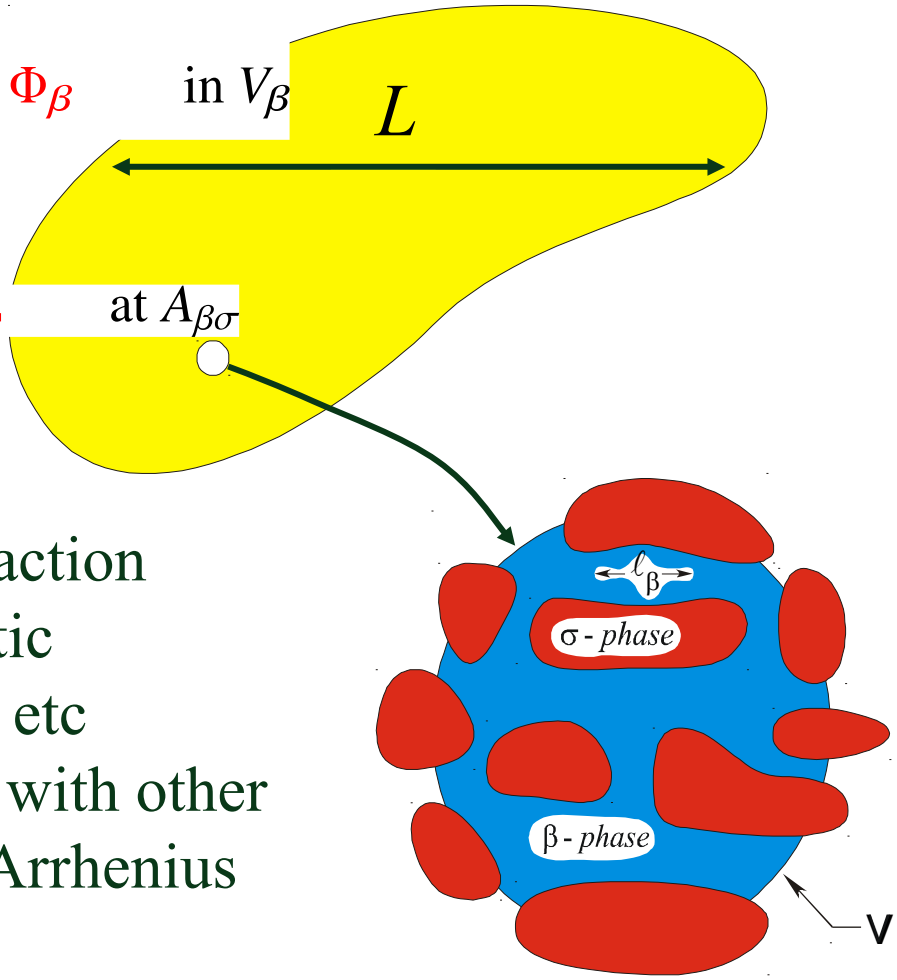
Potential strong coupling: Effect of source terms

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

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

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

$$(\rho c_p)_\sigma \frac{\partial T_\sigma}{\partial t} = \nabla . \left(k_\sigma \nabla T_\sigma \right) + \Phi_\sigma \qquad \text{in } V_\sigma$$



- 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

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

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

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

Note: B.C.2 gives

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

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

Pore-Scale Deviation Problem

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

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

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

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

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

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

Macro-scale models

- **Local equilibrium**

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

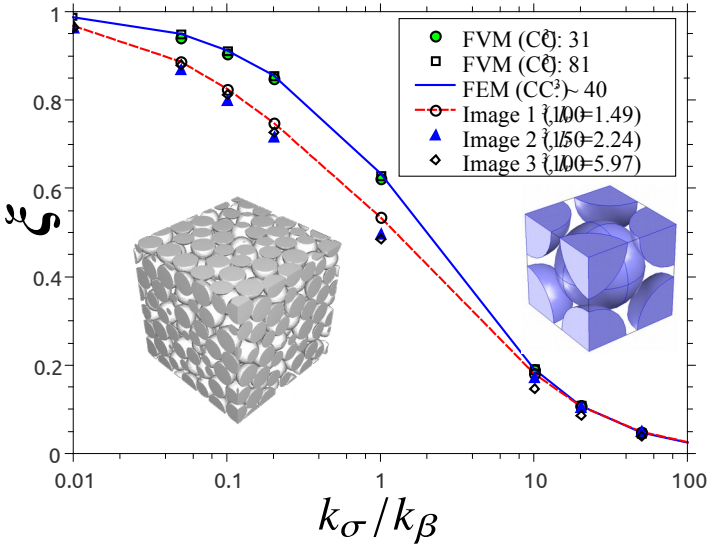
- **2eq model (Quintard & Whitaker, Hdbk Porous Media, 2000; Davit and Quintard, Hdbk Porous Media, 2015)**

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

distribution coefficient

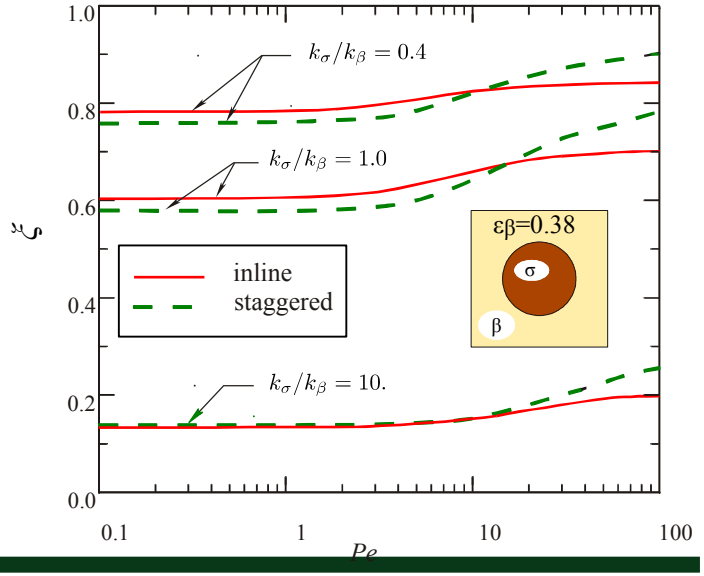
see extension to radiative heat transfer (Leroy et al., 2013), application to combustion (Chen et al., 2014), ...

Calculation of ξ



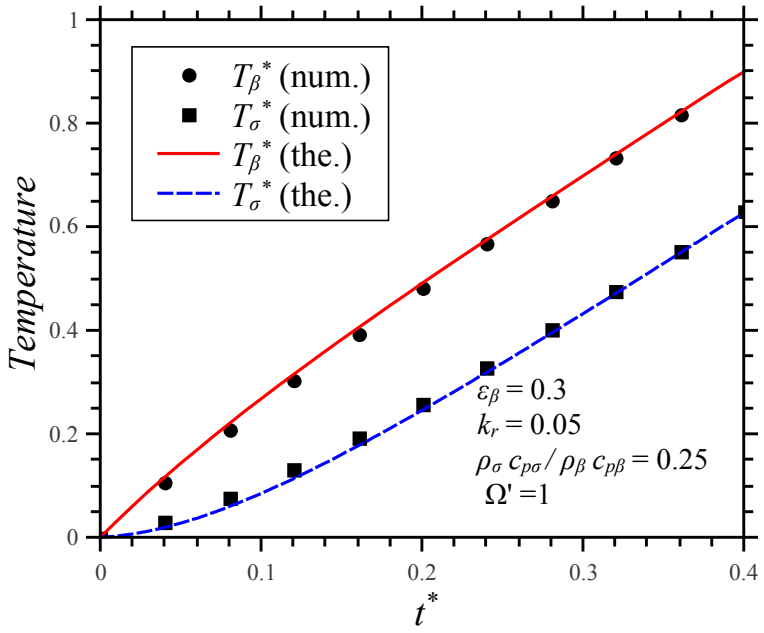
- if $k_\sigma / k_\beta \to \infty$, $\xi \to 0$
  if $k_\sigma / k_\beta \to 0$, $\xi \to 1$

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

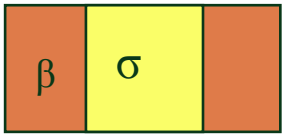


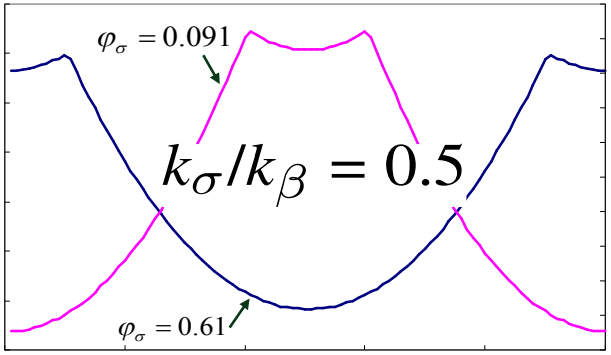
Warning!
Engng practice: ξ → 0

0D "experiment": example of stratified UC



DNS





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

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

- 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

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

$$\varepsilon \left(\rho c_p\right)_\beta \frac{\partial \left\langle T_\beta \right\rangle^\beta}{\partial t} + \left(\rho c_p\right)_\beta \left\langle \mathbf{v}_\beta \right\rangle . \nabla \left\langle T_\beta \right\rangle^\beta - \mathbf{u}_{\beta\beta} \cdot \nabla \left\langle T_\beta \right\rangle^\beta - \mathbf{u}_{\beta\sigma} \cdot \nabla \left\langle T_\sigma \right\rangle^\sigma =$$

$$\nabla \cdot \left(\mathbf{K}_{\beta\beta} . \nabla \left\langle T_\beta \right\rangle^\beta + \mathbf{K}_{\beta\sigma} . \nabla \left\langle T_\sigma \right\rangle^\sigma \right) - h_{2eq} \left(\left\langle T_\beta \right\rangle^\beta - \left\langle T_\sigma \right\rangle^\sigma \right)$$

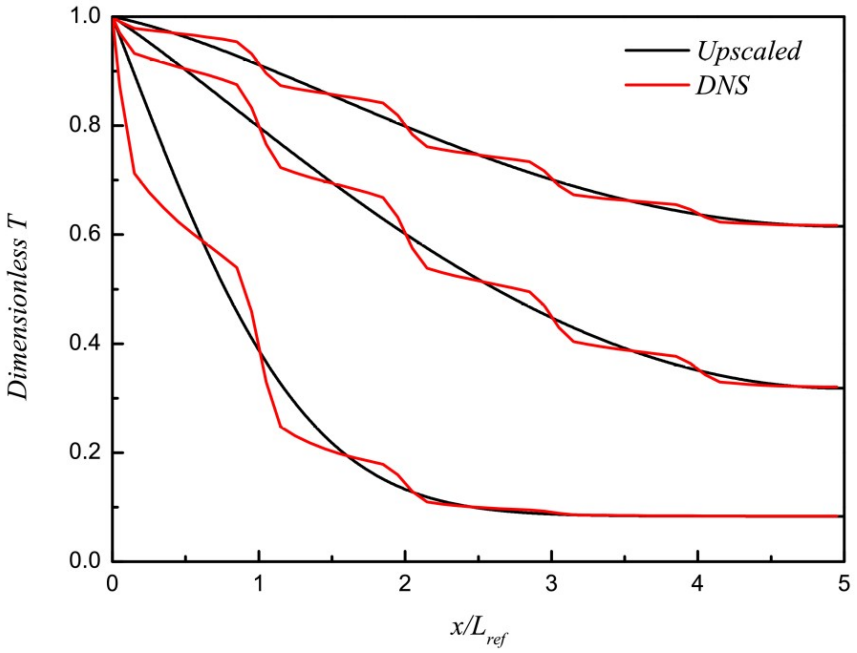
$$+ \varepsilon_\beta \left\langle \Phi_\beta \right\rangle^\beta + a_V \xi \left(1 + w \frac{E}{R \left(\left\langle T_\sigma \right\rangle^\sigma \right)^2} \right) A_0 e^{-E/R\left\langle T_\sigma \right\rangle^\sigma} H_{rxn}$$

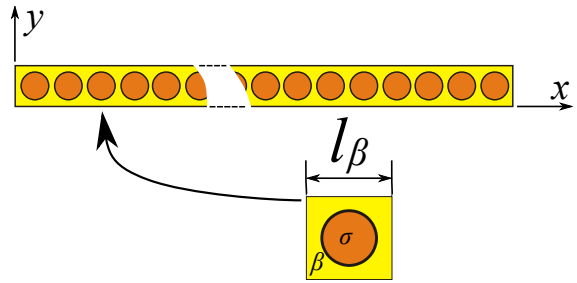
with

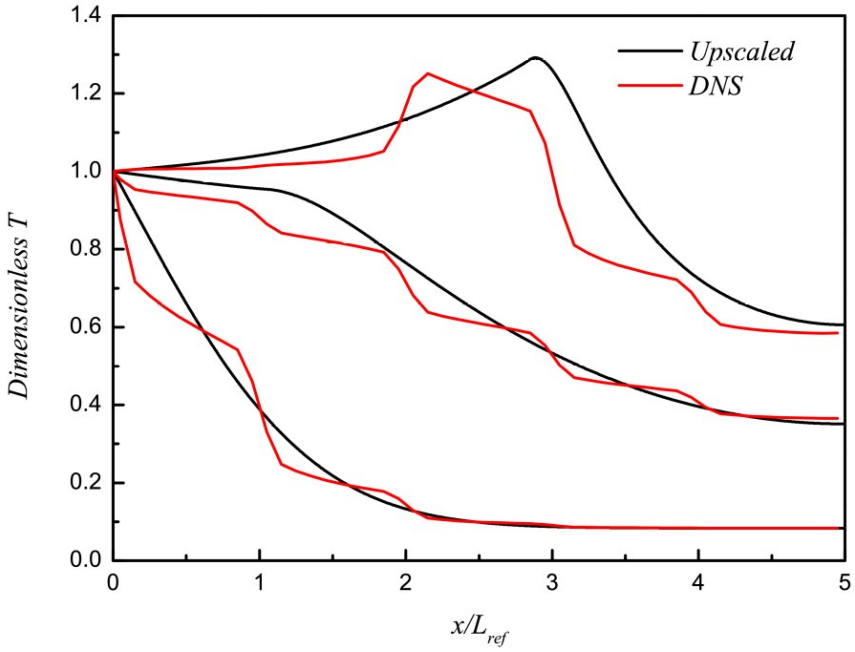
$$w \approx \frac{\frac{E}{R\left(\left\langle T_\beta \right\rangle^\beta\right)^2} e^{-E/R\left\langle T_\beta \right\rangle^\beta} \left(\left\langle T_\sigma \right\rangle^\sigma - \left\langle T_\beta \right\rangle^\beta \right) - \left(e^{-E/R\left\langle T_\sigma \right\rangle^\sigma} - e^{-E/R\left\langle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

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

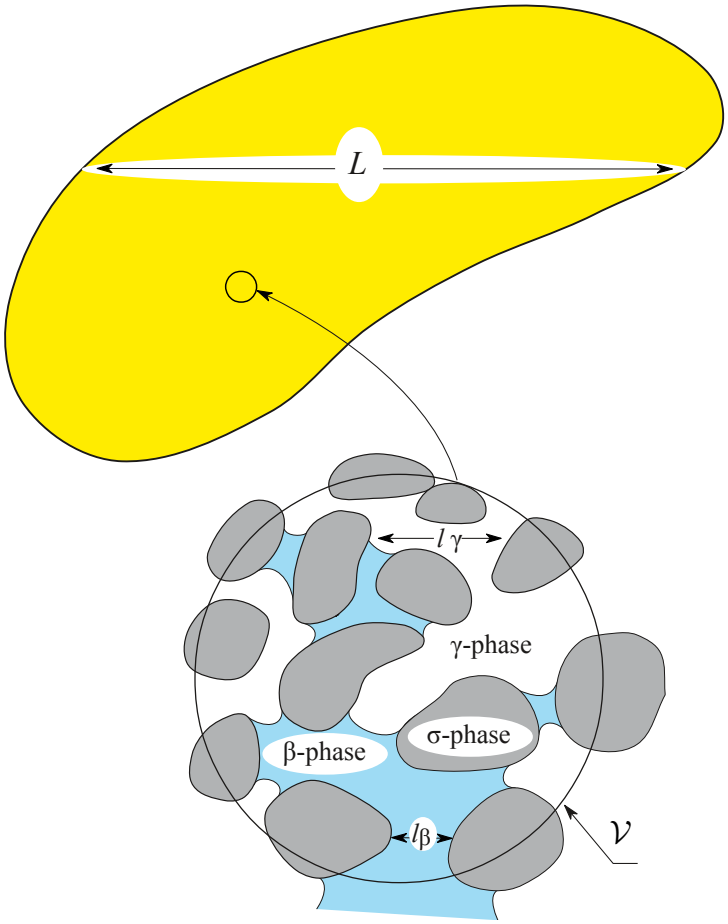
Case with no inert gas!

Mass balances+Momentum balances
+Energy balances

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

$$T_\gamma = T_\beta = T_{sat}(p)$$

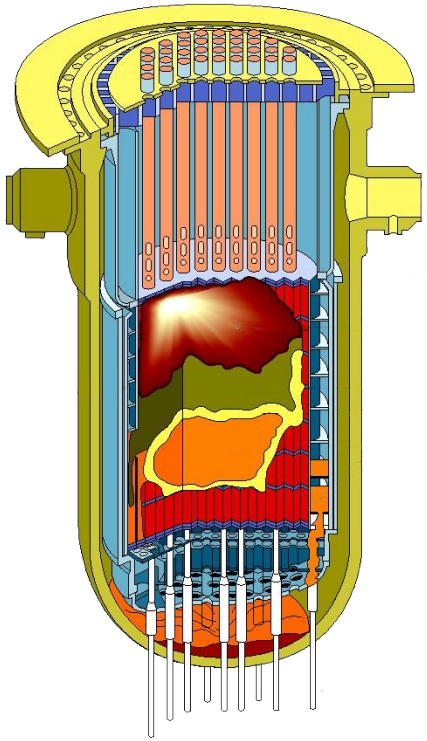
$$\mathbf{n}_{\beta\gamma} \cdot \left(\rho_\gamma \left(\mathbf{v}_{\gamma v} - \mathbf{w}_{\beta\gamma}\right) \delta h_{\beta\gamma}\right) - \mathbf{n}_{\beta\gamma} \cdot \left(k_\gamma \nabla T_\gamma\right) = -\mathbf{n}_{\beta\gamma} \cdot \left(k_\beta \nabla T_\beta\right)$$



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

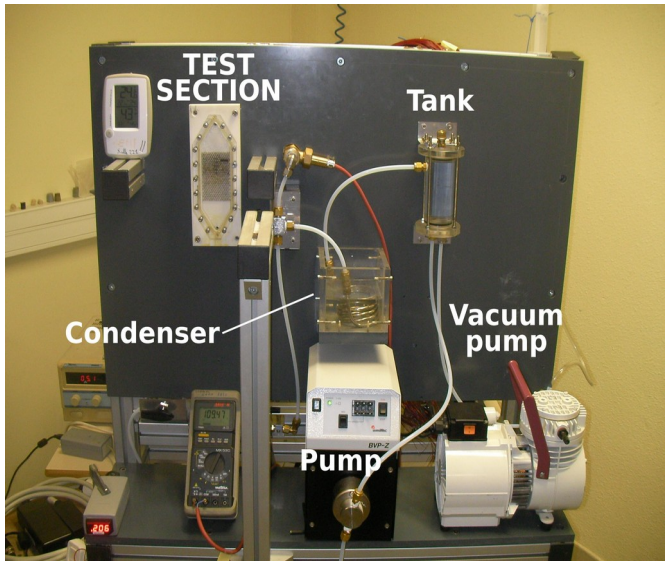
Nuclear LOCA accident

- 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)

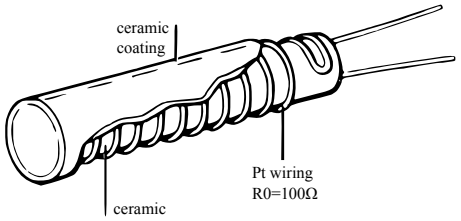


Highly open problem!

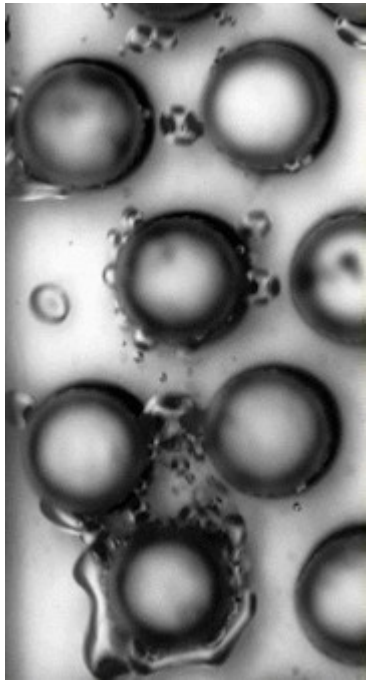
Pore-Scale Experimentations

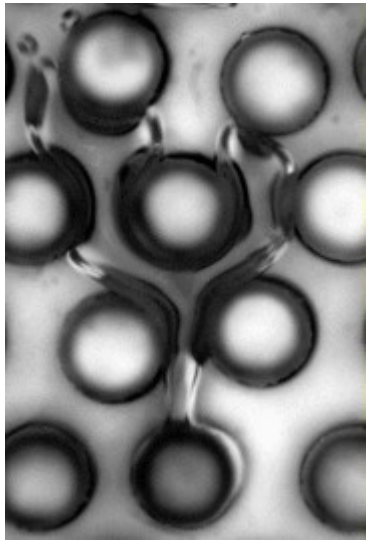


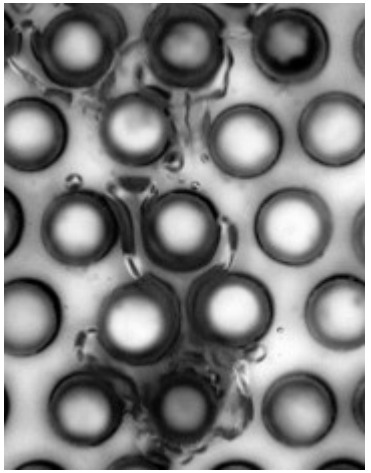
Sapin et al., 2014



Video in slow motion!



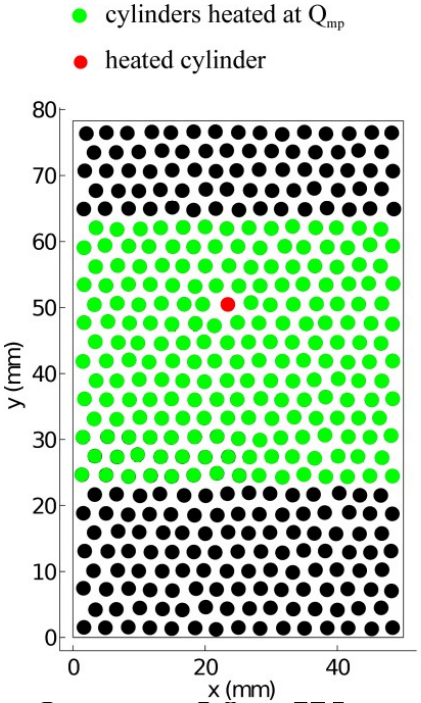


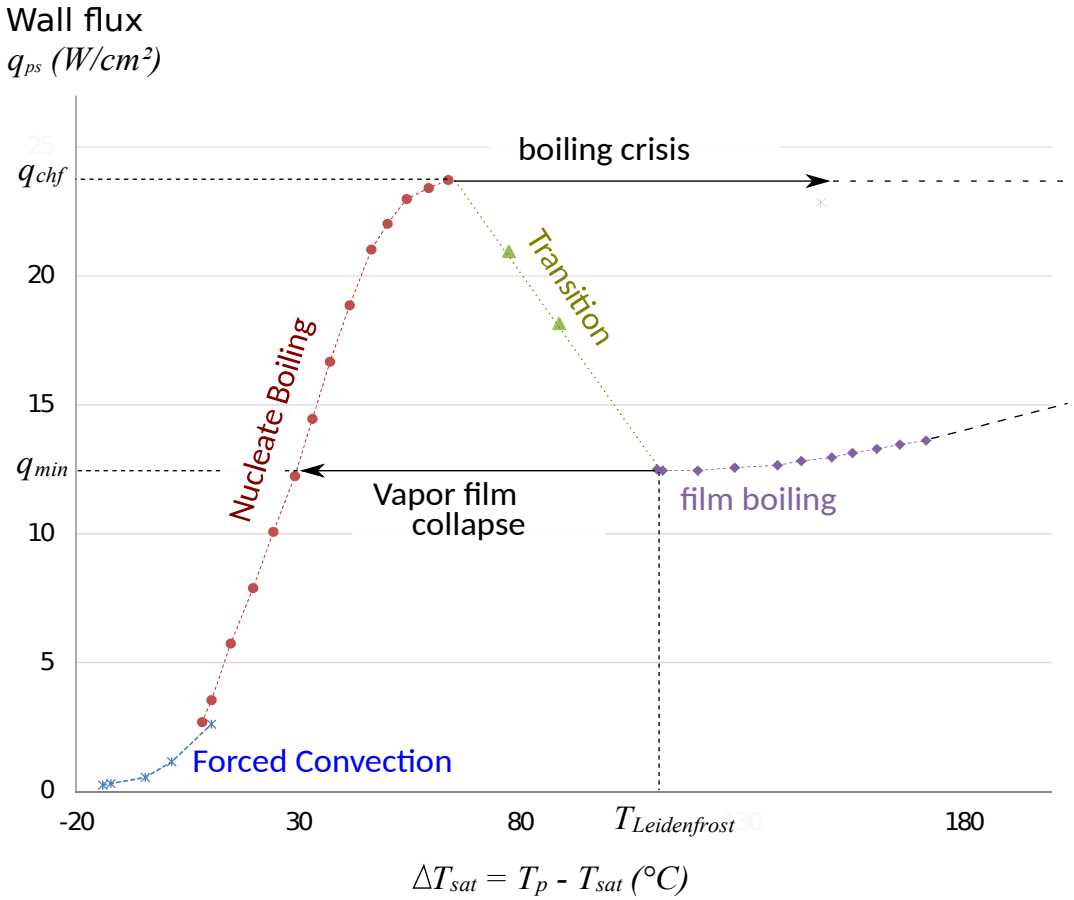


Nucleate Boiling Film Boiling Intense Boiling

Need time-averaging!

Porous Media Nukiyama Curves





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

$$T_l = 24.4°\text{C}$$

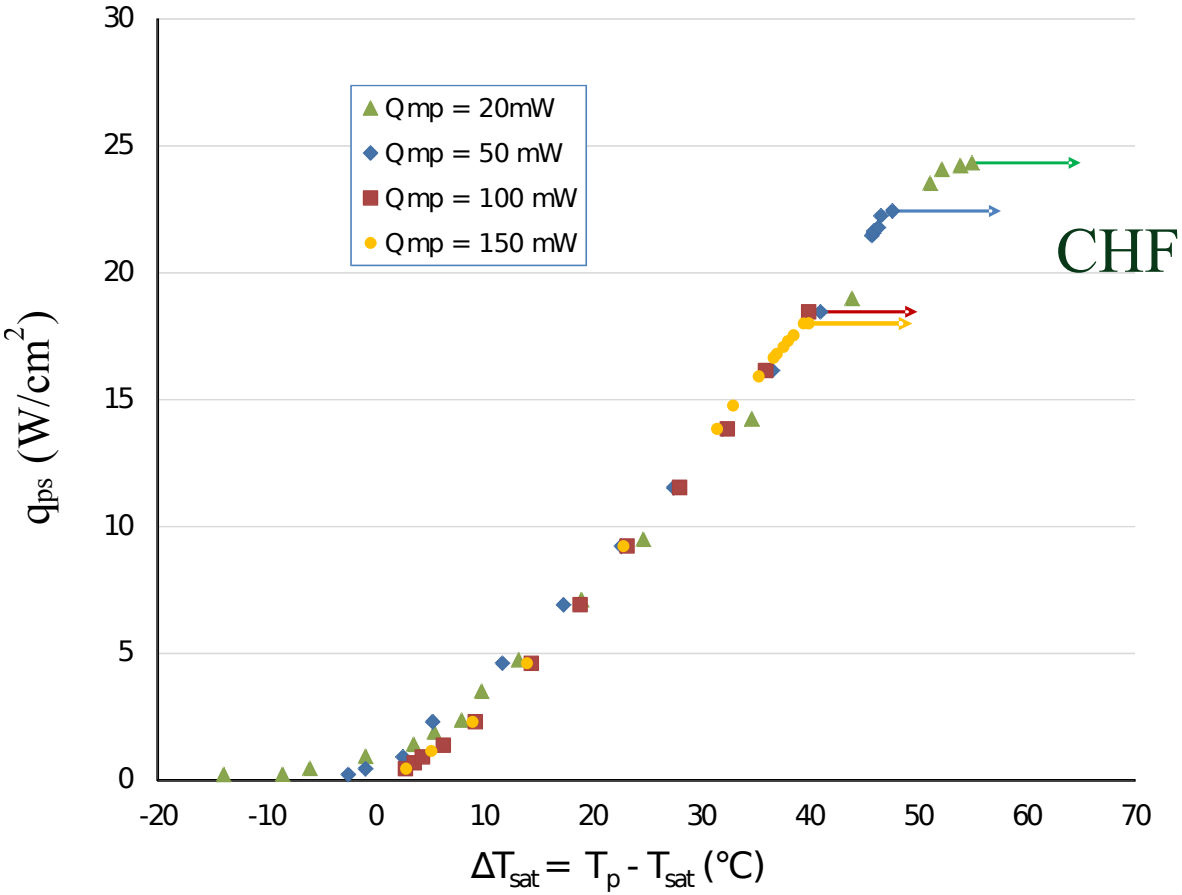
$$P = 1.181\,\text{bar}$$

$$T_{sat} = f(P) = 39.9°\text{C}$$

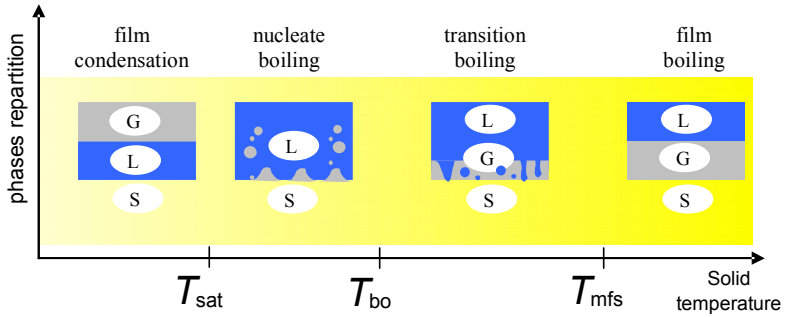
$$v_l = 3.4\,\text{mm/s}$$

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 !

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

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

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

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

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

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

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

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

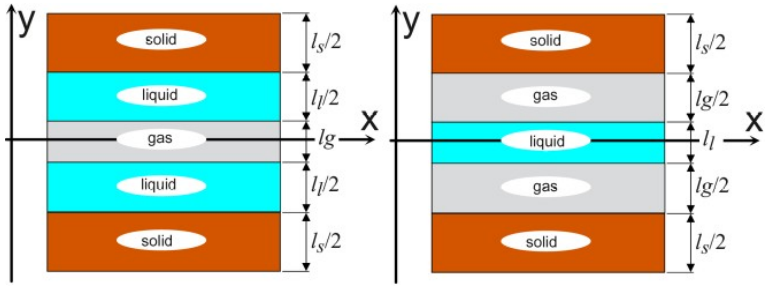
$$\dot{m}_{lg} h_{lg} = Q_{si} + Q_{gi} + Q_{li}$$

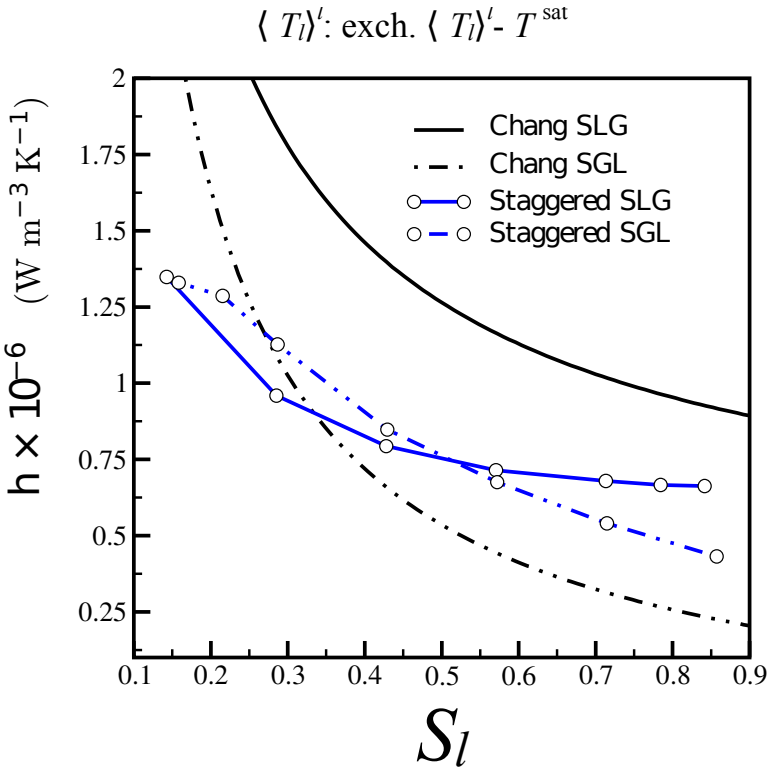
+ generalized Forchheimer

Heat Exchange Terms

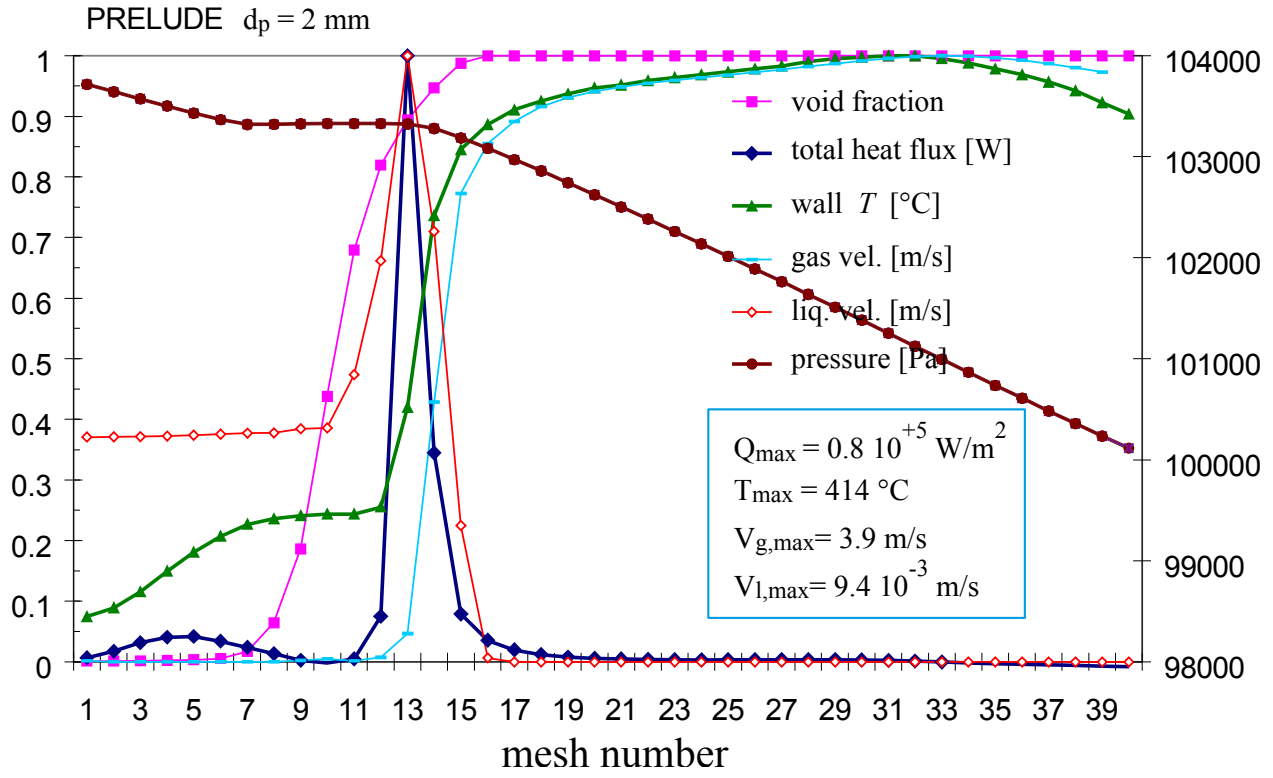
- **Quasi-static two-phase flow theory + inertia terms**

Example: impact of phase configuration!





Example : comparison with experiments

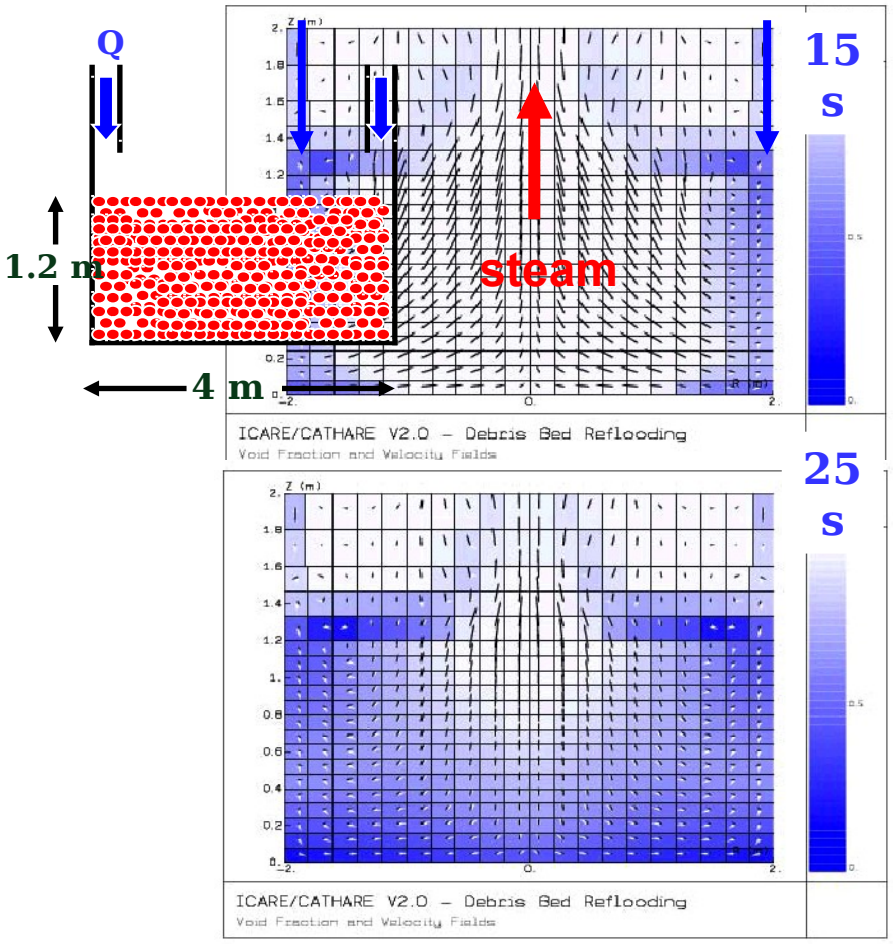


IRSN Experiments:
PRELUDE, SYLPHIDE, ...

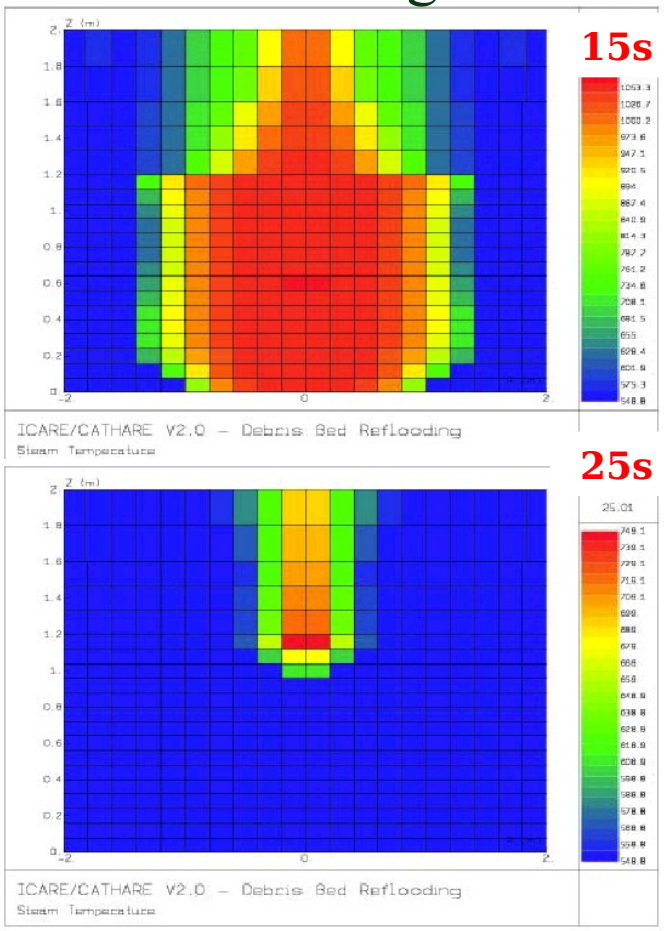
Work confirm main required features (inertia, NLE,...)
→ Macro-scale behavior (heuristic time averaging)
→ Need for adapted correlations

Example of Macro-Scale Simulations (Quenching)

Tregoures et al. (2003)



Water and steam velocities

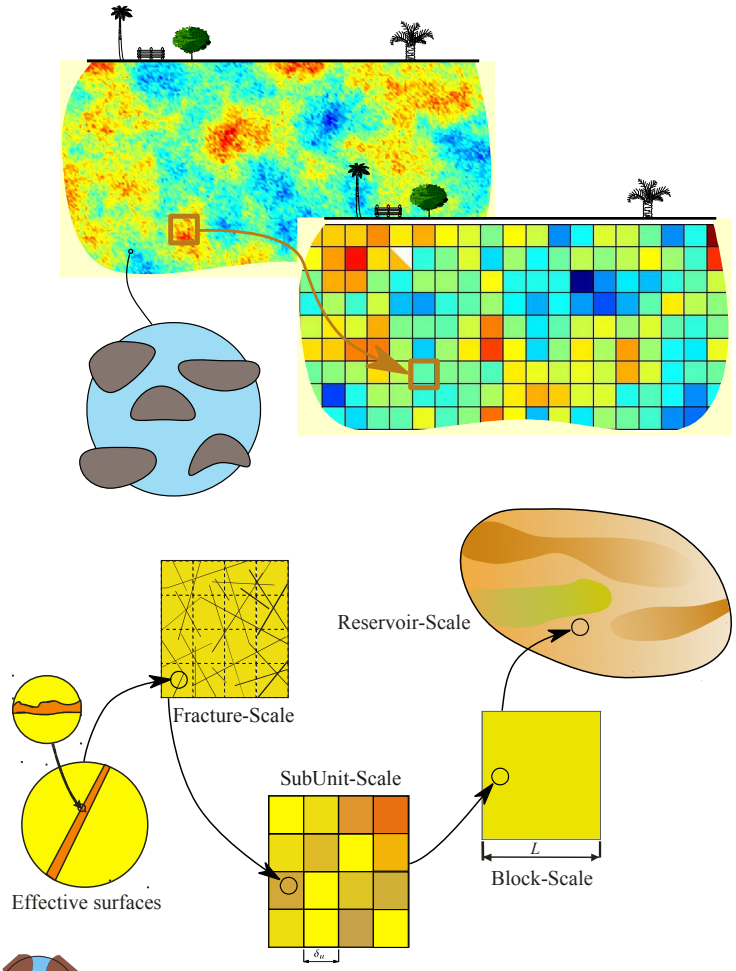


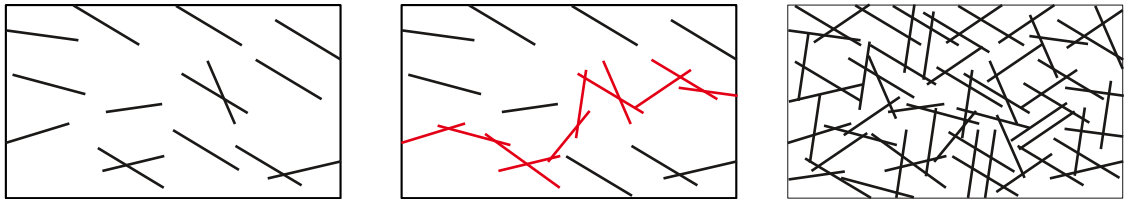
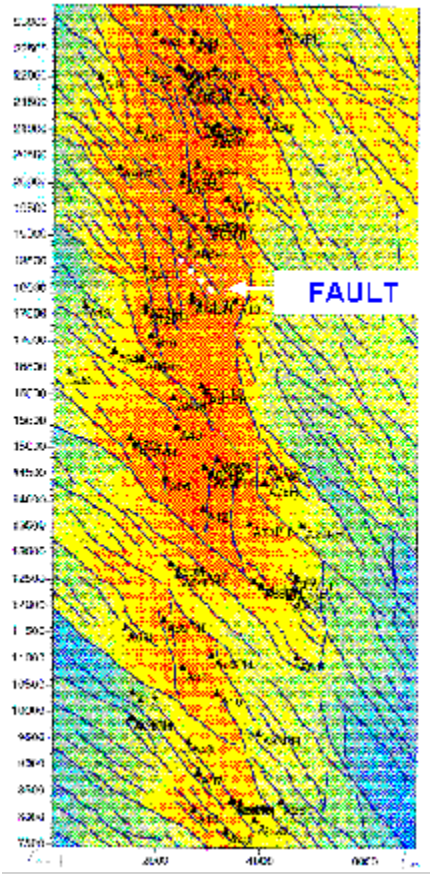
Temperature field

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