INTERPORE @ PURDUE

May 14 - 16, 2012

DERIVATION OF AN ANISOTROPIC DARCY-FORCHHEIMER LAW INCLUDING TURBULENCE EFFECTS AND ITS APPLICATION TO STRUCTURED PACKING

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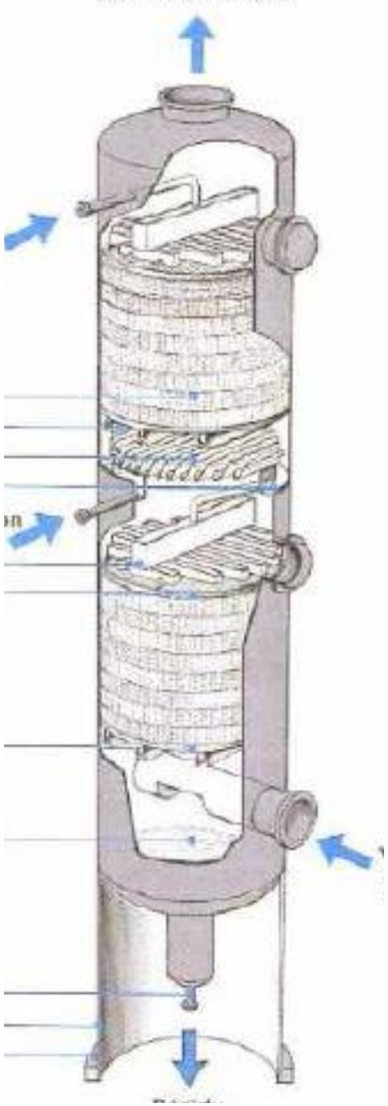
Background : structured packings study



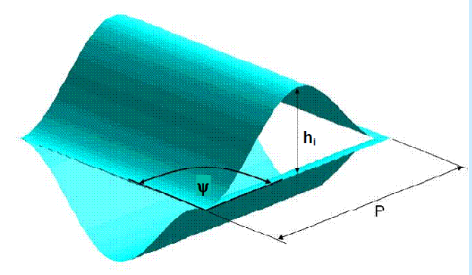
Structured packing

- Replace the fractional distillation
- Large gas-liquide surface to improve separation
- Low pressure loss
- Gas Reynolds number up to 13000
- liquid film flow -> we focus on gas flow

Garnissage structuré
Source Sulzer

Column scale

Seen as a porous media



Representative Elementary Volume (REV)

Characteristic length <1cm

Scientific purposes

How to predict the dry pressure drop in structured packing ?

- Use of CFD simulation on a REV and measurement of the pressure drop (Petre 2003, Raynal 2004 …)

- This method only evaluates the linear pressure drop in the stream direction.

Which law governs the flow at high Reynolds number ?

- Is the Darcy-Forchheimer law still valid in pore-scale turbulent flow regime ?

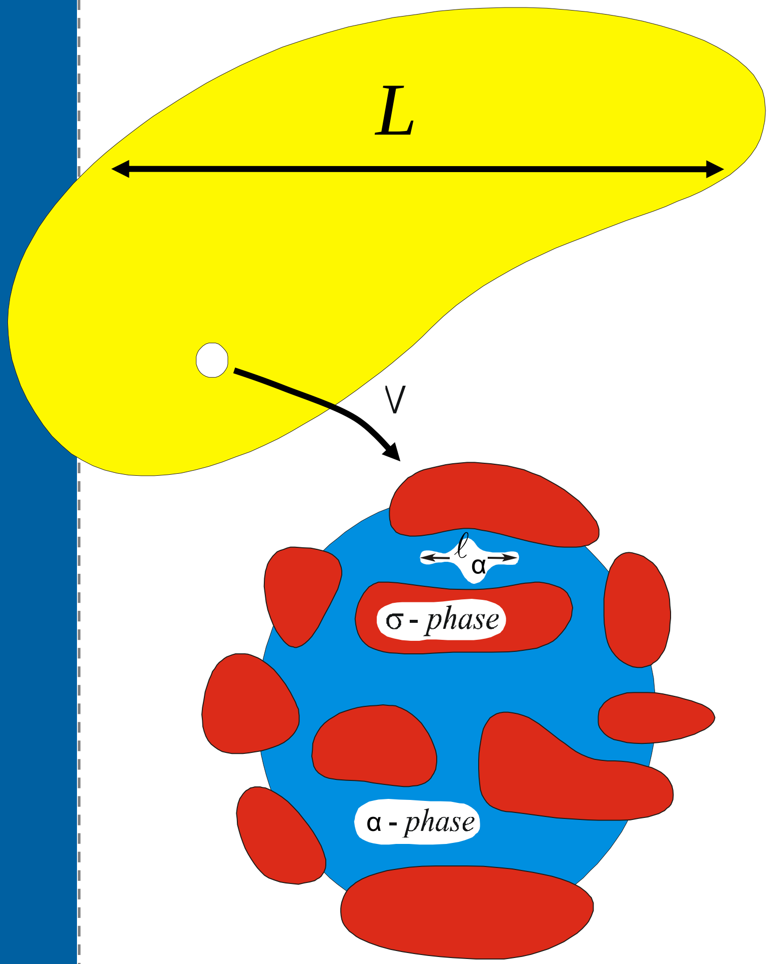
- We look for a methodology to interpret from a macroscopic point of view a turbulent pore-scale simulation

- How to account for large scale anisotropy ?

Single phase flow in porous media : upscaling ?

Re	micro	macro	micro to macro
	Stokes	Darcy's law $$U=-\frac{K}{\mu}(\nabla P-\rho g)$$	Sanchez-Palencia 82 (Asymptotic method) Whitaker 86 (Volume averaging) …
	Laminar Navier-Stokes	Darcy-Forchheimer's law $$U=-\frac{K}{\mu}(\nabla P-\rho g)-F(U)U$$ $$F(U)=\beta\lvert U\rvert^{p}$$ 	Whitaker 96 (Volume averaging) …
	Turbulent Navier-Stokes (DNS, RANS, LES…)	de Lemos, Pinson, Getachew…	

Volume averaging theory



Definitions

$$\langle \psi_\alpha \rangle = \frac{1}{V} \int_{\mathcal{V}_\alpha} \psi_\alpha d\mathcal{V},$$

$$\langle \psi_\alpha \rangle^\alpha = \frac{1}{V_\alpha} \int_{\mathcal{V}_\alpha} \psi_\alpha d\mathcal{V}$$

Main theorems

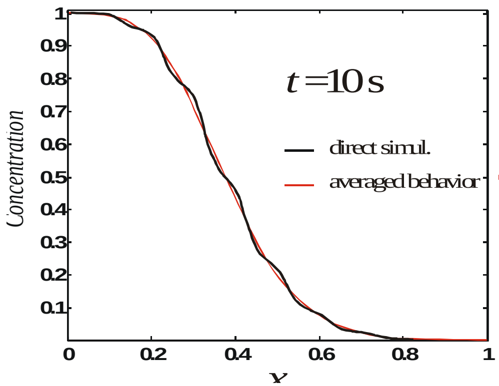
$$\langle \frac{\partial \psi_\alpha}{\partial t} \rangle = \frac{\partial \langle \psi_\alpha \rangle}{\partial t}$$

$$\langle \nabla \psi_\alpha \rangle = \nabla \langle \psi_\alpha \rangle + \frac{1}{V} \int_{\mathcal{A}_{\alpha\sigma}} \mathbf{n}_{\alpha\sigma} \psi_\alpha d\mathcal{A},$$

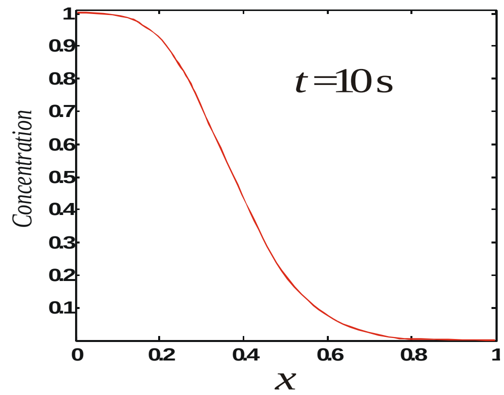
$$\langle \nabla . \mathbf{A}_\alpha \rangle = \nabla . \langle \mathbf{A}_\alpha \rangle + \frac{1}{V} \int_{\mathcal{A}_{\alpha\sigma}} \mathbf{n}_{\alpha\sigma} . \mathbf{A}_\alpha d\mathcal{A}$$

Interfacial effects

Average value and deviation



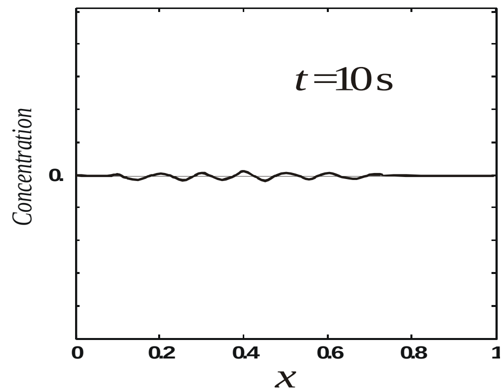
$$c_{A\beta} = \langle c_{A\beta} \rangle^{\beta} + \tilde{c}_{A\beta}$$



Averaged field

$$\langle c_{A\beta} \rangle^{\beta}$$

+



Deviation field

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

closure

- Looking for equations governing the averaged field
- Account for the deviations in the macro-model

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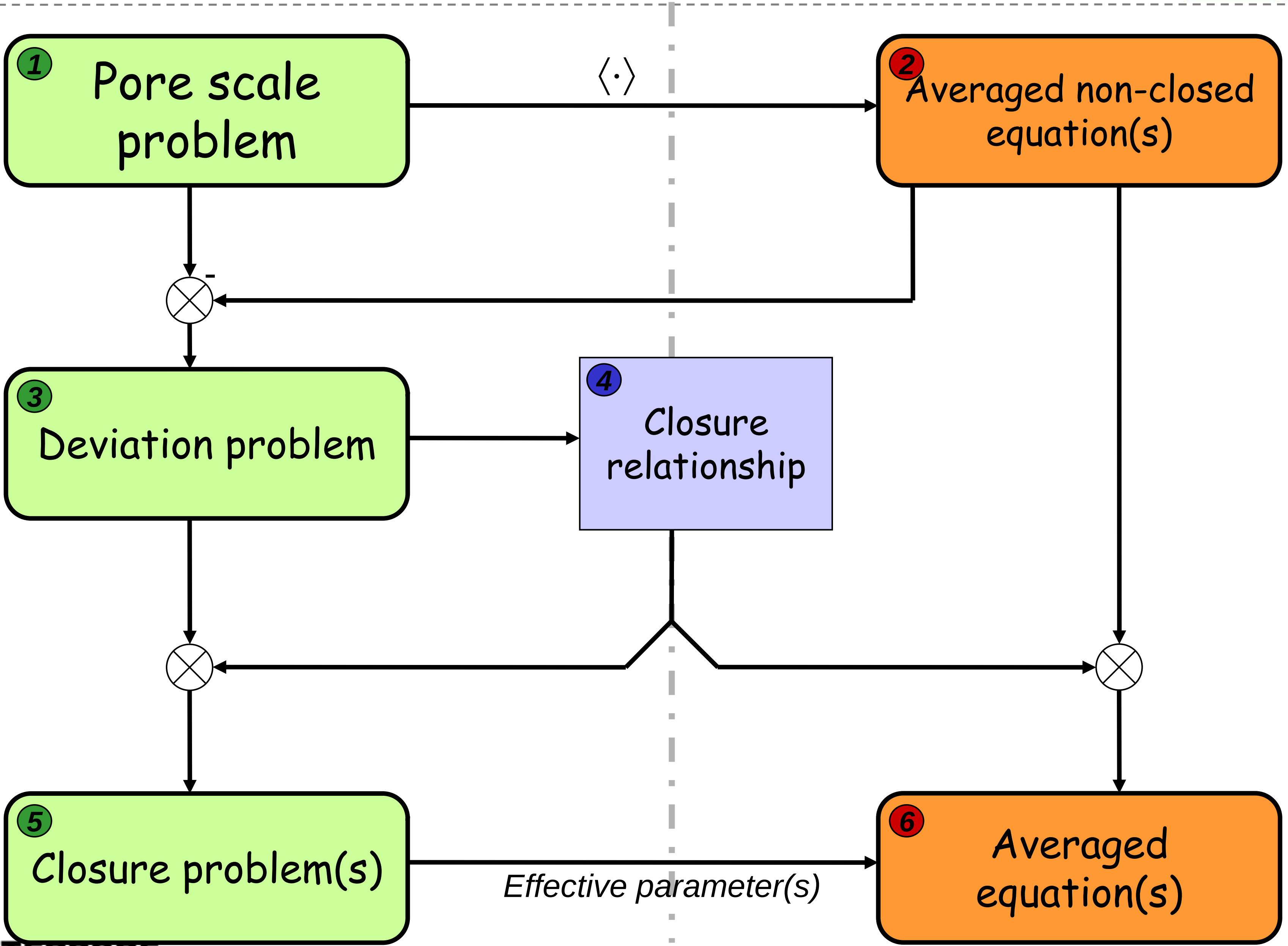
The method of the volume averaging



- **Modeling of gas flow through structured packing in inertial regime**
- **Derivation of a Darcy-Forchheimer law including turbulent effects**
- **Validation of the method and application to structured packing**
- **Conclusions**

Modeling of gas flow through structured packing in inertial regime

Derivation of a Darcy-Forchheimer law including turbulent effects

Validation of the method and application to structured packing

Conclusions

Macro scale model for single phase flow (laminar)

Macroscopic flow model by a Darcy-Forchheimer's law

$$\langle \mathbf{v}_\alpha \rangle = -\frac{\mathbf{K}}{\mu_{\alpha_{mol}}} \cdot \left(\nabla \langle p_\alpha \rangle^\alpha - \rho_\alpha \mathbf{g} \right) - \mathbf{F} \cdot \langle \mathbf{v}_\alpha \rangle \quad = -\frac{\mathbf{K}^*}{\mu_{\alpha_{mol}}} \cdot \left(\nabla \langle p_\alpha \rangle^\alpha - \rho_\alpha \mathbf{g} \right)$$

Permeability tensor

Forchheimer tensor :

- Which form for F(U) ? F(U)=b*U ? F(U)=b*U^p ?
- How to obtain all the tensor composents ?
- Is this law still valid in turbulent flow ?

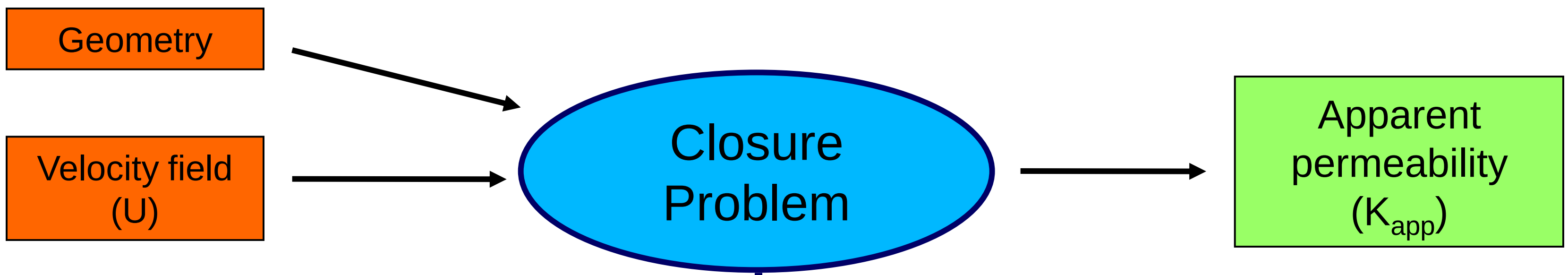
How can the apparent permeability tensor can be evaluated ?

$$\mathbf{K}^* = \begin{pmatrix} K^*_{xx} & K^*_{xy} & K^*_{xz} \\ K^*_{yx} & K^*_{yy} & K^*_{yz} \\ K^*_{zx} & K^*_{zy} & K^*_{zz} \end{pmatrix}$$

- To one pore-scale velocity field corresponds a permeability tensor
- K_{ij}^* depends on the flow direction and magnitude

Evaluation of the apparent permeability tensor in laminar flow regime

- Evaluation of the apparent permeability tensor K_{app} in laminar flow regime using closure problem by *Whitaker 96*



$$(\rho_\beta \mathbf{v}_\beta / \mu_\beta) \cdot \nabla \mathbf{M}$$

$$= -\nabla \mathbf{m} + \nabla^2 \mathbf{M} - \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\mathbf{I}\mathbf{m} + \nabla \mathbf{M})$$

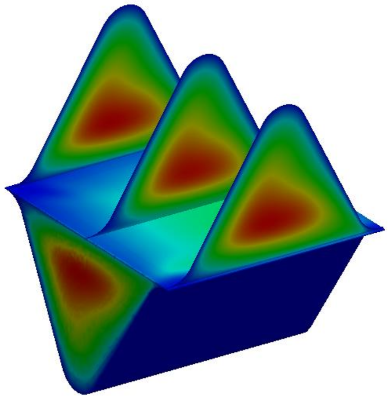
$$\nabla \cdot \mathbf{M} = 0,$$

(B.C.1) $\mathbf{M} = -\mathbf{I}$, at $A_{\beta\sigma}$,

Periodicity: $\mathbf{m}(\mathbf{r} + \ell_i) = \mathbf{m}(\mathbf{r})$, $\mathbf{M}(\mathbf{r} + \ell_i) = \mathbf{M}(\mathbf{r})$,

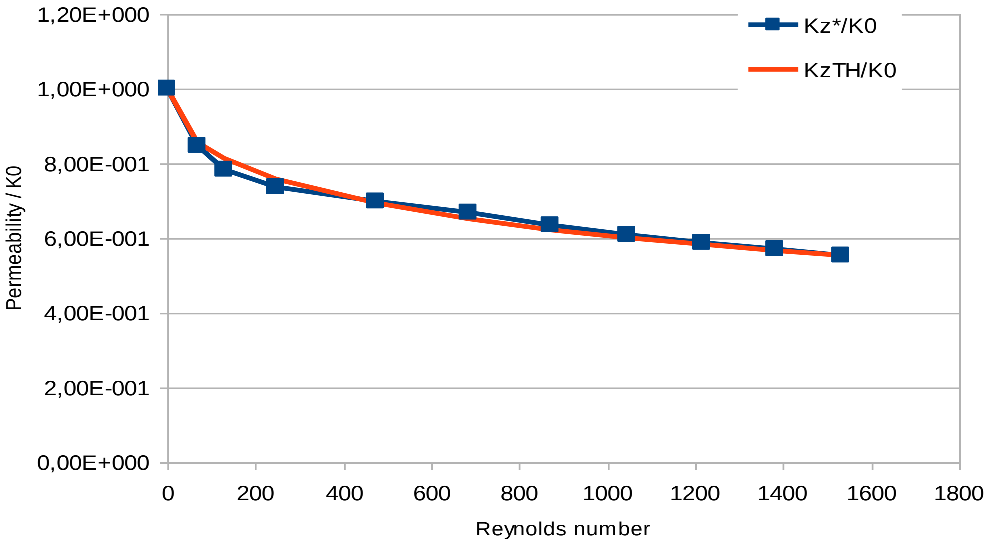
Average: $\langle \mathbf{M} \rangle^\beta = 0$.

Apparent permeability in laminar flow



1. Calculation of the pore scale velocity field using a SIMPLE procedure.

The pressure drop is imposed as a source term in the momentum equation



2. Resolution of the closure problem using Whitaker 96 theory

→ Apparent permeability in the vertical stream direction :

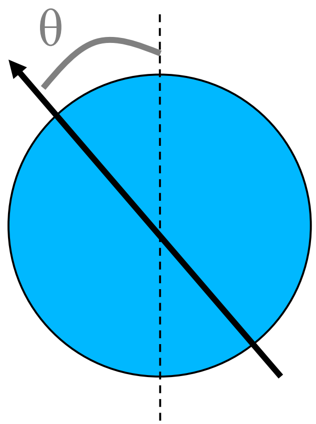
$$\frac{K^*_{yy}}{K_0} = \frac{1}{1+\alpha\sqrt{\text{Re}}}$$

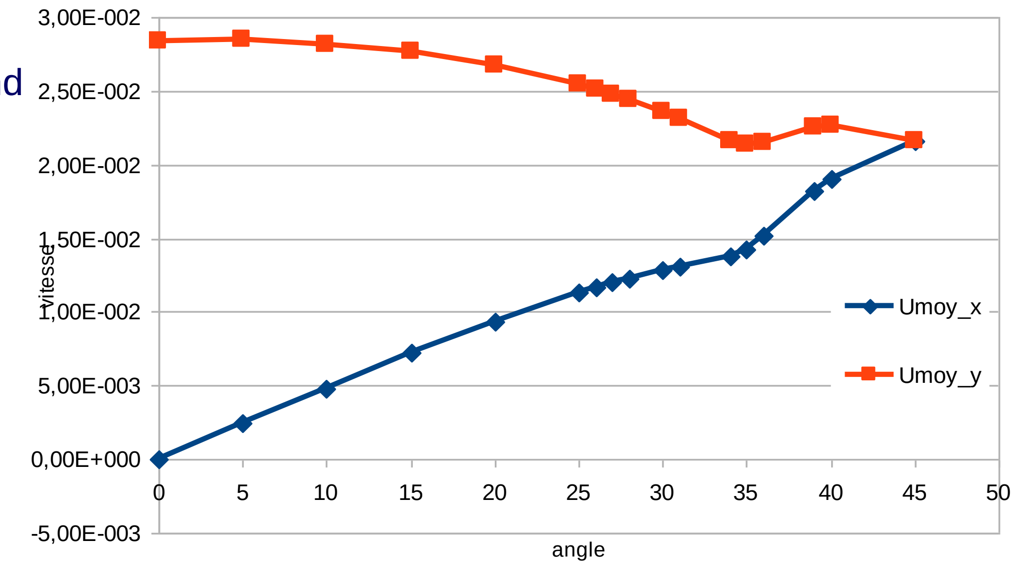
Reminiscent of *Chauveteau and Thirriot* proposal (1965)
See also *Sketjne and Auriault* 1999

Evaluation of the tensor components

1 Calculation of the pore scale velocity field for different flow direction (dP/L is fixed and correspond to Rey=300)

$$\frac{\Delta P}{L}\begin{pmatrix}\sin\theta\\ \cos\theta\\ 0\end{pmatrix}$$

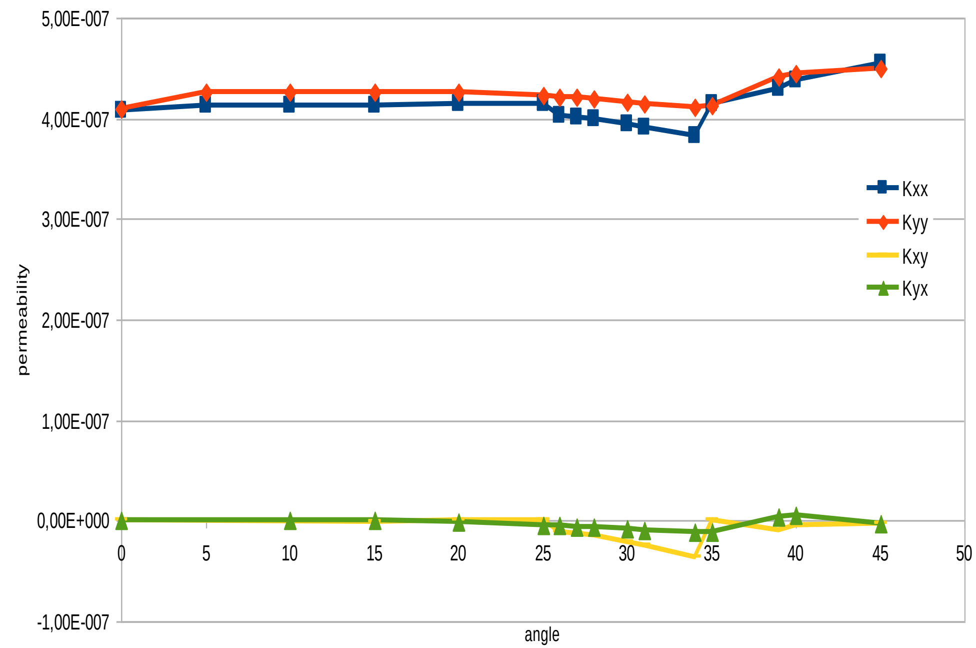




2 Resolution of the closure problem

- non-diagonal coefficient are negligible
- $K_{xx} \approx K_{yy}$ and do not strongly depend on the flow direction

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



Modeling of gas flow through structured packing in inertial regime

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Conclusions

How to model high velocity flow in porous media ?

At macroscale, is a Darcy-Forchheimer law still valid when turbulence effects occur at the smaller scale ?

Experimental results support this statement (Chauveteau & Thirriot 1967, structured packing dry pressure drop correlations…)

More elaborated models for turbulence in porous media

Table 3.1. Classification of turbulence models for porous media (from de Lemos and Pedras, 2001, with permission).

Model class	Authors	General characteristics and treatment of surface integrals	Sequence of integration	Applications
A-L	Lee and Howell (1987), Wang and Takle (1995), Antohe and Lage (1997), Getachewa *et al.* (2000).	Surface integrals are not applied since models are based on macroscopic quantities subjected to time averaging only.	Space–time	Only theory presented. Numerical results using this model are found in Chan *et al.* (2000).
N-K	Masuoka and Takatsu (1996), Kuwahara and Nakayama (1998), Takatsu and Masuoka (1998), Nakayama and Kuwahara (1999).	Masuoka and Takatsu (1996) assumed a non-null value in their Equation (11) for the turbulent shear stress $\mathbf{S}_i = -\rho\overline{\mathbf{u}'\mathbf{u}'}$ along the interfacial area A_i. Takatsu and Masuoka (1998) assume for their volume integral in Equation (14) a different from zero for $\mathbf{d} = (\mu_l/\rho + \mu_t/\sigma_k\rho)\nabla k$ at the interface A_i.	Time–space	Microscopic computations on periodic cell of square rods. Macroscopic model computations presented.
T-C	Gratton *et al.* (1994), Travkin and Catton (1992, 1995, 1998), Travkin *et al.* (1993, 1999).	Morphology-based theory. Surface integrals and volume average operators depend on media morphology.	Time–space	Only theory presented.
P-D	Pedras and de Lemos (2000a,b, 2001b), Rocamora and de Lemos (2000a).	Double-decomposition theory. Surface integrals involving null quantities at surfaces are neglected. The connection between *space–time* and *time–space* theories is unveiled.	Time–space	Microscopic computation on periodic cell of circular rods. Macroscopic computations for porous media presented. Results for hybrid domains are found in de Lemos and Pedras (2000b) and Rocamora and de Lemos (2000b,c,d).

Pore-scale problem

Time-averaged Navier-Stokes equations (k-epsilon example)

$$\nabla \cdot \overline{\mathbf{v}}_\alpha = 0 \ \text{ in } \mathcal{V}_\alpha,$$

$$\rho_\alpha \left(\frac{\partial \overline{\mathbf{v}}_\alpha}{\partial t} + \overline{\mathbf{v}}_\alpha \cdot \nabla \overline{\mathbf{v}}_\alpha \right) = -\nabla \left(\overline{p}_\alpha + \frac{2}{3}\rho k \right) + \rho_\alpha \mathbf{g} + \nabla \cdot \left(\left(\mu_{\alpha_{mol}} + \mu_{\alpha_{turb}}(\mathbf{r}) \right) \nabla \overline{\mathbf{v}}_\alpha \right) \ \text{ in } \mathcal{V}_\alpha,$$

$$\rho_\alpha \left(\frac{\partial k}{\partial t} + \overline{\mathbf{v}}_\alpha \cdot \nabla k \right) = \nabla \cdot \left(\left(\mu_{\alpha_{mol}} + \frac{\mu_{\alpha_{turb}}(\mathbf{r})}{\sigma_k} \right) \nabla k \right) + \mu_{\alpha_{turb}}(\mathbf{r}) \nabla \overline{\mathbf{v}}_\alpha : \nabla \overline{\mathbf{v}}_\alpha - \rho_\alpha \epsilon \ \text{ in } \mathcal{V}_\alpha,$$

$$\rho_\alpha \left(\frac{\partial \epsilon}{\partial t} + \overline{\mathbf{v}}_\alpha \cdot \nabla \epsilon \right) = \nabla \cdot \left(\left(\mu_{\alpha_{mol}} + \frac{\mu_{\alpha_{turb}}(\mathbf{r})}{\sigma_\epsilon} \right) \nabla \epsilon \right) + C_1 \frac{\epsilon^2}{k} \mu_{\alpha_{turb}}(\mathbf{r}) \nabla \overline{\mathbf{v}}_\alpha : \nabla \overline{\mathbf{v}}_\alpha - \rho_\alpha C_2 \frac{\epsilon^2}{k} \ \text{ in } \mathcal{V}_\alpha.$$

$$\mu_{\alpha_{turb}}(\mathbf{r}) = \rho_\alpha C_\mu \frac{k^2}{\epsilon}$$

Volume averaging the RANS problem : the pore scale problem

- We assume that all the turbulent information at pore-scale is included within an effective viscosity and a turbulent pressure
- Energy and dissipation equations are eliminated

$$\nabla \cdot \overline{\mathbf{v}}_\alpha = 0 \ \text{ in } \mathcal{V}_\alpha,$$

$$\rho_\alpha \frac{\partial \overline{\mathbf{v}}_\alpha}{\partial t} + \rho_\alpha \overline{\mathbf{v}}_\alpha \cdot \nabla \overline{\mathbf{v}}_\alpha = -\nabla \overline{p}^*_\alpha + \rho_\alpha \mathbf{g} + \nabla \cdot \left(\mu_\alpha(\mathbf{r}) \nabla \overline{\mathbf{v}}_\alpha \right) \ \text{ in } \mathcal{V}_\alpha,$$

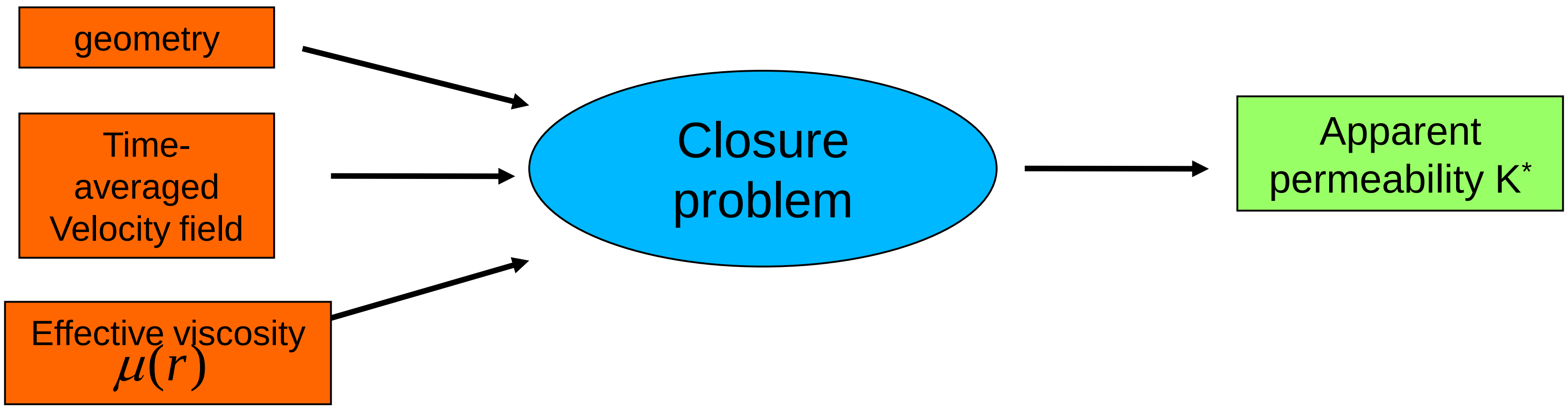
$$\overline{\mathbf{v}}_\alpha = 0 \ \text{ at } \mathcal{A}_{\sigma\alpha}.$$

Macro-scale model

Corresponding macroscale equation : a Darcy-Forchheimer's law

$$\langle \mathbf{v}_\alpha \rangle = -\frac{\mathbf{K}}{\mu_{\alpha_{mol}}}\cdot\left(\nabla\langle p_\alpha\rangle^\alpha - \rho_\alpha \mathbf{g}\right) - \mathbf{F}\cdot\langle \mathbf{v}_\alpha\rangle = -\frac{\mathbf{K}^*}{\mu_{\alpha_{mol}}}\cdot\left(\nabla\langle p_\alpha\rangle^\alpha - \rho_\alpha \mathbf{g}\right)$$

The volume averaging methodology provide a closure problem to evaluate the apparent permeability



Advantages :

- In agreement with experimental studies (Chauveteau & Thirriot 1967, structured packing literature..)
- The method allows the evaluation of all the tensor components
- Does not depend on the turbulent model of the pore-scale simulations (kE, RNG-kE, k-Omega…) but of the actual value of the viscosity field

Difference with Whitaker closure problem

Whitaker 1996	Present work

Closure relationships

Whitaker 1996:

$$\tilde{p}_\beta = \mu_\beta \mathbf{m} \cdot \langle \mathbf{v}_\beta \rangle^\beta$$

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

Present work:

$$\tilde{\mathbf{v}}_\alpha = \mathbf{B}_\alpha \cdot \langle \mathbf{v}_\alpha \rangle^\alpha \quad ; \quad \tilde{p}_\alpha = \mathbf{b}_\alpha \cdot \langle \mathbf{v}_\alpha \rangle^\alpha$$

Closure problem

Whitaker 1996:

$$(\rho_\beta \mathbf{v}_\beta / \mu_\beta) \cdot \nabla \mathbf{M} = -\nabla \mathbf{m} + \nabla^2 \mathbf{M} - \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\mathbf{I}\mathbf{m} + \nabla \mathbf{M})$$

$$\nabla \cdot \mathbf{M} = 0,$$

(B.C.1) $\mathbf{M} = -\mathbf{I}, \quad \text{at} \quad A_{\beta\sigma},$

Periodicity: $\mathbf{m}(\mathbf{r} + \ell_i) = \mathbf{m}(\mathbf{r}), \quad \mathbf{M}(\mathbf{r} + \ell_i) = \mathbf{M}(\mathbf{r}),$

Average: $\langle \mathbf{M} \rangle^\beta = 0.$

Present work:

$$\rho_\alpha \mathbf{v}_\alpha \cdot \nabla \mathbf{B}_\alpha = -\nabla \mathbf{b}_\alpha + \nabla \cdot (\mu_\alpha \nabla \mathbf{B}_\alpha) - \frac{\varepsilon_\alpha^{-1}}{V} \int_{\mathcal{A}_{\alpha\sigma}} \mathbf{n}_{\alpha\sigma} \cdot [-\mathbf{b}_\alpha \mathbf{I} + \mu_\alpha \nabla \mathbf{B}_\alpha] \, d\mathcal{A} \ \text{ in } \mathcal{V}_\alpha,$$

$$\nabla \cdot \mathbf{B}_\alpha = 0 \ \text{ in } \mathcal{V}_\alpha,$$

$$\mathbf{B}_\alpha = -\mathbf{I} \ \text{ at } \mathcal{A}_{\alpha\sigma},$$

$$\mathbf{B}_\alpha(\mathbf{r} + \mathbf{l}_i) = \mathbf{B}_\alpha(\mathbf{r}) \ ; \ \mathbf{b}_\alpha(\mathbf{r} + \mathbf{l}_i) = \mathbf{b}_\alpha(\mathbf{r}) \ ; \ i = 1, 2, 3,$$

$$\langle \mathbf{B}_\alpha \rangle^\alpha = \mathbf{0} \ ; \ \langle \mathbf{b}_\alpha \rangle^\alpha = 0.$$

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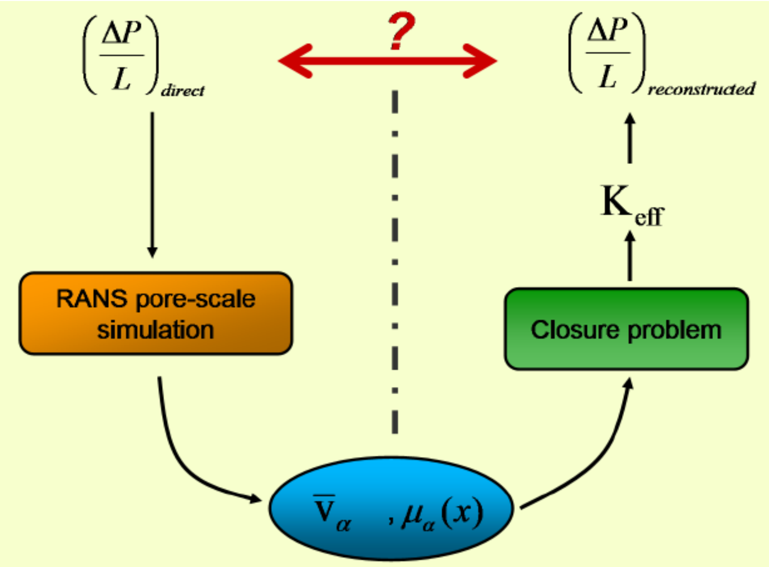
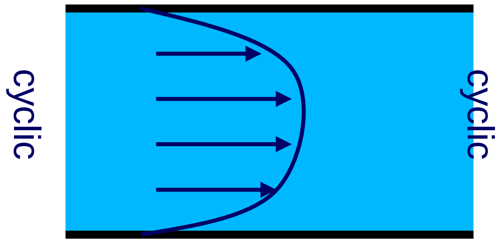
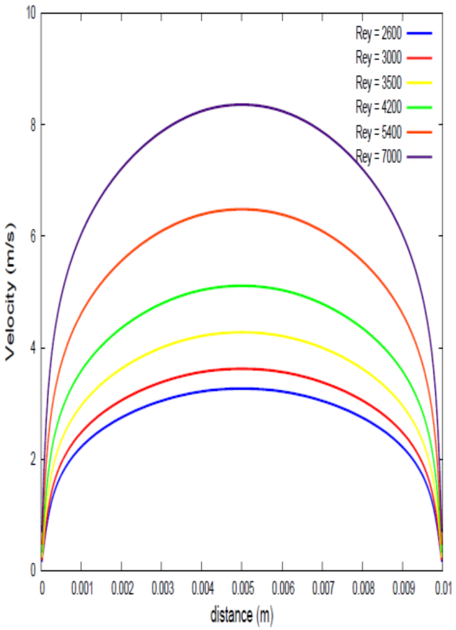
Conclusions

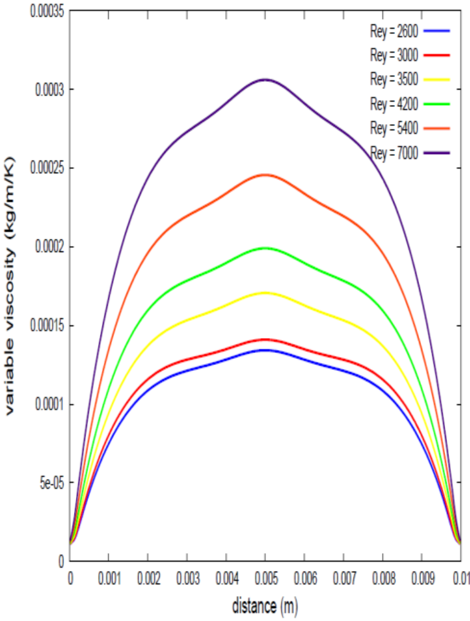
Validation : case of the tube

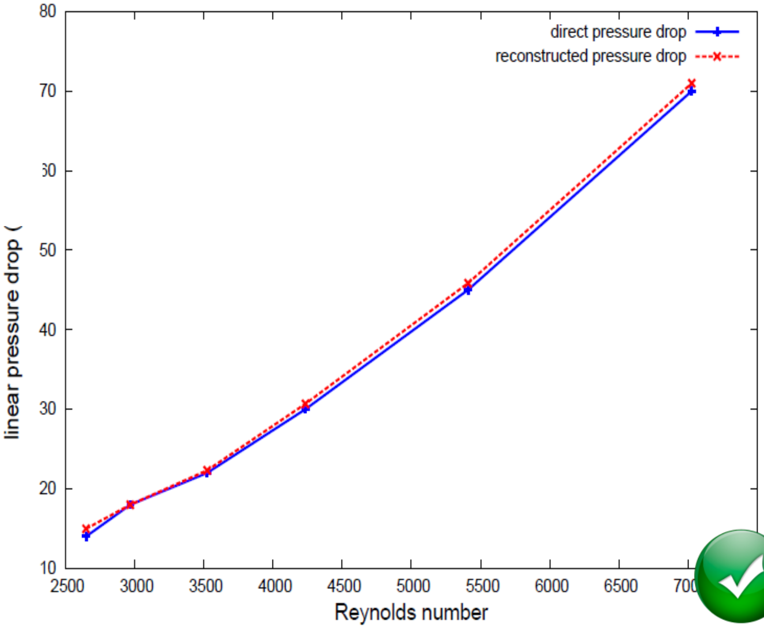




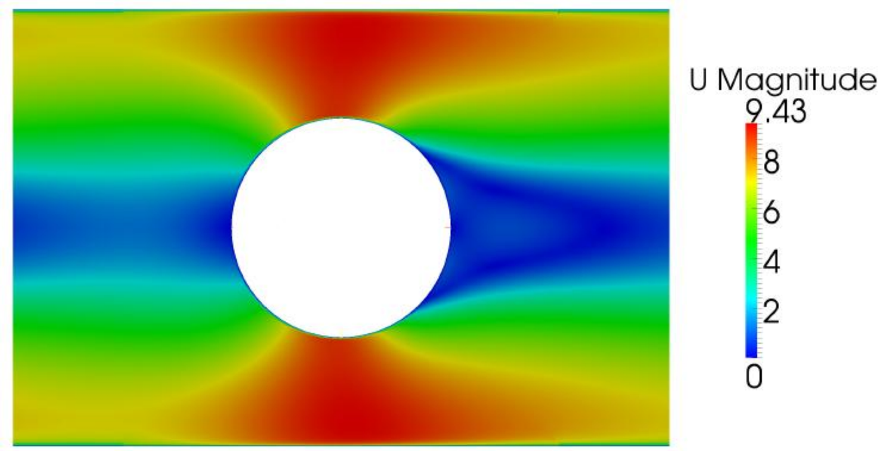
RANS simulations (kEpsilon)



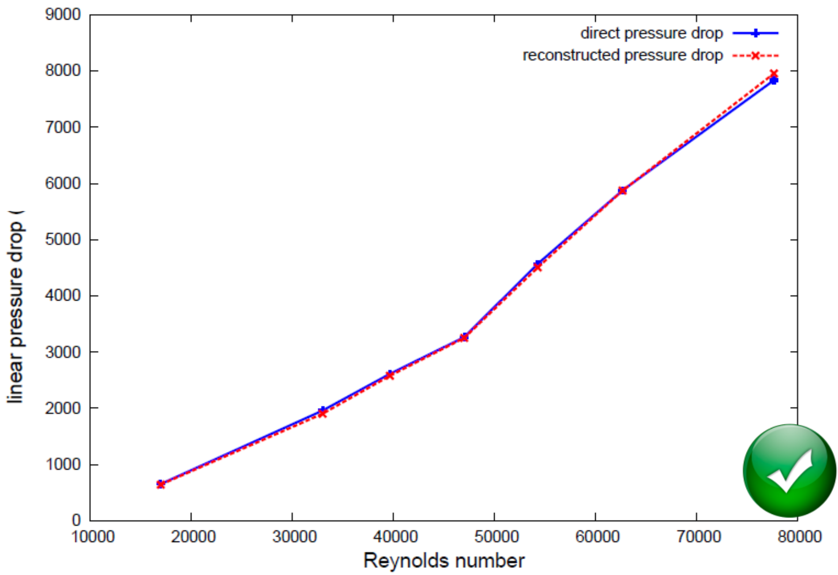


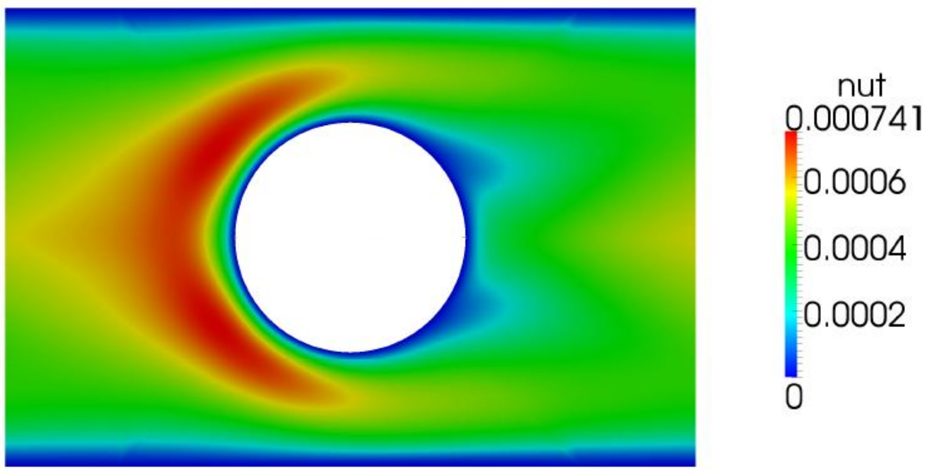


Validation : bead in a tube

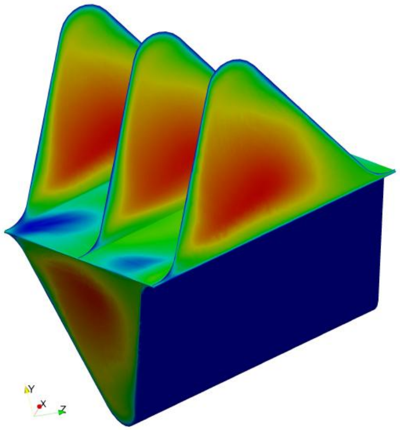


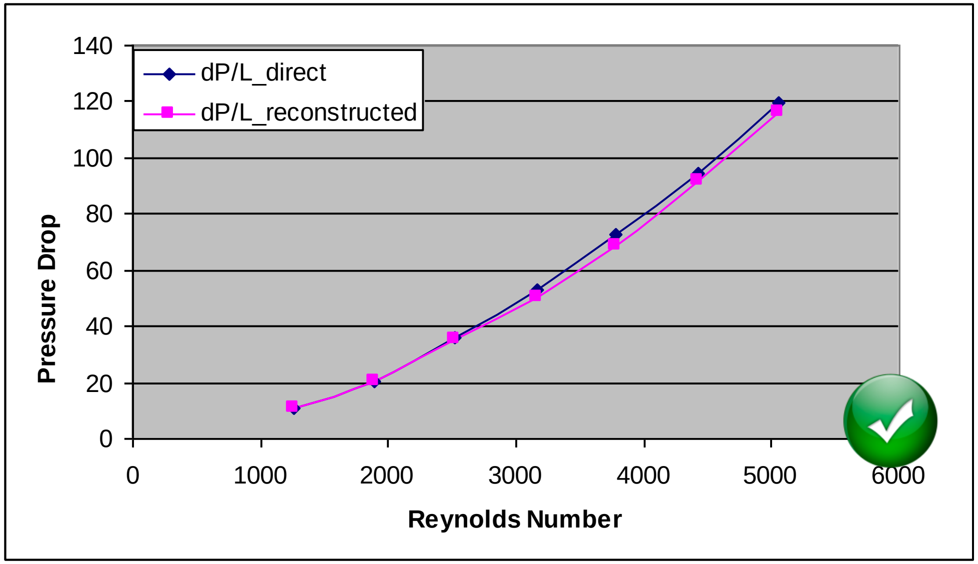
RANS simulations (RNG-kEpsilon)





Application to structured packing (1/2)

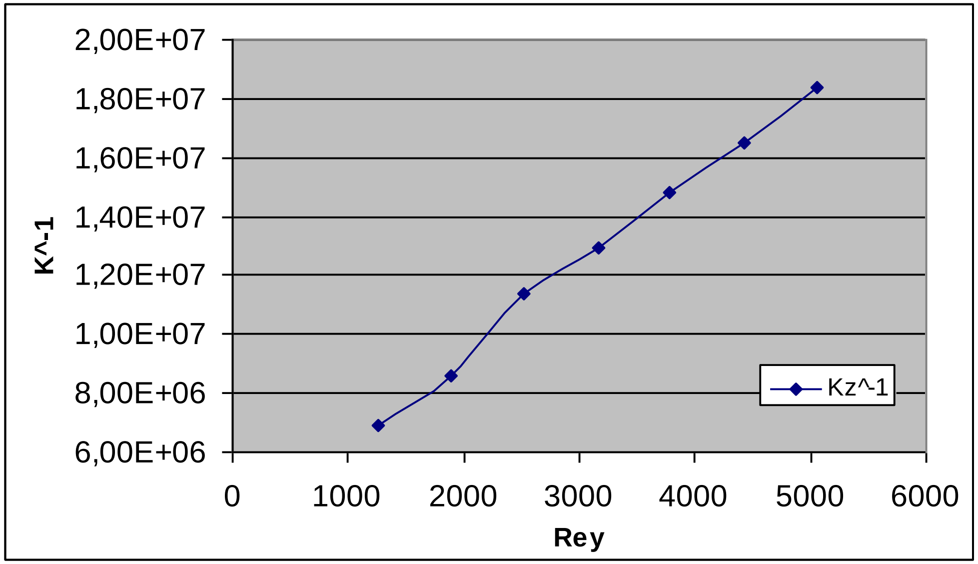




- RANS Simulations (kOmega SST which have proved to give good results (Rafati Saleh 2011, Said 2011…))

- For high Reynolds number, we find a Forchheimer correction that depends on the velocity square

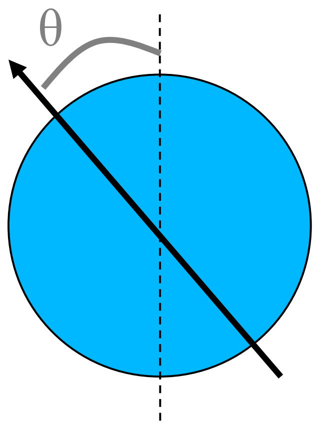
$$K_{yy} = \frac{K_1}{1+\beta \mathrm{Re}}$$

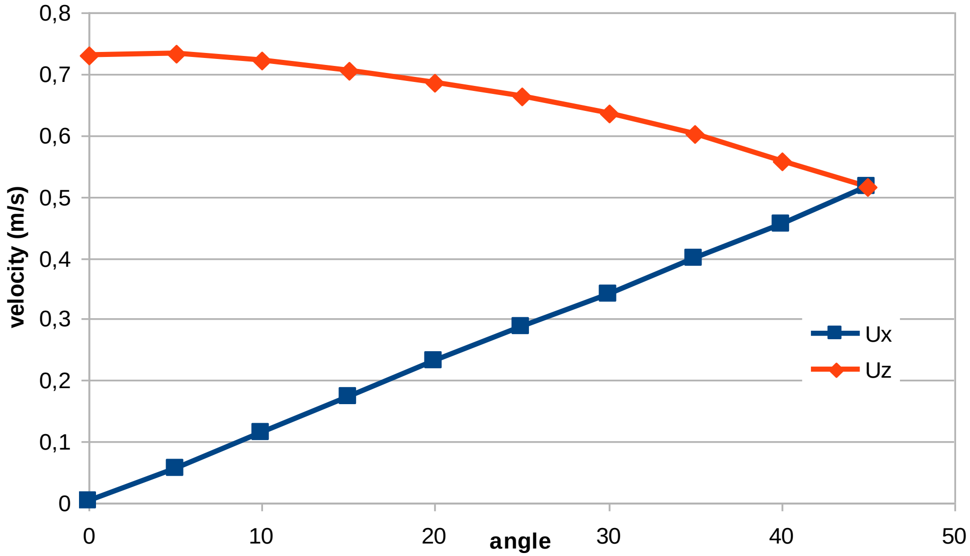


Application to structured packing (2/2)

1. Calculation of the pore scale velocity field for different flow direction (dP/L is fixed and correspond to Rey=4300)

$$\frac{\Delta P}{L}\begin{pmatrix}\sin\theta\\ \cos\theta\\ 0\end{pmatrix}$$

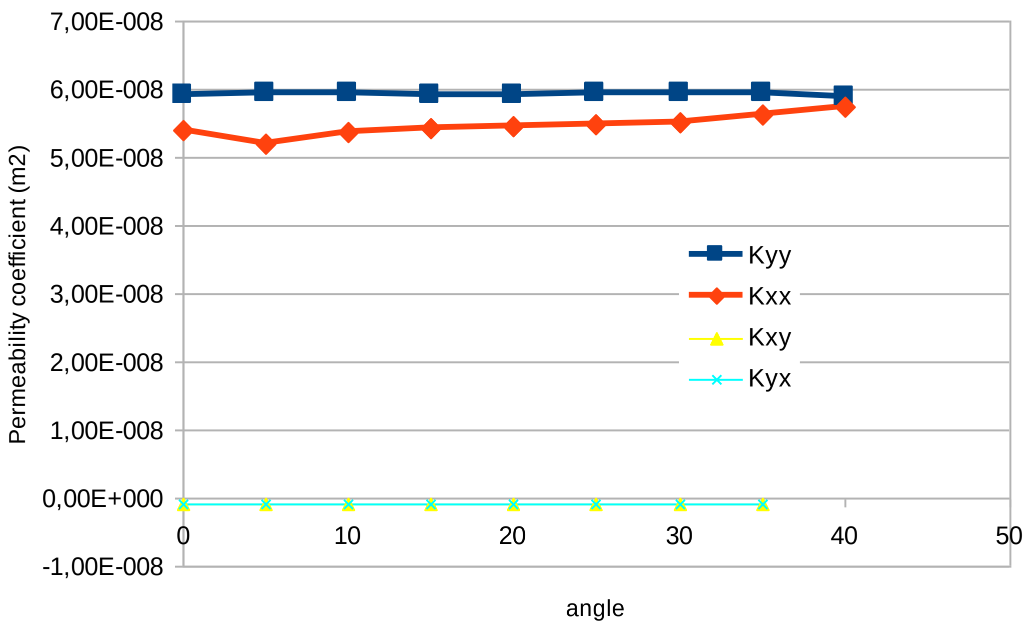




2. Resolution of the closure problem

- non-diagonal coefficients are negligible
- $K^*_{xx} \approx K^*_{yy}$ and do not strongly depend on the flow direction

$$\mathbf{K}^*(Re,\theta) \approx \begin{pmatrix} \frac{K_1}{1+\beta_t Re} & 0 & 0 \\ 0 & \frac{K_1}{1+\beta_t Re} & 0 \\ 0 & 0 & \infty \end{pmatrix}$$



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Conclusions

- We developed a methodology to interpret turbulent pore-scale simulations. Somehow, it is an extension of Whitaker 96

- With this method, the macroscopic flow is governed by a Darcy-Forchheimer-like law

- The method is independent of the tubulence model chosen for the pore-scale simulation. However the actual viscosity field may strongly depend on the turbulence model

- The method has been validated over 2D and 3D calculations

- We applied the methodology to investigate the macroscale behaviour of high Reynold's number flow in structured packing

Thank you for your attention.