AN EFFICIENT METHOD OF DETERMINATION OF THE KLINKENBERG CORRECTION FOR SLIP FLOW IN POROUS MEDIA

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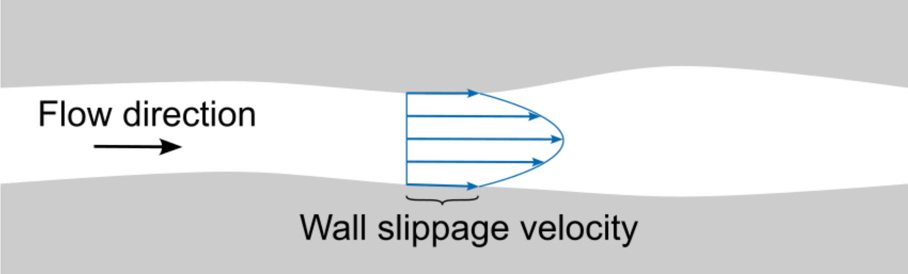
Rarefied gas flow in the slip regime



Slip flow is encountered, for instance

- For non-wetting fluids
- As an effective boundary conditions for flow over rough surfaces
- In rarefied gas flow, when KNUDSEN effects become significant
  - Geological gas storage & extraction, sealing, composite manufacturing…

Rarefied gas flow characterised by the KNUDSEN number

$$\mathrm{Kn} = \frac{\lambda}{\ell}$$

← Gas mean free path ($\propto 1/\rho$)
← Characteristic size (pore size)

For $\mathrm{Kn} \leq \mathcal{O}(10^{-1})$, the flow is in the slip regime

- Flow modelled using NAVIER-STOKES equations with first-order slip boundary condition at the walls
  - $\mathcal{O}(\mathrm{Kn})$ approximation to the BOLTZMANN equation

One-phase microscopic slip flow model

Pore-scale microscopic flow model (slightly compressible, isothermal, creeping flow)

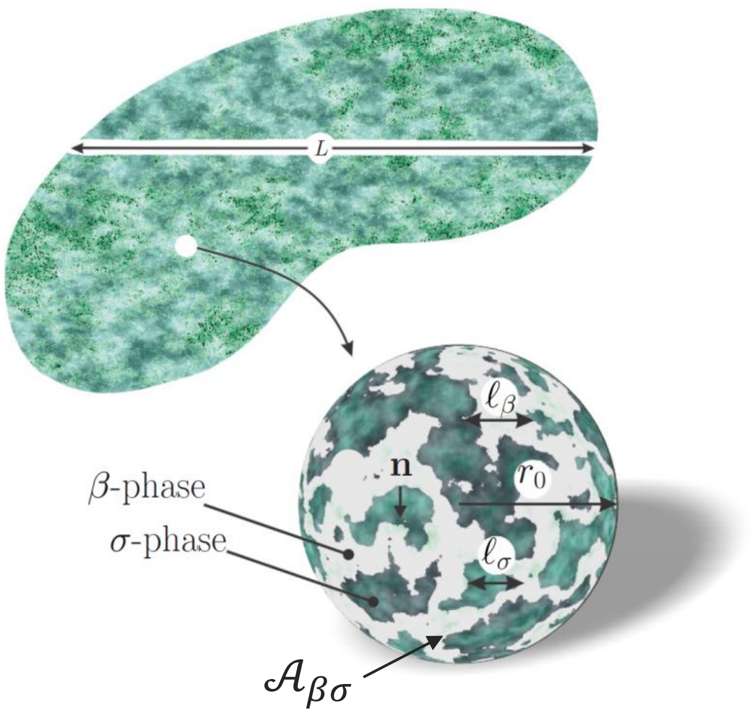
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0 \qquad \text{in } \mathcal{V}_\beta \qquad (1.1)$$

$$-\nabla p + \mu \nabla^2 \boldsymbol{v} = 0 \qquad \text{in } \mathcal{V}_\beta \qquad (1.2)$$

$$\rho = \varphi(p) \qquad \text{in } \mathcal{V}_\beta \qquad (1.3)$$

Slip BC

$$\boldsymbol{v} = -\xi\lambda \mathbf{P} \cdot \left(\boldsymbol{n} \cdot \left(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^{\mathrm{T}}\right)\right) \qquad \text{on } \mathcal{A}_{\beta\sigma} \qquad (1.4)$$



with

- $\mathbf{P} = \mathbf{I} - \boldsymbol{nn}$ the tangential projection tensor ($\mathbf{P} = \mathbf{P}^{\mathrm{T}} \geq 0, \quad \mathbf{P} = \mathbf{P} \cdot \mathbf{P}$)
- ξ the accommodation coefficient of the gas at the walls
- $\xi\lambda$ is identified as local slip length
  - For other slip mechanisms (non wetting flow, effective BC over rough surface): generally replaced by a slip length l.

Lasseux et al., *Phys. Fluids*, **26**, 053102 (2014)

Macroscopic flow model with slip

Definition of averaging operators

Porosity

$$\langle \bullet \rangle^\beta = \frac{1}{V_\beta} \int_{\mathcal{V}_\beta} \bullet \, \mathrm{d}V \qquad \langle \bullet \rangle = \frac{1}{V} \int_{\mathcal{V}_\beta} \bullet \, \mathrm{d}V = \varepsilon \langle \bullet \rangle^\beta$$

After upscaling, considering slightly compressible flow ($\rho \approx \langle \rho \rangle^\beta$, $\lambda \approx \bar{\lambda} \propto 1/\langle \rho \rangle^\beta$), we obtain

Macroscopic model

$$\varepsilon \frac{\partial \langle \rho \rangle^\beta}{\partial t} + \boldsymbol{\nabla} \cdot \left(\langle \rho \rangle^\beta \langle \boldsymbol{v} \rangle \right) = 0 \qquad (2.1)$$

$$\langle \boldsymbol{v} \rangle = -\frac{\mathbf{K}}{\mu} \cdot \boldsymbol{\nabla} \langle p \rangle^\beta \qquad (2.2)$$

$$\langle \rho \rangle^\beta = \varphi\left(\langle p \rangle^\beta \right) \qquad (2.3)$$

Unit cell closure problem

$\boldsymbol{\nabla} \cdot \mathbf{D} = \mathbf{0}$	in $\mathcal{V}_\beta$	(3.1)
$\boldsymbol{\nabla} \cdot \mathbf{S} + \mathbf{I} = \mathbf{0}$	in $\mathcal{V}_\beta$	(3.2)
$\mathbf{S} = -\mathbf{I}\boldsymbol{d} + \boldsymbol{\nabla}\mathbf{D} + \boldsymbol{\nabla}\mathbf{D}^{\mathrm{T}_{12}}$	in $\mathcal{V}_\beta$	(3.3)
$\mathbf{D} = -\xi \bar{\lambda} \mathbf{P} \cdot (\boldsymbol{n} \cdot \mathbf{S})$	on $\mathcal{A}_{\beta\sigma}$	(3.4)
$\boldsymbol{d}, \mathbf{D}$ periodic, $\langle \boldsymbol{d} \rangle = \mathbf{0}$		(3.5)
$\mathbf{K} = \langle \mathbf{D} \rangle$	Dependence on $\xi \bar{\lambda}$	(3.6)

Apparent permeability tensor

It can be shown that $\mathbf{K}$ is symmetric and positive definite.

Lasseux et al., *J. Fluid Mech.*, **805**, 118-146 (2016) ; Lasseux et al., *J. Fluid Mech.*, **923**, A37 (2021)

Viscous and slip contributions

To isolate purely viscous effects from slip effects, power series in $\xi\bar{\lambda}$ are proposed as

$$\boldsymbol{d} = \sum_{j=0}^{+\infty} \boldsymbol{d}_j (\xi\bar{\lambda})^j \qquad \mathbf{D} = \sum_{j=0}^{+\infty} \mathbf{D}_\mathrm{j} (\xi\bar{\lambda})^j \qquad \mathbf{K} = \sum_{j=0}^{+\infty} \mathbf{K}_\mathrm{j} (\xi\bar{\lambda})^j = \mathbf{K_0} + \xi\bar{\lambda}\mathbf{K_1} + (\xi\bar{\lambda})^2 \mathbf{K_2} + \cdots$$

Identification at the different orders leads to sequentially coupled, intrinsic, closure problems

For $j = 0$

$\boldsymbol{\nabla}\cdot\mathbf{D_0} = \mathbf{0}$	in $\mathcal{V}_\beta$	(4.1)
$\boldsymbol{\nabla}\cdot\mathbf{S_0} + \mathbf{I} = \mathbf{0}$	in $\mathcal{V}_\beta$	(4.2)
$\mathbf{S_0} = -\mathbf{I}\boldsymbol{d}_0 + \boldsymbol{\nabla}\mathbf{D_0} + \boldsymbol{\nabla}\mathbf{D}_0^{\mathrm{T}_{12}}$	in $\mathcal{V}_\beta$	(4.3)
$\mathbf{D_0} = \mathbf{0}$	on $\mathcal{A}_{\beta\sigma}$	(4.4)
$\boldsymbol{d}_0, \mathbf{D_0}$ periodic, $\langle \boldsymbol{d}_0 \rangle = \mathbf{0}$		(4.5)
$\mathbf{K_0} = \langle \mathbf{D_0} \rangle$		(4.6)

Intrinsic permeability tensor (no-slip)

For $j \geq 1$

$\boldsymbol{\nabla}\cdot\mathbf{D_j} = \mathbf{0}$	in $\mathcal{V}_\beta$	(5.1)
$\boldsymbol{\nabla}\cdot\mathbf{S_j} = \mathbf{0}$	in $\mathcal{V}_\beta$	(5.2)
$\mathbf{S_j} = -\mathbf{I}\boldsymbol{d}_j + \boldsymbol{\nabla}\mathbf{D_j} + \boldsymbol{\nabla}\mathbf{D}_j^{\mathrm{T}_{12}}$	in $\mathcal{V}_\beta$	(5.3)
$\mathbf{D_j} = -\mathbf{P}\cdot(\boldsymbol{n}\cdot\mathbf{S_{j-1}})$	on $\mathcal{A}_{\beta\sigma}$	(5.4)
$\boldsymbol{d}_j, \mathbf{D_j}$ periodic, $\langle \boldsymbol{d}_j \rangle = \mathbf{0}$		(5.5)
$\mathbf{K_j} = \langle \mathbf{D_j} \rangle$	Coupling	(5.6)

j^{th} order slip correction tensor

Alternative expressions of the correction tensors

Up to now, we have sequentially coupled intrinsic closure problems

- To obtain the j^{th} order correction: need to solve for $j+1$ problems
- Potentially time consuming
- Prone to propagation of numerical errors

☝ Alternative expressions for $\mathbf{K_j}$ are hoped for

Considering the following GREEN reciprocity formula

$$\int_{\mathcal{V}_\beta} \mathbf{D_p}^{\mathrm{T}} \cdot (\nabla \cdot \mathbf{S_q}) - (\nabla \cdot \mathbf{S_p})^{\mathrm{T}} \cdot \mathbf{D_q} \,\mathrm{d}V = \int_{\mathcal{A}_{\beta\sigma}} \mathbf{D_p}^{\mathrm{T}} \cdot (\boldsymbol{n} \cdot \mathbf{S_q}) - (\boldsymbol{n} \cdot \mathbf{S_p})^{\mathrm{T}} \cdot \mathbf{D_q} \,\mathrm{d}A$$

Letting $p = 0$ and $q = j$, we obtain

Using transpose of slip BC (5.4)

$$\mathbf{K_j} = -\frac{1}{V} \int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n} \cdot \mathbf{S_0})^{\mathrm{T}} \cdot \underbrace{\mathbf{D_j}} \,\mathrm{d}A = \frac{1}{V} \int_{\mathcal{A}_{\beta\sigma}} \overbrace{(\boldsymbol{n} \cdot \mathbf{S_0})^{\mathrm{T}}} \cdot \underbrace{\mathbf{P} \cdot (\boldsymbol{n} \cdot \mathbf{S_{j-1}})} \mathrm{d}A = -\frac{1}{V} \int_{\mathcal{A}_{\beta\sigma}} \overbrace{\mathbf{D_1}^{\mathrm{T}}} \cdot (\boldsymbol{n} \cdot \mathbf{S_{j-1}}) \,\mathrm{d}A$$

Using slip BC (5.4)

Lasseux et al., *Phys. Rev. Fluids*, **8**, 053401 (2023)

Alternative expressions of the correction tensors

For $p, q \neq 0$, the volume integral in GREEN's formula is identically zero ($\boldsymbol{S}_\mathbf{j}$ are solenoidal), giving

$$\int_{\mathcal{A}_{\beta\sigma}} \mathbf{D_p}^\mathrm{T} \cdot (\boldsymbol{n} \cdot \mathbf{S_q})\,\mathrm{d}A = \int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n} \cdot \mathbf{S_p})^\mathrm{T} \cdot \mathbf{D_q}\,\mathrm{d}A$$

Using $p = 1$ et $q = j - 1$, we obtain

$$\mathbf{K_j} = -\frac{1}{V} \int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n} \cdot \mathbf{S_0})^\mathrm{T} \cdot \mathbf{D_j}\,\mathrm{d}A = -\frac{1}{V} \int_{\mathcal{A}_{\beta\sigma}} \mathbf{D_1}^\mathrm{T} \cdot (\boldsymbol{n} \cdot \mathbf{S_{j-1}})\,\mathrm{d}A = -\frac{1}{V} \int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n} \cdot \mathbf{S_1})^\mathrm{T} \cdot \mathbf{D_{j-1}}\,\mathrm{d}A$$

Repeating the process recursively until $p = q = \lfloor j/2 \rfloor$, we finally obtain

$$\mathbf{K_j} = \begin{cases} -\dfrac{1}{V} \displaystyle\int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n} \cdot \mathbf{S}_{j/2})^\mathrm{T} \cdot \mathbf{D}_{j/2}\,\mathrm{d}A & j \text{ even} \\ \dfrac{1}{V} \displaystyle\int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n} \cdot \mathbf{S}_{(j-1)/2})^\mathrm{T} \cdot \mathbf{P} \cdot (\boldsymbol{n} \cdot \mathbf{S}_{(j-1)/2})\mathrm{d}A & j \text{ odd} \end{cases} \tag{6}$$

Alternative expressions of the correction tensors

This gives for the first few tensors $\mathbf{K_j}$

$$\mathbf{K_0} = \frac{1}{V}\int_{\mathcal{V}_\beta} \mathbf{D_0}\,\mathrm{d}V \qquad \mathbf{K_1} = \frac{1}{V}\int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n}\cdot\mathbf{S_0})^{\mathrm{T}}\cdot\mathbf{P}\cdot(\boldsymbol{n}\cdot\mathbf{S_0})\mathrm{d}A$$

Requires only solution to 0th order closure

$$\mathbf{K_2} = -\frac{1}{V}\int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n}\cdot\mathbf{S_1})^{\mathrm{T}}\cdot\mathbf{D_1}\,\mathrm{d}A \qquad \mathbf{K_3} = \frac{1}{V}\int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n}\cdot\mathbf{S_1})^{\mathrm{T}}\cdot\mathbf{P}\cdot(\boldsymbol{n}\cdot\mathbf{S_1})\mathrm{d}A$$

Requires only solution to 1st order closure

Each closure problem now provides 2 slip correction tensors!

- Computational expense divided by 2 to reach a given correction order

Specifically, KLINKENBERG's correction (1st order truncation, $\mathbf{K} \approx \mathbf{K_0} + \xi\bar{\lambda}\mathbf{K_1}$) can be obtained by solving the no-slip 0th order closure only!

Lasseux et al., *Phys. Rev. Fluids*, **8**, 053401 (2023)

Properties of the correction tensors

We have the following equivalent expressions for $j \geq 1$

$$\mathbf{K_j} = \begin{cases} -\frac{1}{V}\int_{\mathcal{V}_\beta} \frac{1}{2}\left(\nabla\mathbf{D_{j/2}} + \nabla\mathbf{D}_{j/2}^{\mathrm{T}_{12}}\right)^{\mathrm{T}_{13}} : \left(\nabla\mathbf{D_{j/2}} + \nabla\mathbf{D}_{j/2}^{\mathrm{T}_{12}}\right) \mathrm{d}V & j \text{ even} \\ \frac{1}{V}\int_{\mathcal{A}_{\beta\sigma}} \left(\boldsymbol{n}\cdot\mathbf{S}_{(j-1)/2}\right)^{\mathrm{T}} \cdot \mathbf{P} \cdot \left(\boldsymbol{n}\cdot\mathbf{S}_{(j-1)/2}\right)\mathrm{d}A & j \text{ odd} \end{cases} \tag{7}$$

⟵ Integrand of the form $\mathbf{A}^{\mathrm{T}_{13}} : \mathbf{A}$ (j even)

⟵ Integrand of the form $\mathbf{A}^{\mathrm{T}} \cdot \mathbf{A}$ (j odd)

For the first few tensors, we have

$$\mathbf{K_0} = +\frac{1}{V}\int_{\mathcal{V}_\beta} \frac{1}{2}\left(\nabla\mathbf{D_0} + \nabla\mathbf{D}_0^{\mathrm{T}_{12}}\right)^{\mathrm{T}_{13}} : \left(\nabla\mathbf{D_0} + \nabla\mathbf{D}_0^{\mathrm{T}_{12}}\right)\mathrm{d}V \qquad \mathbf{K_1} = +\frac{1}{V}\int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n}\cdot\mathbf{S_0})^{\mathrm{T}} \cdot \mathbf{P} \cdot (\boldsymbol{n}\cdot\mathbf{S_0})\mathrm{d}A$$

$$\mathbf{K_2} = -\frac{1}{V}\int_{\mathcal{V}_\beta} \frac{1}{2}\left(\nabla\mathbf{D_1} + \nabla\mathbf{D}_1^{\mathrm{T}_{12}}\right)^{\mathrm{T}_{13}} : \left(\nabla\mathbf{D_1} + \nabla\mathbf{D}_1^{\mathrm{T}_{12}}\right)\mathrm{d}V \qquad \mathbf{K_3} = +\frac{1}{V}\int_{\mathcal{A}_{\beta\sigma}} (\boldsymbol{n}\cdot\mathbf{S_1})^{\mathrm{T}} \cdot \mathbf{P} \cdot (\boldsymbol{n}\cdot\mathbf{S_1})\mathrm{d}A$$

Which proves that

- All $\mathbf{K_j}$ are symmetric
- and form an alternate series for $j \geq 1$ ($\mathbf{K_j} \leq 0$ for j even, $\mathbf{K_j} \geq 0$ for j odd)

PADÉ approximant

Having the power series for $\mathbf{K}$ at hand, we propose to construct the PADÉ approximant, $\widetilde{\mathbf{K}}_{(1,1)}$

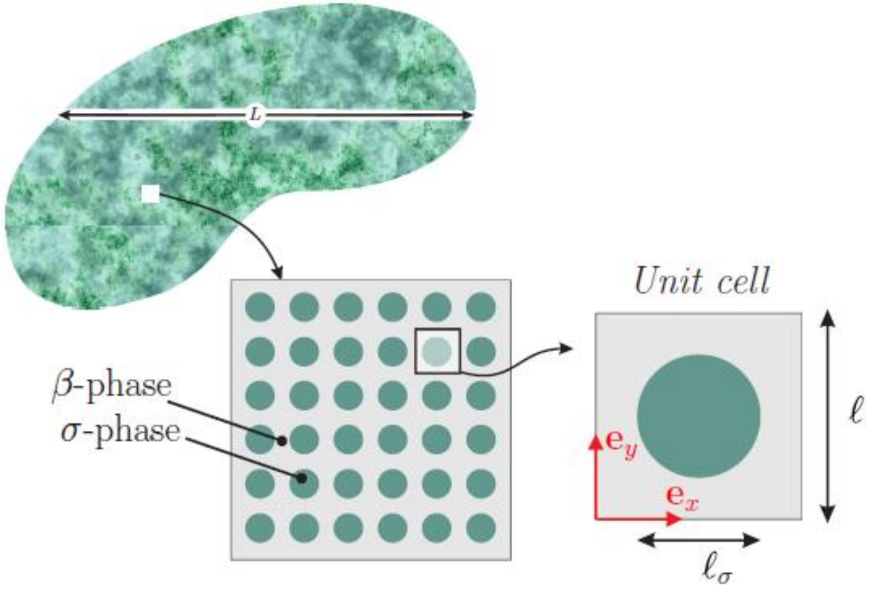
- From the solutions of the first 2 closure problems only (providing $\mathbf{K}_0$, $\mathbf{K}_1$, $\mathbf{K}_2$, $\mathbf{K}_3$)
- Same expansion as the power series up to order 2 in $\xi\bar{\lambda}$
- Constant asymptotic behaviour as $\xi\bar{\lambda} \to +\infty$ (perfect slip) Lasseux *et al.*, *J. Fluid Mech.* **997**, A65 (2024)
- Better extrapolation properties than a polynomial

$$\widetilde{\mathbf{K}}_{(1,1)} = \underbrace{\left(\mathbf{K}_0 + \xi\bar{\lambda}\left(\mathbf{K}_1 - \mathbf{K}_0 \cdot \mathbf{K}_1^{-1} \cdot \mathbf{K}_2\right)\right)}_{\text{“Numerator”}} \cdot \underbrace{\left(\mathbf{I} - \xi\bar{\lambda}\mathbf{K}_1^{-1} \cdot \mathbf{K}_2\right)}_{\text{“Denominator”}}{}^{-1}$$

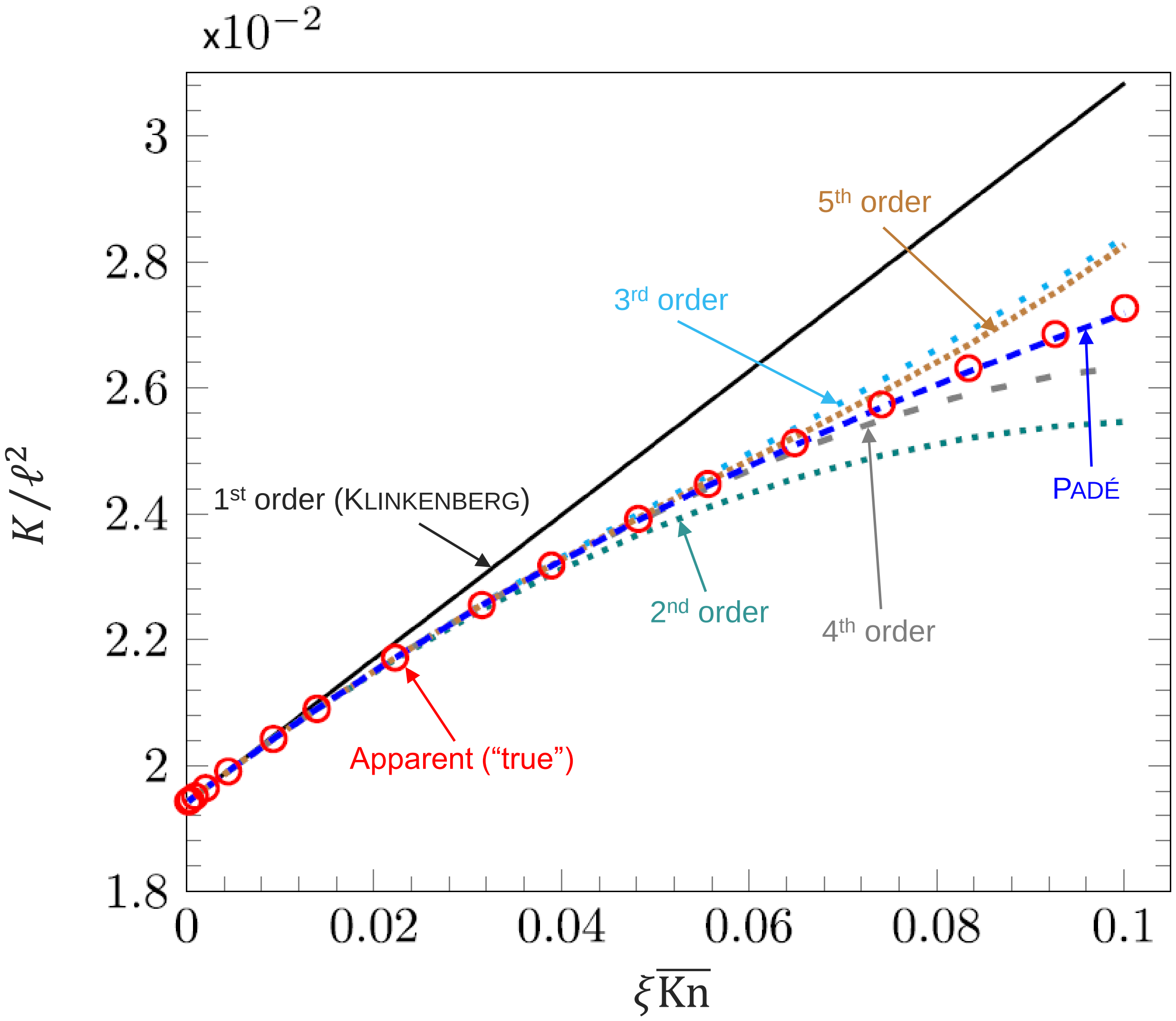
$\widetilde{\mathbf{K}}_{(1,1)}$ is symmetric

Numerical example

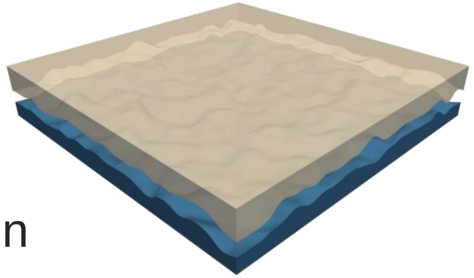
Consider the bundle of cylinders



$$\varepsilon = 0.8, \quad \overline{\mathrm{Kn}} = \frac{\bar{\lambda}}{\ell_\beta}, \quad \ell_\beta = \sqrt{\frac{12K_0}{\varepsilon}}$$



Case of a rough fracture



After upscaling, we obtain the macroscopic 2D REYNOLDS equation

2D porosity

Macroscopic model

$$\varepsilon_\beta \langle h \rangle \frac{\partial \langle \rho \rangle^\beta}{\partial t} + \boldsymbol{\nabla} \cdot \langle \boldsymbol{q} \rangle = 0 \qquad (8.1)$$

$$\langle \boldsymbol{q} \rangle = -\langle \rho \rangle^\beta \frac{\mathbf{K}}{\mu} \cdot \boldsymbol{\nabla} \langle p \rangle^\beta \qquad (8.2)$$

$$\langle \rho \rangle^\beta = \varphi\left(\langle \rho \rangle^\beta\right) \qquad (8.3)$$

Unit cell closure problem

$$\boldsymbol{\nabla} \cdot \mathbf{F} = \mathbf{0} \quad \text{in } \mathcal{A}_\beta \qquad (9.1)$$

$$\mathbf{F} = \bar{k}(\mathbf{I} + \boldsymbol{\nabla} \boldsymbol{b}) \quad \text{in } \mathcal{A}_\beta \qquad (9.2)$$

$$\bar{k} = k_0 + 6\xi\bar{\lambda}k_1 \quad \text{in } \mathcal{A}_\beta \qquad (9.3)$$

$$\boldsymbol{n} \cdot \mathbf{F} = \mathbf{0} \quad \text{on } \mathcal{C}_{\beta\sigma} \qquad (9.4)$$

$$\boldsymbol{b} \text{ periodic, } \langle \boldsymbol{b} \rangle = \mathbf{0} \qquad (9.5)$$

$$\mathbf{K} = \langle \mathbf{F} \rangle \qquad (9.6)$$

Apparent transmissivity tensor

With $\boldsymbol{b} = \boldsymbol{b}_0 + 6\xi\bar{\lambda}\boldsymbol{b}_1 + \left(6\xi\bar{\lambda}\right)^2 \boldsymbol{b}_2 + \cdots$ $\qquad \mathbf{K} = \mathbf{K}_0 + 6\xi\bar{\lambda}\mathbf{K}_1 + \left(6\xi\bar{\lambda}\right)^2 \mathbf{K}_2 + \cdots$

We are able to obtain

$$\mathbf{K}_0 = \left\langle k_0 (\mathbf{I} + \boldsymbol{\nabla} \boldsymbol{b}_0)^{\mathrm{T}} \cdot (\mathbf{I} + \boldsymbol{\nabla} \boldsymbol{b}_0) \right\rangle \qquad \mathbf{K}_1 = \left\langle k_1 (\mathbf{I} + \boldsymbol{\nabla} \boldsymbol{b}_0)^{\mathrm{T}} \cdot (\mathbf{I} + \boldsymbol{\nabla} \boldsymbol{b}_0) \right\rangle$$

$$\mathbf{K}_{\mathbf{j}} = \begin{cases} -\left\langle k_0 \boldsymbol{\nabla} \boldsymbol{b}_{j/2}{}^{\mathrm{T}} \cdot \boldsymbol{\nabla} \boldsymbol{b}_{j/2} \right\rangle, & j \text{ even} \\ \left\langle k_1 \boldsymbol{\nabla} \boldsymbol{b}_{(j-1)/2}{}^{\mathrm{T}} \cdot \boldsymbol{\nabla} \boldsymbol{b}_{(j-1)/2} \right\rangle, & j \text{ odd} \end{cases}, \qquad j \geq 2$$

(almost) perfect analogy with 3D porous media case

Zaouter et al., *J. Fluid Mech.*, **969**, A9 (2023)

Conclusion

- Each closure problem gives access to 2 slip correction tensors
- Solving the first n closure problems provide $2n$ permeability and slip correction tensors $(\mathbf{K_0}, \mathbf{K_1}, \cdots, \mathbf{K_{2n-1}})$
- KLINKENBERG's model can be obtained from the intrinsic no-slip 0^{th} order closure problem only!
- All tensors are symmetric and alternatively positive and negative definite, forming an alternate series
- PADÉ approximant can be built upon the power series to better capture the dependence of $\mathbf{K}$ with $\xi\overline{\mathrm{Kn}}$

References

Porous case

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Fracture case

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Thank you for your attention!

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