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Non-Newtonian Flows in Porous Media: upscaling problems

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https://www.dropbox.com/s/mcgg0ifpogsznv2/non_newtonian_V00.pdf?dl=0
Objective/Outline

- **Motivation:** flow of polymer solutions, question about heuristic models in Res. Engng
- **Upscaling**
  - Introduction (generalized Stokes)
  - Transition
  - Induced anisotropy, effect of disorder, effect of size of the UC, ...
- **Further problems:** exclusion zone, viscoelastic
- **Conclusions**
Multi-Scale Analysis

- Sequential multi-scale pattern
- Used in DRP, Res. Engng, Hydro., etc...
- Objectives of macro-scale theories:
  - Smoothing operator $\langle . \rangle \rightarrow$ Macro variables, Eqs & BCs
  - Micro-macro link $\rightarrow$
    Determination of Effective Properties
- Needs Scale Separation:
  $$l_\beta, l_\sigma \ll \text{REV?} \ll L$$
  (process dependent)
Multi-Scale Analysis: Upscaling Techniques

- **Form of the equations?**
  - averaging and TIP (Marle, Gray, Hassanizadeh, ...)
  - averaging and closure (Whitaker, ...)
  - homogenization (Bensoussan et al., Sanchez-Palencia, Tartar, ...), also “closure”
  - stochastic approaches (Dagan, Gelhar, ...)

- **Effective properties calculations?**
  - Assuming the form of Eqs: interpret experiments or DNS
  - Upscaling with “closure” (averaging, homogenization, stochastic): provides local Unit Cell problems

- **Many Open Problems**: High non-linearities, Strong couplings, Evolving pore-scale structure, ...
A simple introduction to upscaling with “closure”

\[ \nabla \cdot (k(x) \nabla \langle c \rangle) = 0 \]

Closure:

\[ \bar{c} = b \cdot \nabla \langle c \rangle + O(\ell^2/L^2) \]

\[ \nabla \cdot (k \cdot \nabla b) = -\nabla \cdot \bar{k} \]

\[ \nabla \cdot (k \nabla \bar{c}) = -\nabla \cdot (\bar{k} \nabla \langle c \rangle) + \nabla \langle k \nabla \bar{c} \rangle \]

Macro-scale Equation

\[ \nabla \left( K_{eff} \nabla \langle c \rangle \right) = 0 \]

Effective property

\[ K_{eff} = \langle k \rangle + \langle k \cdot \nabla b \rangle \]

- Tomography
- Reconstruction
- Geostatistics
- ...
Flow of a non-Newtonian fluid

Case of Generalized Stokes equation

- **Pore-Scale problem (Re~0)**

\[ \nabla \cdot \left[ \mu_\beta (\dot{\gamma}) \left( \nabla v_\beta + ^T \left( \nabla v_\beta \right) \right) \right] - \nabla p_\beta + \rho_\beta g = 0 \quad \text{in } V_\beta \]
\[ \nabla \cdot v_\beta = 0 \text{ in } V_\beta ; \quad n_\beta \sigma \cdot v_\beta = 0 \text{ at } A_\beta \sigma \]

**Rheology:**

\[ \mu_\beta = \mu_0 \hat{\mu} (\dot{\gamma}) \quad \dot{\gamma} = \frac{1}{2} \left( \nabla v_\beta + ^T \left( \nabla v_\beta \right) \right) : \left( \nabla v_\beta + ^T \left( \nabla v_\beta \right) \right) \]

- **Upscaling:** (vol. aver. \( \langle \psi_\beta \rangle = \hat{\epsilon}_\beta \langle \psi_\beta \rangle^\beta \) with \( \hat{\epsilon}_\beta = V_\beta / V \))?

\[ p_\beta = \langle p_\beta \rangle^\beta + \tilde{p}_\beta ; \quad v_\beta = \langle v_\beta \rangle^\beta + \tilde{v}_\beta \]
Typical local (over a REV) features

\[ \nabla \langle v_\beta \rangle \approx 0 \]
\[ \nabla \langle p_\beta \rangle^\beta - \rho_\beta g \approx \text{Constant} \]

Remark (far from BCs)

\[ \langle v_\beta \rangle = -K_{\text{gen}} \left( \langle v_\beta \rangle \right) \cdot \left( \nabla \langle p_\beta \rangle^\beta - \rho_\beta g \right) \]

\[ \nabla p_\beta - \rho_\beta g = \nabla \tilde{p}_\beta + \nabla \langle p_\beta \rangle^\beta - \rho_\beta g \]

constant \( h \)

velocity

viscosity

Pressure dev.

30°
Upscaling flow of a non-Newtonian fluid

- Averaging (vol. aver. $\langle \psi_\beta \rangle = \varepsilon_\beta \langle \psi_\beta \rangle$ with $\varepsilon_\beta = V_\beta / V$)

\[
\nabla \langle v_\beta \rangle = 0
\]

\[
macro \begin{cases}
- \varepsilon_\beta \left( \nabla \langle p_\beta \rangle - \rho_\beta g \right) + \frac{1}{V} \int_{A_{\beta\sigma}} n_{\beta\sigma} \cdot \left[ \mu_\beta \left( \tilde{\gamma} \right) \left( \nabla \tilde{v}_\beta + ^T \left( \nabla \tilde{v}_\beta \right) \right) - \tilde{p}_\beta \right] dA = 0
\\
\text{Closure?} + \ldots
\end{cases}
\]

\[
\begin{align*}
0 &= -\nabla \tilde{p}_\beta + \nabla \cdot \left( \mu_\beta \left( \nabla \tilde{v}_\beta + \nabla \tilde{v}_\beta^T \right) \right) - \left( \nabla \langle p_\beta \rangle - \rho_\beta g \right) \\
\nabla . (\tilde{v}_\beta) &= 0 \\
\tilde{v} &= -\langle v_\beta \rangle^\beta \text{ at } A_{\beta\sigma}
\end{align*}
\]

$\Rightarrow$ Problem must be solved for each value of $\langle v_\beta \rangle^\beta$!
"Closure"?

Under several constraints: scale separation, far from BCs, ...

⇒

\[
\langle \mathbf{v} \rangle^\beta = \mathbf{B} \cdot \langle \mathbf{v}_\beta \rangle^\beta + ... \\
\langle \mathbf{p} \rangle^\beta = \mu_0 \mathbf{b} \cdot \langle \mathbf{v}_\beta \rangle^\beta + ...
\]

Tentatively:

\[
(\nabla \cdot [\mu (\mathbf{\hat{\gamma}}) (\nabla \mathbf{B} + \nabla^T (\nabla \mathbf{B}))] - \nabla \mathbf{b}) \cdot \langle \mathbf{v}_\beta \rangle^\beta = \langle \nabla \cdot [\mu (\mathbf{\hat{\gamma}}) (\nabla \mathbf{B} + \nabla^T (\nabla \mathbf{B}))] - \nabla \mathbf{b} \rangle^\beta \cdot \langle \mathbf{v}_\beta \rangle^\beta
\]

\[
(\nabla \cdot \mathbf{B}) \cdot \langle \mathbf{v}_\beta \rangle^\beta = 0 ; \quad \mathbf{B} \cdot \langle \mathbf{v}_\beta \rangle^\beta = -\mathbf{I} \cdot \langle \mathbf{v}_\beta \rangle^\beta \text{ at } A_{\beta \sigma}
\]

\[
\mathbf{B} (\mathbf{r}) = \mathbf{B} (\mathbf{r} + h \mathbf{e}_i) \quad \text{and} \quad \mathbf{b} (\mathbf{r}) = \mathbf{b} (\mathbf{r} + h \mathbf{e}_i) \quad \text{for } i = 1, 2, 3 \quad \text{(periodicity)}
\]

\[
\langle \mathbf{b} \rangle = 0
\]

with

\[
\mathbf{\hat{\gamma}} = \left\| (\nabla \mathbf{B} + \nabla^T \mathbf{B}) \cdot \mathbf{e}_\beta \right\| \left\| \langle \mathbf{v}_\beta \rangle^\beta \right\|
\]

\[
\mathbf{e}_\beta = \langle \mathbf{v}_\beta \rangle^\beta / \left\| \langle \mathbf{v}_\beta \rangle^\beta \right\|
\]

⇒ Problem must be solved for each value of \( \langle \mathbf{v}_\beta \rangle^\beta \)!
A classical story: the linear case and Darcy’s law (see Sanchez-Palencia, Whitaker, ….)

- **Closure** (any solution is a linear combination of elementary solutions for \( \langle \mathbf{v}_\beta \rangle^\beta = e_i \) for \( i = 1, 2, 3 \))

\[
\vec{v}_\beta = \mathbf{B} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \ldots
\]
\[
\tilde{p}_\beta = \mu_0 \mathbf{b} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \ldots
\]

\[
(\nabla \cdot (\nabla \mathbf{B}^T (\nabla \mathbf{B})) - \nabla \mathbf{b}) = \langle \nabla \cdot (\nabla \mathbf{B}^T (\nabla \mathbf{B})) - \nabla \mathbf{b} \rangle^\beta
\]

\[
(\nabla \cdot \mathbf{B}) = 0 \quad ; \quad \mathbf{B} = -\mathbf{I} \quad \text{at} \quad A_{\beta \sigma} \quad \text{over a UC!}
\]

\( \mathbf{B}(\mathbf{r}) = \mathbf{B}(\mathbf{r} + h\mathbf{e}_i) \) and \( \mathbf{b}(\mathbf{r}) = \mathbf{b}(\mathbf{r} + h\mathbf{e}_i) \) for \( i = 1, 2, 3 \) (periodicity)

\[
\langle \mathbf{b} \rangle = 0
\]

- **Macro-Scale equation and effective properties**

Darcy’s law:

\[
\langle \mathbf{v}_\beta \rangle = -\frac{1}{\mu_0} \mathbf{K}_0 \cdot \langle \nabla \langle \mathbf{p}_\beta \rangle^\beta - \rho_\beta \mathbf{g} \rangle
\]

Intrinsic permeability:

\[
\mathbf{K}_0^{-1} = \frac{1}{V} \int_{V_\beta} (\nabla \cdot (\nabla \mathbf{B}^T (\nabla \mathbf{B})) - \nabla \mathbf{b}) \, dV
\]

Important: Proof of symmetry of \( \mathbf{K}_0 \) requires periodicity!
Calculations of the permeability

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

- 3 possibilities
  - Initial closure problem
  - Transformation of closure problem into ~Stokes with source term and periodic pressure and velocity
  - “permeameters”: no-periodicity

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

See discussion in Guibert et al., 2015
Calculations over non-periodic images

- “permeameters”
  - All methods have bias
  - $\langle \nu_x \rangle^\beta \neq 0$
  - $K_{xy} \neq K_{yx}$

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; ...
Non-Linear Case: Non-Newtonian Fluid

- **Fluid rheology**

\[
\mu = \begin{cases} 
\mu_0 & \text{if } \dot{\gamma} < \dot{\gamma}_c, \\
\mu_0 \left( \frac{\dot{\gamma}}{\dot{\gamma}_c} \right)^{n-1} & \text{else.}
\end{cases}
\]

- **Representation as a deviation from Darcy’s law**

\[
\langle \mathbf{v}_\beta \rangle = -\frac{1}{\mu_0} k_n \mathbf{P} \cdot \mathbf{K}_0 \cdot \left( \nabla \langle p_\beta \rangle^\beta - p_\beta \mathbf{g} \right)
\]

- **No generic closure independent of fluid velocity! Generic macro-scale law:**

\[
\langle \mathbf{v}_\beta \rangle = -K_{gen} \langle \langle \mathbf{v}_\beta \rangle \rangle \cdot \left( \nabla \langle p_\beta \rangle^\beta - p_\beta \mathbf{g} \right)
\]

- **PLCO**

\[
\mu = \begin{cases} 
\mu_0 & \text{if } \dot{\gamma} < \dot{\gamma}_c, \\
\mu_0 \left( \frac{\dot{\gamma}}{\dot{\gamma}_c} \right)^{n-1} & \text{else.}
\end{cases}
\]
Test cases

2D

Clashach Bentheimer

(a) A1
(b) P1
(c) C1
(d) B1

(f) A2
(g) P2
(h) C2
(i) B2

HPC center EOS-Calmip:
Typically: $10^8$ mesh cells
$10^5$ cores $\times$ hours

} often limited to
~ mm$^3$!

Needs very fine grid!
Resolution with OpenFoam

- FVM with OpenFOAM (SIMPLE, second-order scheme)
- Use of HPC, calculations up to 100 millions mesh elements
- A total of 100000 hours of CPU time.
- Conform orthogonal hexahedral elements.
- Multi-criteria grid convergence study = OK.
Results

- Computations allows to analyze various features:
  - Properties of pore-scale fields (PDFs)
  - Transition:
    - Starts in a few narrow constrictions
    - Scaling for transition?

\[
\langle \psi \rangle_{\text{FL}} = \text{intrinsic fluid average}
\]
Normalized pdf ~similar between Newtonian and non-Newtonian flow! Not valid for pdf of $\nabla \langle p_\beta \rangle^\beta$
Transition Scaling

\[ U^* = \frac{\langle U \rangle_{\text{FL}}}{(\dot{\gamma}_c \sqrt{K_0})} \]

(a) \( k^* \) vs \( \langle U \rangle_{\text{FL}} \) \( \mu \text{m} \cdot \text{s}^{-1} \)

\[ k^* = \frac{K_{\text{app}}}{K_0} \]

(b) \( k^* \) vs \( U^* \)

\[ \dot{\gamma}_c = 1 \text{s}^{-1} ; \quad n = 0.75 \]

Zami-Pierre et al., 2015

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Transport in Porous Media
Impact of Domain Size

- Anisotropy induced by non-linear behavior decreases with ↗ $L$ for disordered media
- Effective property variance decreases with ↗ $L$

$\gamma_c = 1 \text{s}^{-1}$ ; $n = 0.70$

$\theta = 22^\circ$  \quad $U^* \gg 1$
Impact of Domain Size

\[ \theta = 22^\circ \]

\[ U^* \gg 1 \]

Disorder → no anisotropy induced by non-linearity if \( L \) large enough!

\[ B \text{ medium: } \alpha \]
\[ \text{B medium: } \beta \]

\[ R_{eq} \text{ (pore size)} \]
Impact of disorder and velocity

![Graph showing the impact of disorder and velocity on transport in porous media. The graphs illustrate the dependence of $k_n$ and the angle $\alpha$ of $P$ on the dimensionless velocity $U^*$. Different colors and symbols represent different values of $A_1^\sigma$.]

- $k_n$ increases with $U^*$ for $A_1^\sigma=0$ and decreases for $A_1^\sigma=0.05, 0.10, 0.20, 0.30$.
- The angle $\alpha$ of $P$ decreases significantly for $A_1^\sigma=0.30$, indicating a change in the direction of transport.

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Transport in Porous Media
21/27
Practical Consequences

- Eng. Practice: apparent Darcy’s law

\[ \langle v_\beta \rangle = -\frac{1}{\mu(\dot{\gamma}_{eq})} K_0 \cdot (\nabla \langle p_\beta \rangle^\beta - \rho_\beta g) \]

- Discussion:
  - P=I for all \( \langle v_\beta \rangle^\beta \) if isotropic disordered media and REV (→ need tests for various sizes)!
  - Apparent permeability \( \sim \) scales with \( (K_0)^{1/2} \) → classical scaling “may” introduce artificial dependence upon parameters such as porosity:

\[ \langle U_c \rangle_{FL} = \alpha' \dot{\gamma}_c \sqrt{K_0} \quad \text{versus} \quad \langle U_c \rangle_{FL} = \frac{1}{\alpha \sqrt{2\varepsilon_\beta}} \dot{\gamma}_c \sqrt{K_0} \]

- Description of transition near the critical velocity may not be well described by an apparent viscosity (no observed angle in the apparent permeability in the case of PLCO)
Further upscaling

- Depletion layer treated as an effective BC

\[ \mathbf{v}_\beta = -\ell \mathbf{n} \cdot \left( \nabla \mathbf{v}_\beta + (\nabla \mathbf{v}_\beta)^T \right) \cdot (\mathbf{I} - \mathbf{n n}^T) \]

Zami-Pierre et al., 2017

see Chauveteau (1982), Sorbie & Huang (1991) (double-layer model)
Further upscaling

- **Viscoelastic fluids**

\[
\rho_l \frac{\partial \mathbf{v}_l}{\partial t} + \rho_l \mathbf{v}_l \cdot \nabla \mathbf{v}_l = -\nabla p_l + \rho_l \mathbf{g} + \nabla \cdot \left( \mu_s \left( \nabla \mathbf{v}_l + \nabla \mathbf{v}_l^T \right) \right) + \nabla \cdot \mathbf{\tau}_v
\]

\[
\frac{\nabla}{\tau_v} = \frac{\partial \mathbf{\tau}_v}{\partial t} + \mathbf{v}_l \cdot \nabla \mathbf{\tau}_v - \nabla \mathbf{v}_l^T \cdot \mathbf{\tau}_v - \mathbf{\tau}_v \cdot \nabla \mathbf{v}_l
\]

upper convected Derivative

- **Rheological models**

**FENE-P:**

\[
f (\tau_v) = \frac{\tau_v}{2} a \mu_p \left( \nabla \mathbf{v}_l + \nabla \mathbf{v}_l^T \right)
\]

\[
f (\tau_v) = 1 + \frac{3 a + (\lambda/\mu_p) \text{tr} (\mathbf{\tau}_v)}{L^2}; \quad a = \frac{L^2}{L^2 - 3}
\]

\[
L^2 \to \infty \text{ gives Oldroyd-B model (no-elongation limit)}
\]
Example of results: De et al., soft matter, 2018

Steady-state!
Deborah number: \[ \text{De} = \frac{\lambda U_r}{L_r} \]

...also Weissenberg number 😊

De= 0.001 0.1
Normal stress along average flow direction

-see previous discussion on “apparent permeability”, etc…
- elastic turbulence?
Further perspectives: N-momentum equations, multi-component aspects, ...

- Superfluid: 2 momentum equations $\rightarrow$ complex behavior $\rightarrow$ macro-scale model?
  
  see Allain et al. (2010, 2013, 2015), Soulaine et al. (2015, 2017)

- Polymer solution as multi-component systems:
  - Mechanical segregation, degradation (bio., mech.)
  - Model?
    - Momentum balances:
      - diffusion theory or
      - N-momentum equations
    - Composition:
      - Continuous models or
      - PBM (population balance model), ...

\[ \text{pdf} \]
\[ \text{mol. weight} \]
Conclusions

- Upscaling tells that this is not always possible to separate in an apparent Darcy’s law permeability and viscosity
- Specific anisotropy effects
- Simplifications arise for disordered media
- Various results published in the literature for various rheology: power-law (...), Ellis and Herschel–Bulkley fluids (Sochi & Blunt, 2008), Yield-Stress Fluids (Sochi, 2008), etc...
- Additional problems: retention effects, Inaccessible Pore Volume (IPV), mobile/immobile effects
- Perspectives: viscoelastic, multicomponent, coupling with other transport problems (transport of species, heat transfer, etc...), ...