Simulation of particle deposition in porous media: computational fluid dynamics and population balance modelling

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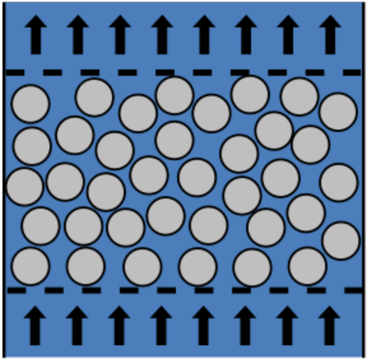
September 29, 2015

Motivation of the work

Many fields of interest

- Packed bed reactors
- Filtration
- Chromatographic Separation
- Aquifer Remediation
- Enhanced Oil Recovery



- Fluid flowing through an arrangement of stationary solid grains.
- The flowing fluid can contain liquid droplets, gas bubbles or solid particles.

Computational models structure

Porous medium generation

- Experimental:
  · μ-CT, X-ray, SEM
- Algorithmic reconstruction:
  · DEM, particle-based
  · Rigid body simulation
  $\rightarrow$ Blender (opensource)

Flow, transport simulation

- Computational Fluid Dynamics
  · Ansys FLUENT (commercial)
  · OpenFOAM (opensource)

$\Rightarrow$ Model of porous medium with **Blender**
$\Rightarrow$ Meshing and CFD simulation with **OpenFOAM**

Dispersion in 3D Porous Media

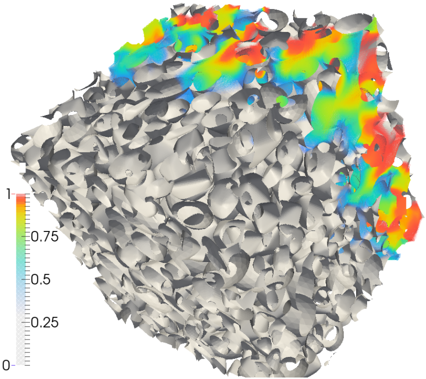
Simulation Setup

Geometry

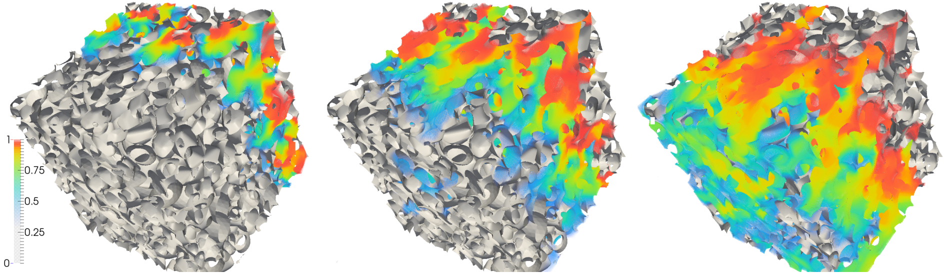
- 2mm cubic sample
- 3000 grains
- 40M cells

Operating Conditions

- Particle diameter: $d_p = 1 \div 1000$ nm
- Superficial velocity: $q = 10^{-6} \div 0.1$ ms^{-1}
- $10^{-4} <$ Re < 300
- $10^{-2} <$ Pe $= \dfrac{qD_g}{\mathcal{D}_m} < 10^7$



Hydrodynamic Dispersion



Snapshots of particle concentration at three different times

- Hydrodynamic dispersion enlarges and smoothens out the particle concentration front over time
- This effect increases for higher Péclet numbers

Particle Deposition

Deposition Efficiency

Brownian Diffusion

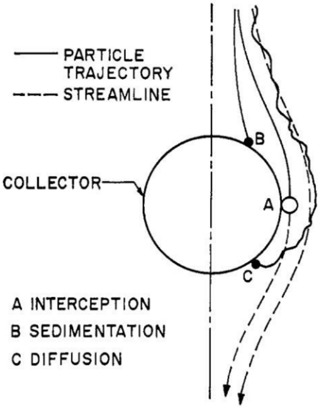
$\eta_B = 4.04\mathrm{Pe}^{-\frac{2}{3}}$ Yao-Levich

$\eta_B = 4As^{\frac{1}{3}}\mathrm{Pe}^{-\frac{2}{3}}$ Happel

Interception

$\eta_I = \frac{3}{2}\left(\frac{d_p}{D_g}\right)^2 = \frac{3}{2}N_R^2$ Yao-Levich

$\eta_I = \frac{3}{2}AsN_R^2$ Happel



Particles Modeling

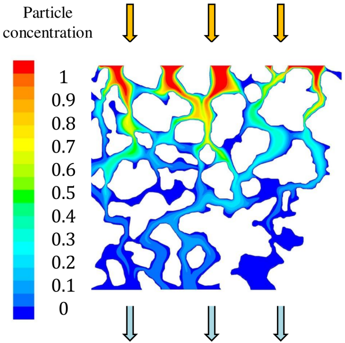
Particles are transported by convective and diffusive phenomena

BOUNDARY CONDITION

- C = 1 at inlet
- C = 0 on grain surface (assumed "perfect sink" B.C.)

OPERATING CONDITIONS

- Particle diameter: $d_p = 1 \div 1000$ nm
- Superficial velocity: $q = 10^{-6} \div 0.01$ ms^{-1}

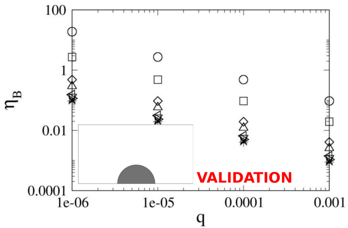


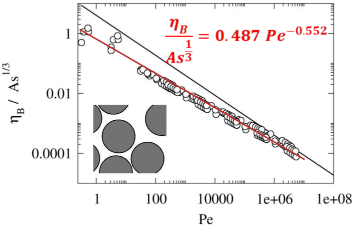
Collector deposition efficiency, η calculated with packed bed performance equation

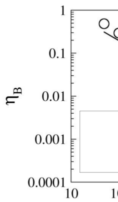
$$\frac{dC}{dx} = -\frac{3}{2}\frac{1-\varepsilon}{\varepsilon D_g}\eta C$$

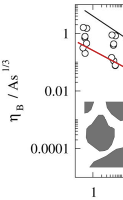
Results: Particle Deposition

Deposition Efficiency: Brownian Diffusion









Population Balance Modelling

Population balance equation

$\rightarrow$ evolution of the particle size distribution

$\rightarrow$ possibility of treating a polydisperse particle population

Solution of the PBE in the CFD code with the Method of Moments

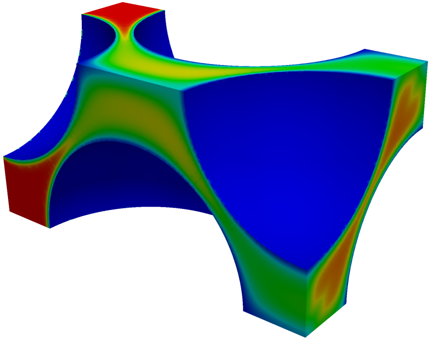
$$\frac{\partial m_k}{\partial t} + \frac{\partial \mathbf{u} m_k}{\partial \mathbf{x}} = \frac{\partial}{\partial \mathbf{x}} \left(\Gamma_0 \frac{\partial m_{k-1}}{\partial \mathbf{x}} \right)$$

Deposition of polydisperse particle populations

Simulation Setup

Geometry

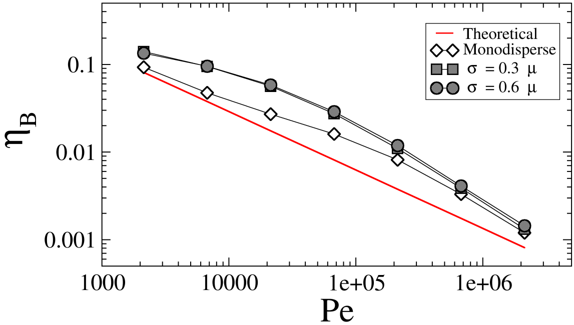
- Domain = one grain
- Face-centered cubic
- 260k cells



Operating Conditions

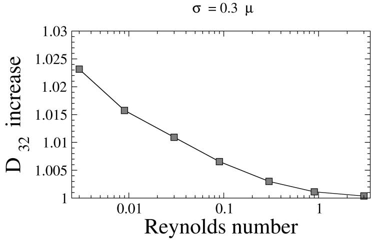
- Mean particle diameter: $\mu = 300$ nm
- $10^{-3} < \text{Re} < 3$
- Two lognormal distributions:
  $\rightarrow \sigma = 0.3\ \mu$
  $\rightarrow \sigma = 0.6\ \mu$

Results: Deposition rates of polydisperse particle populations



- Very different η-Pe relationship w.r.t to monodisperse case and theoretical prediction.
- Weak effect of particle population polidispersity.

Results: Increase in average diameter



- Higher σ means more deposition of smaller particles, hence an increase of average particle diameter.
- Behaviour of particle population changes in space during the evolution of the dispersion process
  $\rightarrow$ e.g. effect on reaction rates, dispersion coefficient, et c.

Conclusions

Micro-scale modeling is essential
to the derivation of effective macro-scale models

Classic deposition laws fail with:

→ realistic (non-spherical) geometries

→ polydisperse particle populations

- Possibility of treating packings of arbitrary grain shape with BLENDER
- Treatment of polydisperse particle populations via population balance modelling shows an improvement over theoretical predictions

Acknowledgements - People

DIATI - Politecnico di Torino (I)

- Tiziana Tosco (Ass. Prof.)
- Francesca Messina (Post-Doc. Res.)

Warwick University (UK)

- Matteo Icardi (Assistant Professor)

Acknowledgements - Resources

Financial Resources

- AQUAREHAB (FP7, Grant Agreement no. 226565)
- PRIN Project 2008:
  "Disaggregazione, stabilizzazione e trasporto di ferro zerovalente nanoscopico"

Computational Resources

- PRACE Research Infrastructure
- CINECA

Thank you!