Pore-scale simulation of particle transport and deposition in 3D porous media

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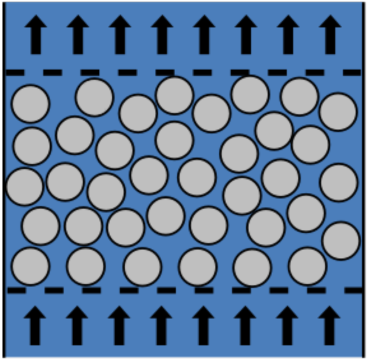
Motivation of the work

Many fields of interest

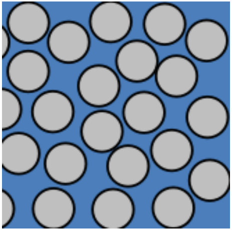
- Packed bed reactors
- Filtration
- Chromatographic Separation
- Aquifer Remediation
- Enhanced Oil Recovery



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

Necessity of mathematical modeling for porous media

- More info w.r.t. experiments
- Possible to explore micro-scale behaviour



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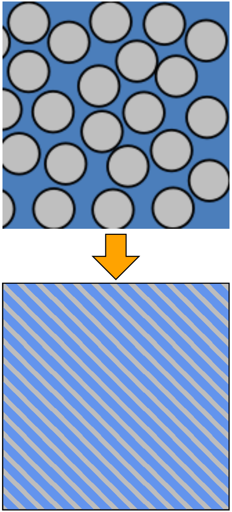

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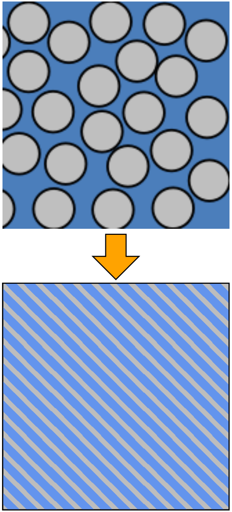
- Estimation of parameters:

Porosity	ε
Permeability	k
Dispersion	$\mathbf{D}$
Deposition eff.	η



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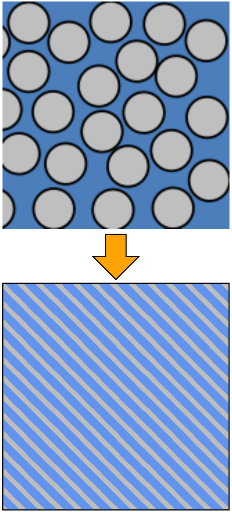

Verification and validation:

- experimental data
- empirical relationships
- theoretical models (analytical solutions)

Computational models structure

Computational models structure

Porous medium generation

- Experimental:
  - μ-CT, X-ray, SEM

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- Computational Fluid Dynamics

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⇒ Model of porous medium with **Blender**

⇒ Meshing and CFD simulation with **OpenFOAM**

Workflow

Model generation

- A grain shape and grain size distribution is chosen
- The porous media model is generated with **Blender**

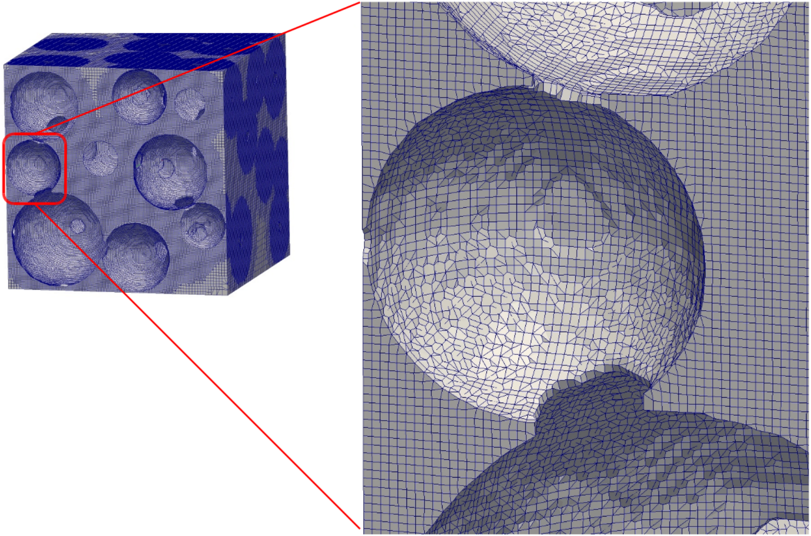
Mesh Generation

SNAPPYHEXMESH

- Good control of final mesh quality
  (care must be given to meshing parameters)
- Simple handling of zone refinement
- Contact points are not problematic

$\Rightarrow$ Description of contacts is as precise as mesh resolution is, and is never a problem during meshing

Mesh Quality



Workflow

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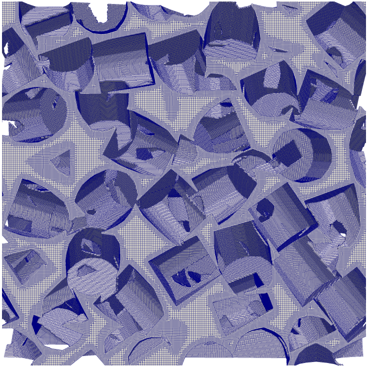

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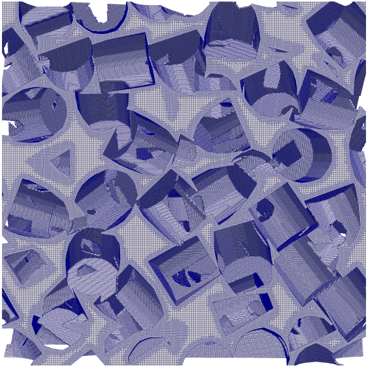
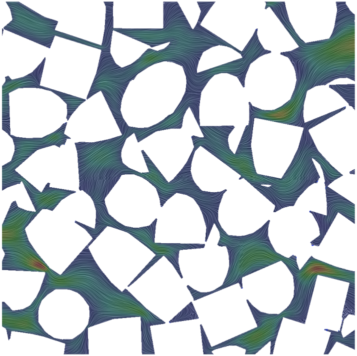
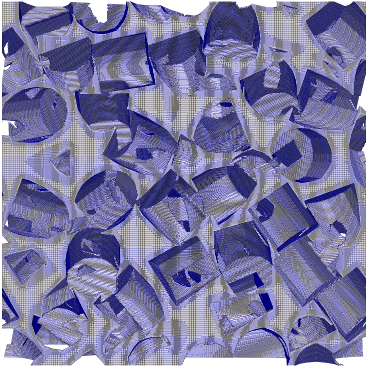


Simulation



Workflow

Meshing



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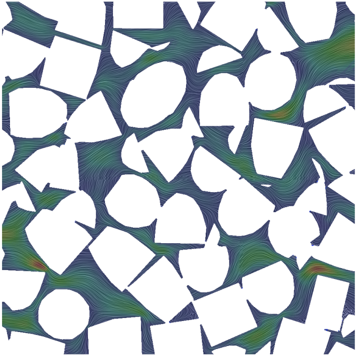

OpenFOAM is used both for the meshing process and the CFD simulation

Theoretical Background: Fluid Flow

Macroscale Continuum Approach

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Macroscale Continuum Approach

- **Re** < 1: creeping flow / linear relationship

DARCY'S LAW

$$\frac{\Delta P}{L} = \frac{\mu}{k} q$$

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- Packing of spherical particles (**wide range of Re**)

$$\Delta P^* = \frac{\Delta P \rho D_g \varepsilon^3}{L G_0^2 (1-\varepsilon^3)}$$

$$\mathrm{Re}^* = \frac{D_g G_0}{(1-\varepsilon)\mu}$$

ERGUN'S LAW
$$\Delta P^* = \frac{150}{\mathrm{Re}^*} + 1.75$$

$$G_0 = \rho q$$

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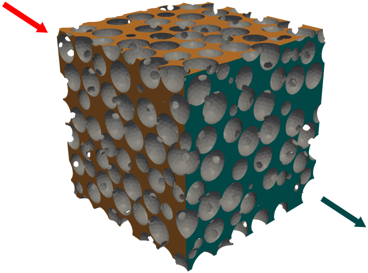
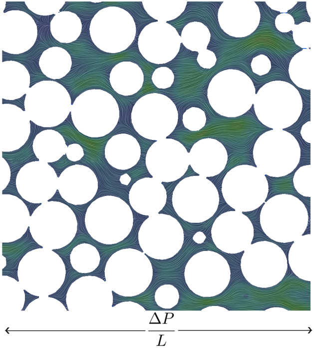
- Extension of Ergun's law to non-spherical objects

Simulation Setup





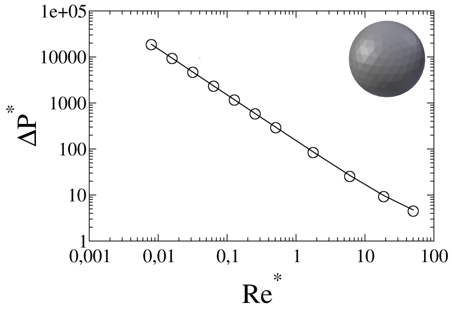
- Different grain shapes analyzed (spheres, cylinders, trilobes)

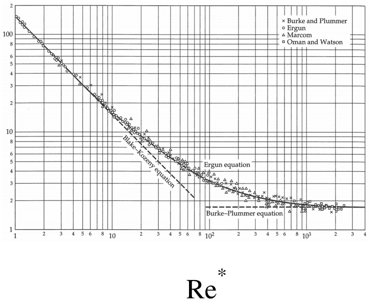
- Range of fluid flow velocity:
$$10^{-3} < \mathrm{Re} = \frac{qD_g}{\nu} < 100$$

Pressure drop calculated and compared with Ergun's law predictions

Validation: Pressure Drop

Model: Spheres

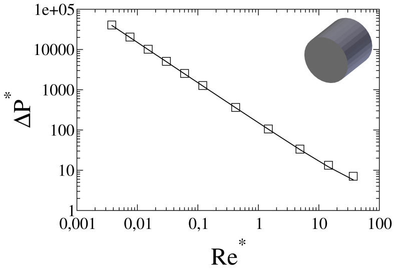


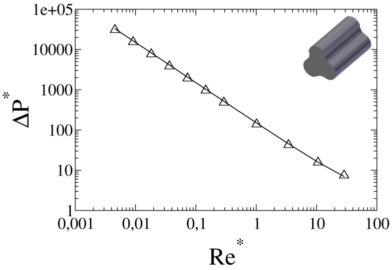


Relative error between Ergun's law predictions and CFD results are less than 10%

Validation: Pressure Drop

Models: Cylinders and Trilobes





Pressure drop is correctly predicted with Ergun's law even in the case of cylindrical and trilobe-shaped grains

Dispersion in 3D Porous Media

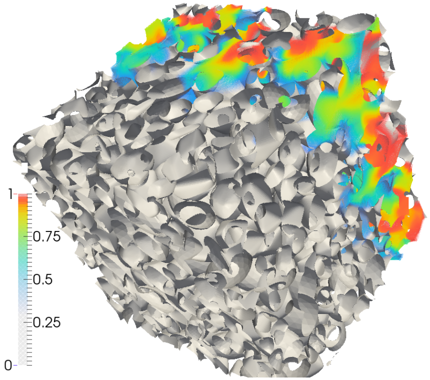
Simulation Setup

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}
- $10^{-4} < \text{Re} < 300$
- $10^{-2} < \text{Pe} = \dfrac{qD_g}{\mathcal{D}_m} < 10^7$



Dispersion in 3D Porous Media

Simulation Setup

GEOMETRY

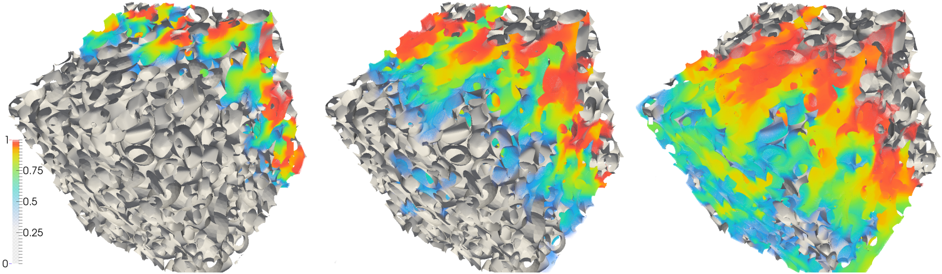
- 2mm cubic sample
- 3000 grains
- 40M cells

NEED FOR HPC!

- Very large domains needed for realistic geometries
- DISPERSION: long time scales needed to study transient behaviour
- DEPOSITION: high concentration gradients at the walls require finer mesh

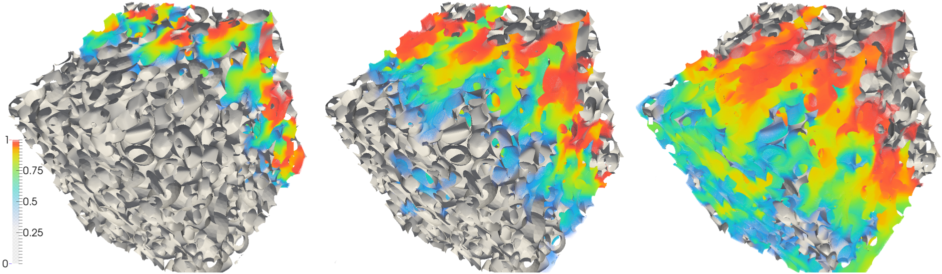
$\Rightarrow$ Huge memory requirements

Hydrodynamic Dispersion



Snapshots of particle concentration at three different times

Hydrodynamic Dispersion



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- Hydrodynamic dispersion enlarges and smoothens out the particle concentration front over time

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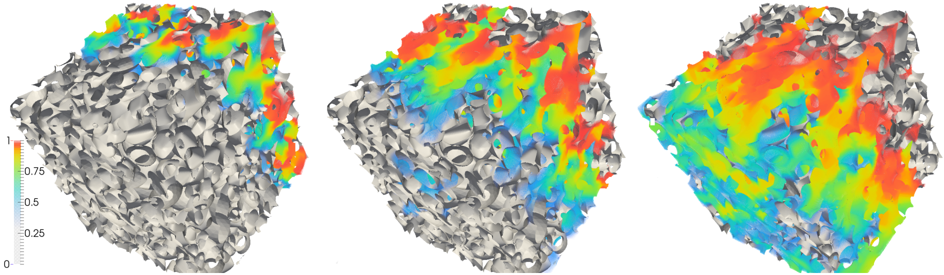
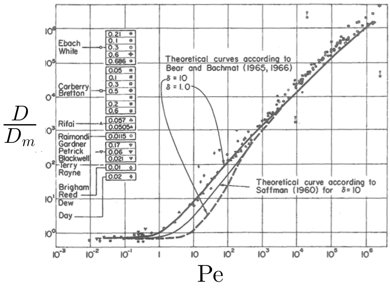


Snapshots of particle concentration at three different times

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

Validation: Hydrodynamic Dispersion



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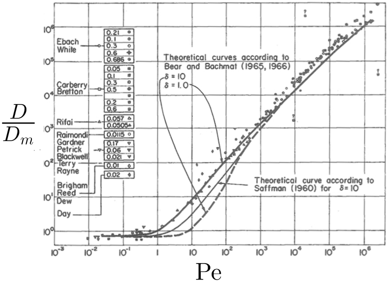
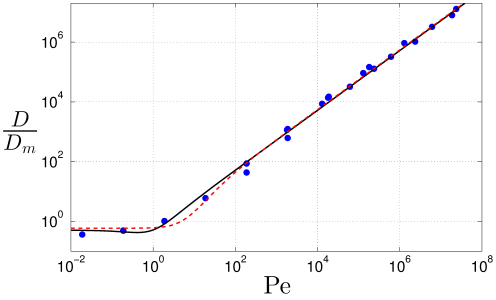




Values of hydrodynamic dispersion $\mathcal{D}$ are favourably comparable experimental data and empirical relationships

Particle Deposition

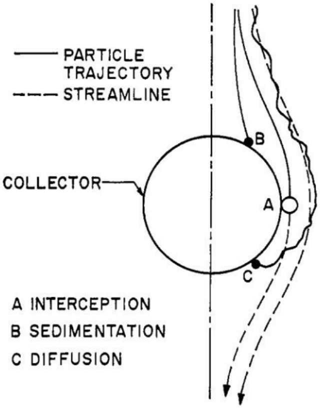
Deposition Efficiency

BROWNIAN DIFFUSION

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

INTERCEPTION

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



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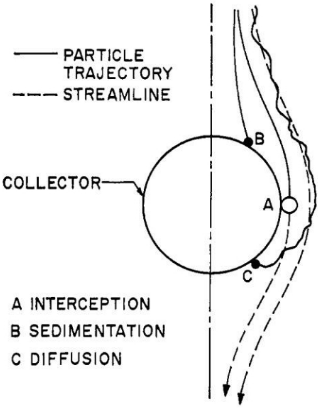

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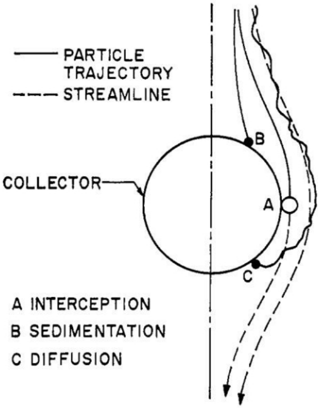


Particles Modeling

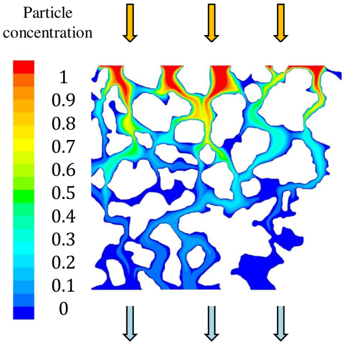
Particles are transported by convective and diffusive phenomena

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: Overview

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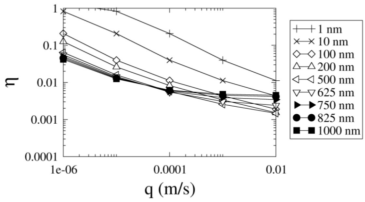

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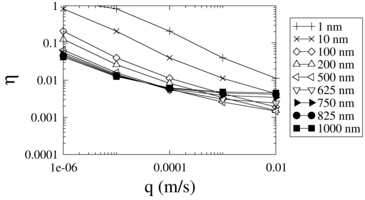
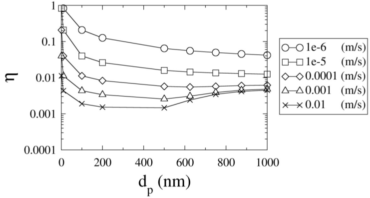


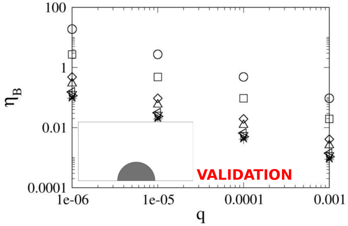


- Efficiency η decreases for higher superficial velocities q (low residency times)

- Efficiency η decreases for higher particle diameter (low $\mathcal{D}$) until a certain d_p value, then increases for the steric interception effect.

Results: Particle Deposition

Deposition Efficiency: Brownian Diffusion



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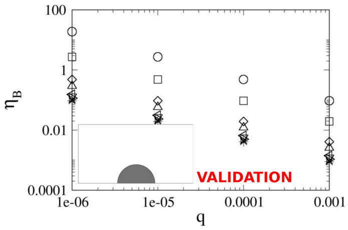

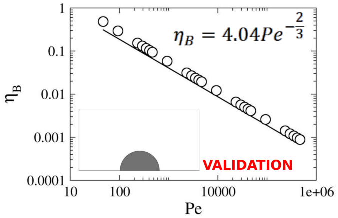

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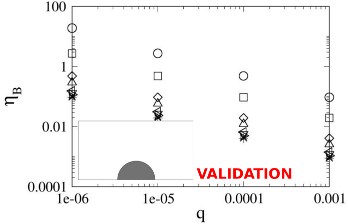

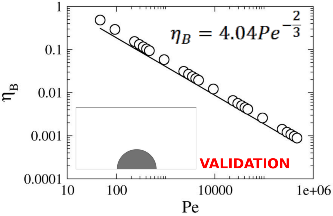

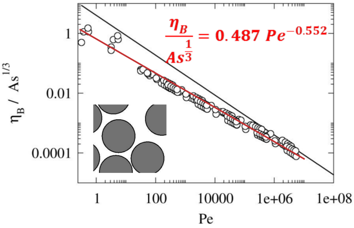

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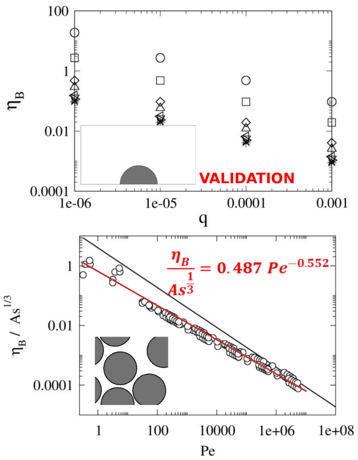

Conclusions

Algorithmic packing generation and CFD simulation:
viable methodology?

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→POSSIBILITY TO TREAT PACKINGS OF ARBITRARY GRAIN SHAPE

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→Possibility to treat packings of arbitrary grain shape

→Results validated by experimental data

- pressure drop prediction, hydrodynamic dispersion

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→Results validated by experimental data

- pressure drop prediction, hydrodynamic dispersion

→Micro-scale modeling essential

OpenFOAM and HPC

- Meshing of complicated geometries easy with snappyHexMesh
- Large memory requirements to simulate realistic domains

Acknowledgements - People

DIATI - Politecnico di Torino (I)

- Tiziana Tosco (Ass. Prof.)
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- Yacine Haroun (Res.)
- Daniel Ferre (Res.)

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- Daniel Tartakovsky (Full Prof.)

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!

Validation: Porosity (radial distribution)

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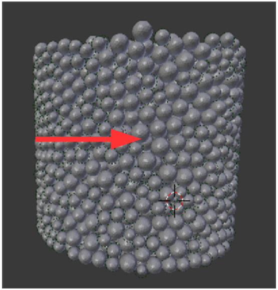

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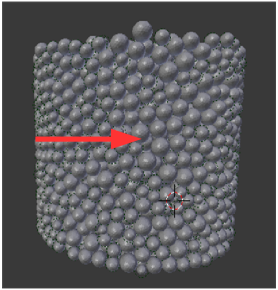

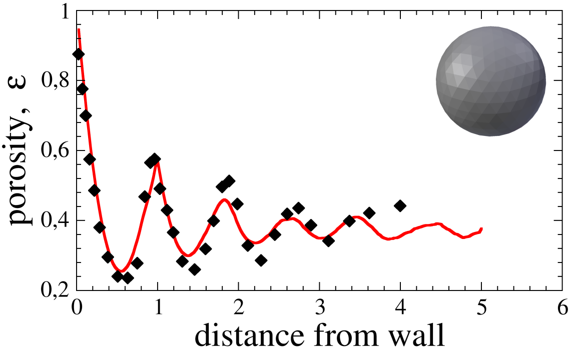

Good accordance between experimental radial distribution profiles and Blender simulation results

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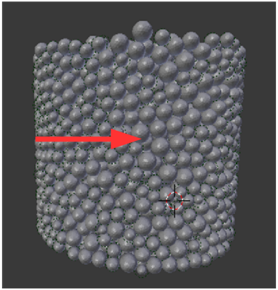
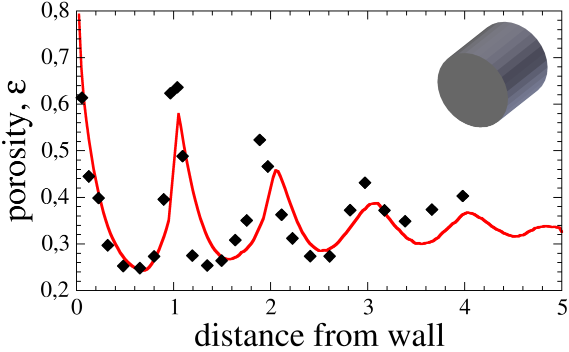




Also for non-spherical catalytic particles:
→ good accordance with experiments

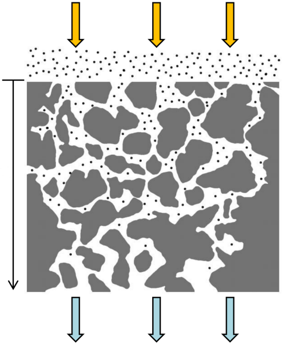
Theoretical Background: Particle Deposition

Macroscale 1D Advective-Diffusion Equation

$$\frac{\partial C}{\partial t} + q\frac{\partial C}{\partial x} - \mathcal{D}\frac{\partial^2 C}{\partial x^2} = \text{Source}$$

$$\text{Source} = -K_d C$$

$$K_d = \frac{3}{2}\,\frac{1-\varepsilon}{\varepsilon}\,\frac{q}{D_g}\,\alpha\,\eta$$



η : Collector Deposition Efficiency

Darcy's law and permeability limit

$$\frac{\Delta P}{L} = \frac{\mu}{k} q \rightarrow \frac{q\mu}{\Delta P/L} = k$$

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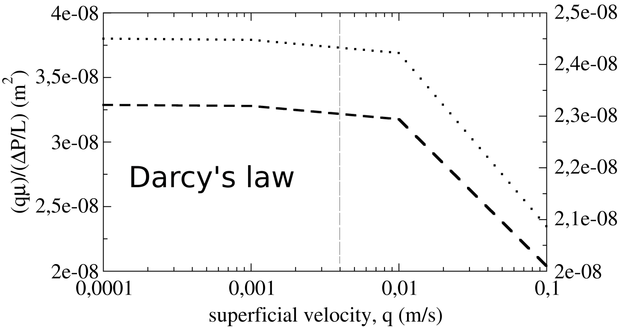

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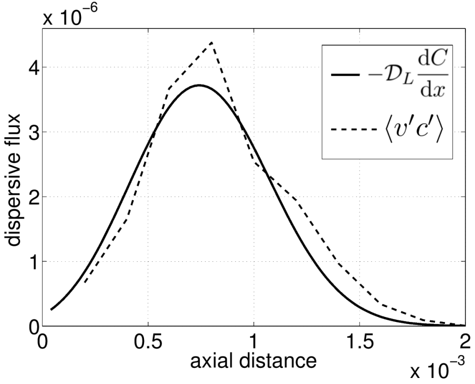

$$J = \langle v'c' \rangle \overset{?}{\approx} -\mathcal{D}_L \frac{\mathrm{d}C}{\mathrm{d}x}$$

Comparison of the term $\langle v'c' \rangle$ with $-\mathcal{D}_L \frac{\mathrm{d}C}{\mathrm{d}x}$ demonstrates the assumption of Fickian transport in the system for the dispersive term

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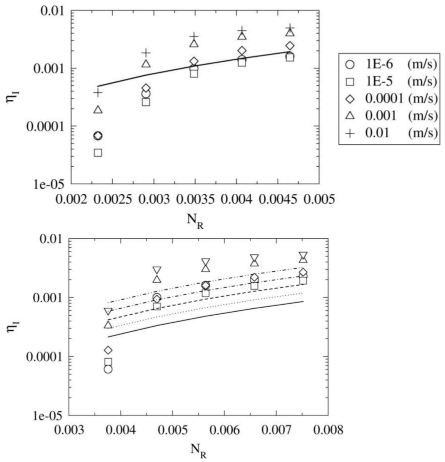
Deposition Efficiency: Interception



Theoretical law:

$$\eta_I = \frac{3}{2} As N_R^2$$

$$As = As(\varepsilon); N_R = \frac{d_p}{D_g}$$

- Results appear in line with theoretical predictions but are strongly dispersed, with great variations at different q

$$\eta_I = 1.116 As N_R^2 \text{Re}^{0.145}$$