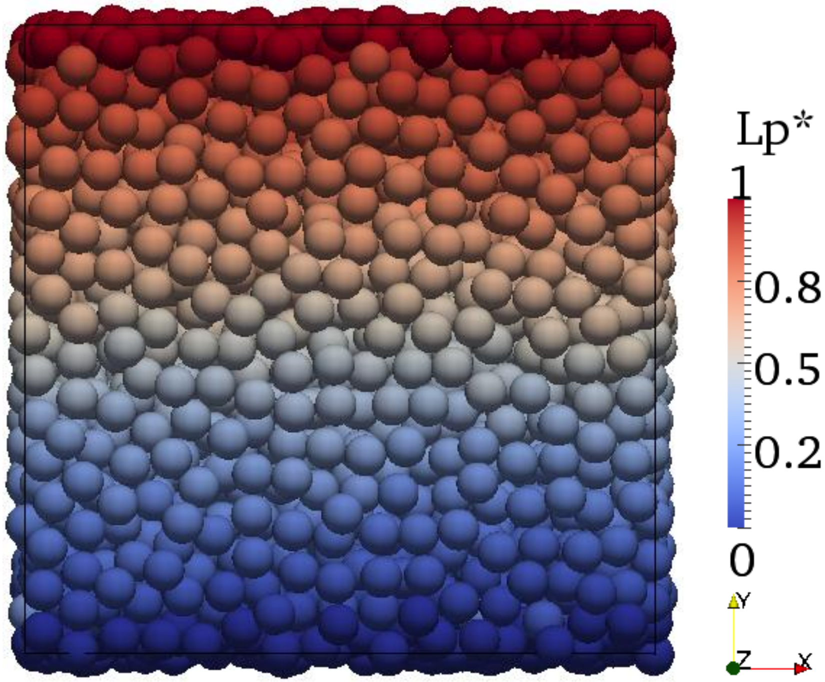
Jahrestreffen der Fachgruppe Computational Fluid Dynamics, Mischvorgänge und Rheologie

Predictive Capabilities of Microscopic Models for Conductive Transport in Sheared Particle Beds

Bhageshvar Mohan, Johannes G.Khinast, Stefan Radl



February 24, 2014

Talk : 5371

Würzburg, Germany

(20mins)

Outline

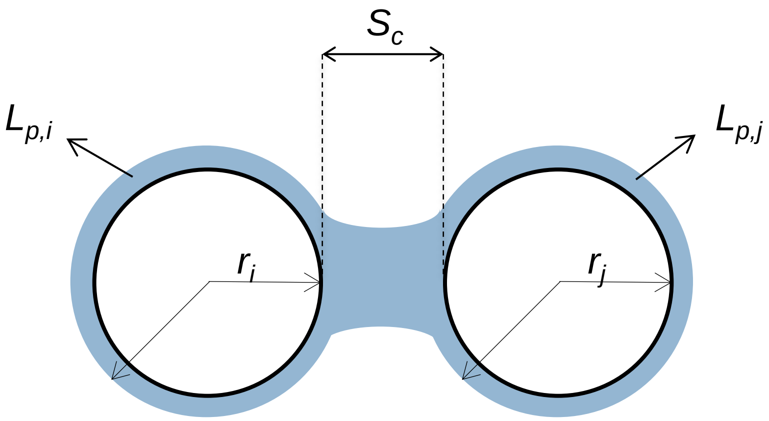
- **Introduction**
- **Proposed models**
- **Single particle-particle collision**
- **Sheared particle beds**
- **Conclusions**

Introduction

- Granular materials show extremely complex flow features.
- Prediction of wet granular flow difficult due to difficulties in describing liquid exchange during particle-particle collisions.
- A more rigorous model that is valid for all regimes would be of paramount industrial importance, e.g., to predict the distribution of liquid between particles more reliably in a
  - **granulation**,
  - **mixing**,
  - **drying or coating** applications
- Four liquid transfer models to predict the formation and rupture of liquid bridges and model for the conductive liquid flux for different flow regimes.

Proposed Models

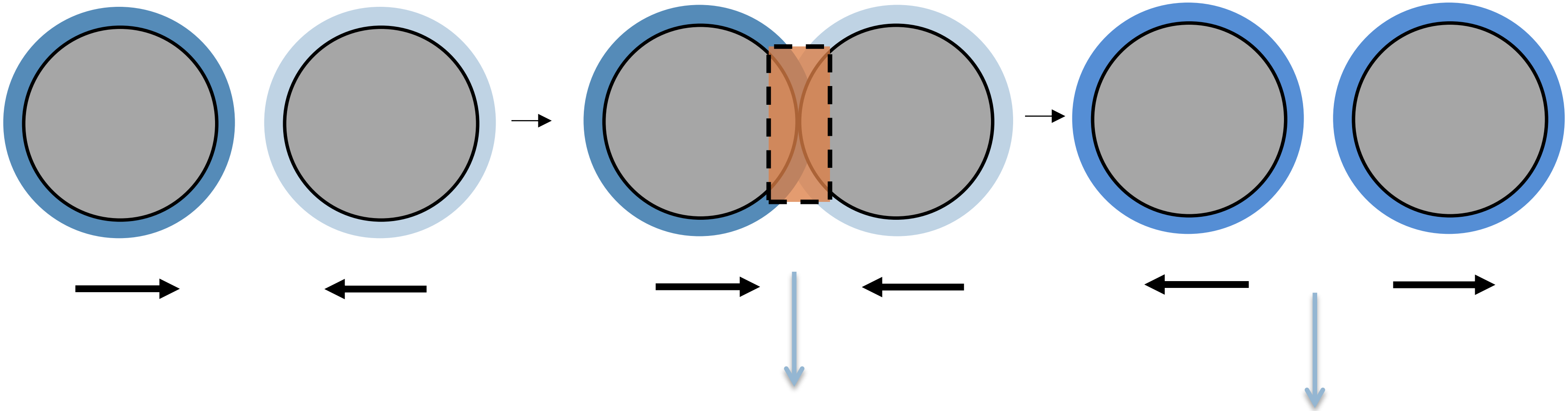
- **Model – A**
  - Conduction based simple liquid transfer rate model[1]
- **Model – B1**
  - Instantaneous liquid transfer model based on surface contact of particles[2]
- **Model – B2**
  - Instantaneous liquid bridge formation and rupture
- **Model – C**
  - Filling rate based model for drainage of liquid into the bridge



[1] Tomassone et al, Powder Technology 2012

[2] Shi and McCarthy, Powder Technology 2008

Proposed Models



Liquid transfer happens

Liquid transfer happens

Model A

Model B1

Transfer rate based on Γ

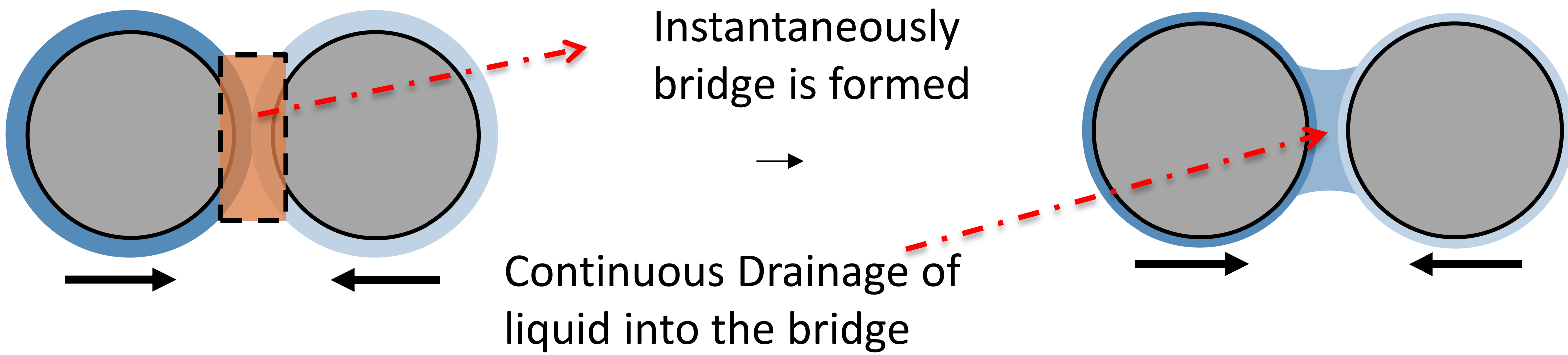
Calculation of bridge volume[2]

Transfer of liquid between particles instantaneously

[2] Shi and McCarthy, Powder Technology 2008

Proposed Models

Formation of liquid bridge



Model B2

Explicit Calculation of bridge volume[2]

Instantaneous transfer of liquid into the bridge

Model C

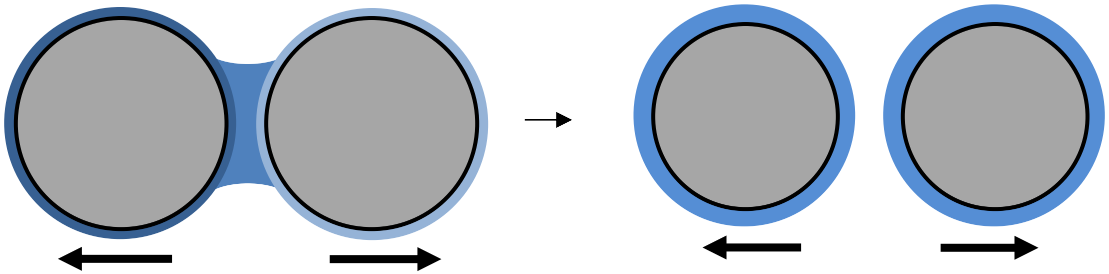
Drainage of liquid from the film into the bridge based on t_{ref}

$$t_{ref} = r_{eff} \cdot \frac{\mu_l}{\sigma_l}$$

Backflow of liquid from the bridge to liquid film is possible

Proposed Models

Rupture of liquid bridges



Calculation of rupture distance

$$s_c = \|\boldsymbol{\delta}\| - r_i - r_j$$

$$s_r = (1 + 0.5\theta)\, V_b^{1/3}$$ [3]

$$s_c \geq s_r$$

On rupture of liquid bridges

$$Q_i = \frac{V_b \cdot n}{\triangle t}$$

$$Q_j = \frac{V_b \cdot (1 - n)}{\triangle t}$$

[3] Lian et al., Journal of colloid and interface science 161, 138–147

Proposed Models

Key differences	Model A	Model B1	Model B2	Model C
Account of liquid Film thickness	No	No	**Yes**	**Yes**
Explicit calculation of Bridge volume	No	Not really (just at the end of collision)	**Yes**	**Yes**
Rupture distance	No	No	**Yes**	**Yes**
Effect of liquid viscosity and surface tension	**Yes**	No	No	**Yes**

Dimensional analysis

$$\gamma^{*} = \gamma d_p^{3/2} / \sqrt{k_n / \rho_p}$$

Dimensionless shear rate
Range[4] : **10^{-4} to 1**

Based on dimensional analysis of main influencing parameters, we get two dimensionless numbers

$$\Gamma = t_{ref}/t_{shear} = \gamma \cdot r_{eff} \cdot \mu_l/\sigma_l$$

$$\varepsilon = h_o/r_{eff}$$

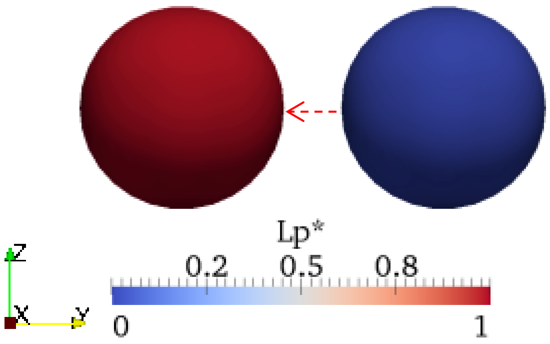
Range : **10^{-3} to 1**

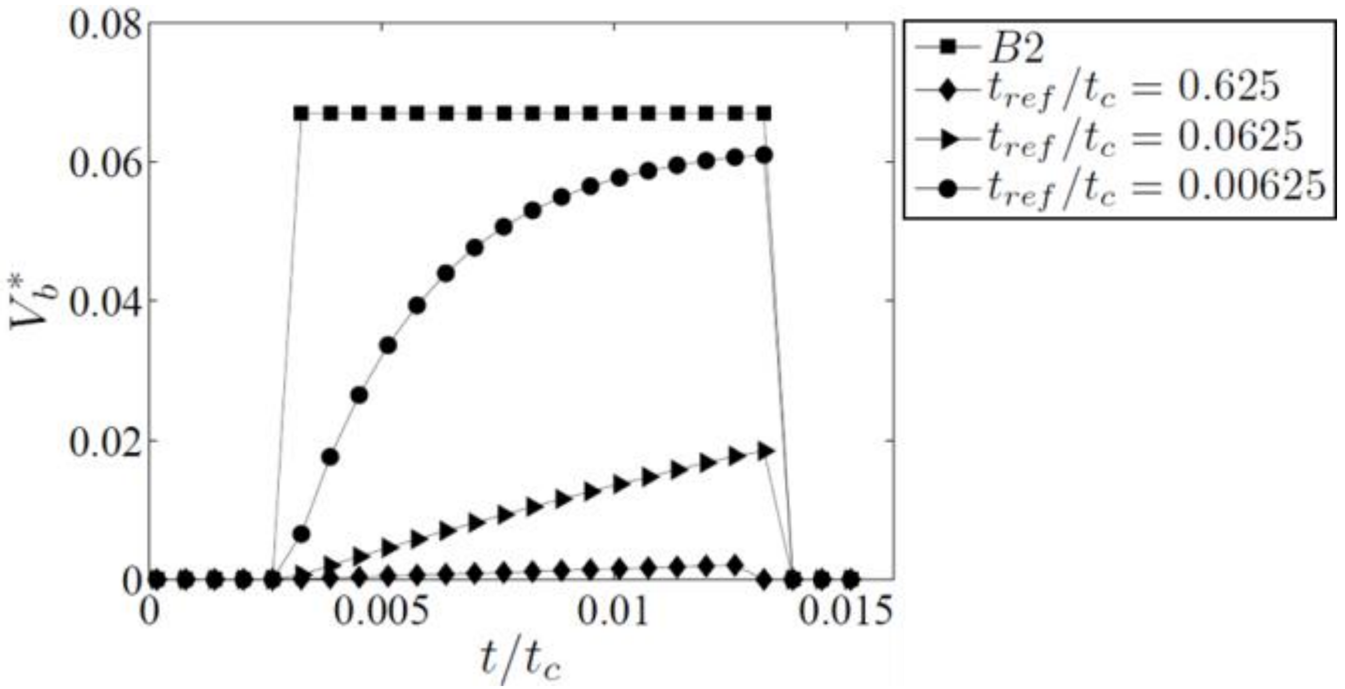
Dimensionless liquid film thickness

[4] Chialvo et al, Physical Review E. 85 (2012).

Model setup

Single particle-particle collision setup



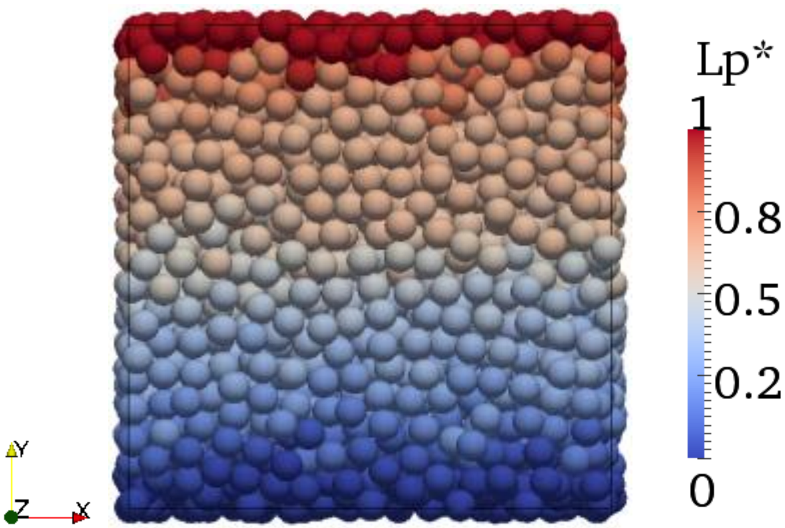


$$t_{ref} = r_{eff} \cdot \frac{\mu_l}{\sigma_l}$$

- Smooth
- Equal sized particles
- No force models

Sheared Particle Beds

Simulation Setup



$$\mathbf{q}^{cond} = \frac{1}{V}\sum_{c} Q \cdot \mathbf{r}_{ij}$$

$$q_s = -\gamma \cdot \nabla_y L_{p,i} / d_p$$

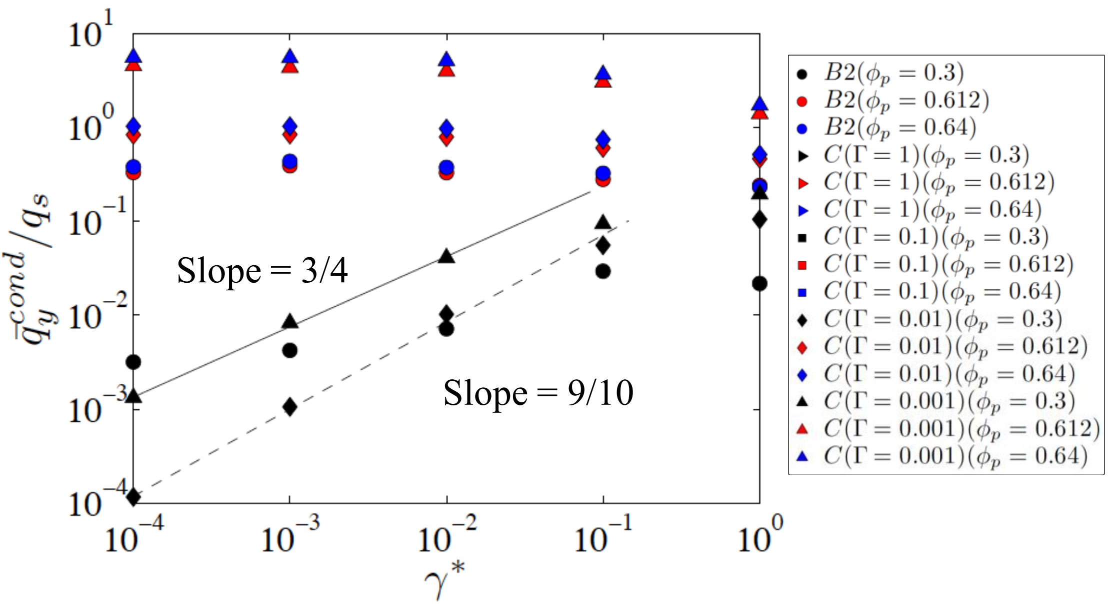
- Particles placed in a **periodic box** ($H/d_p=15$).
- Particles stiffness based on dimensionless shear rate
- Volume of liquid on the particle based on dimensionless liquid film thickness.
- Particles near the **top boundary were fixed to be wet (L_p^* = 1)** and near the **bottom boundary were fixed to be dry (L_p^* = 0)**.
- Lees-Edwards boundary conditions[5] used.
- Conductive liquid flux (q_y^{cond}) made dimensionless using q_s as the reference conductive liquid flux in the solid material the particles are made of.

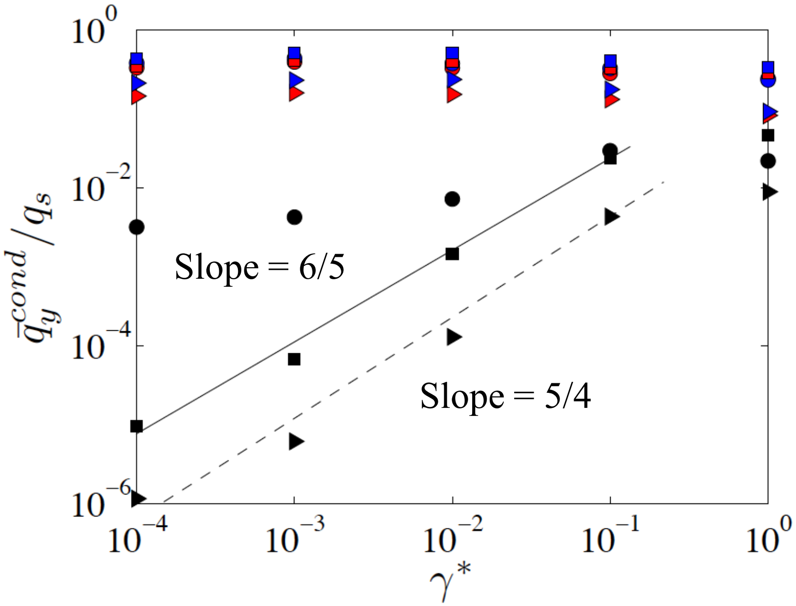
[5] Lees and Edwards, Journal of Physics C: Solid State Physics 1921 (2001).

Sheared Particle Beds

Summary of conductive liquid flux vs dimensionless shear rate

$$\Gamma = 10^{-3}, 10^{-2} \qquad \varepsilon = 2.6\cdot 10^{-6} \qquad \Gamma = 10^{-1}, 1$$





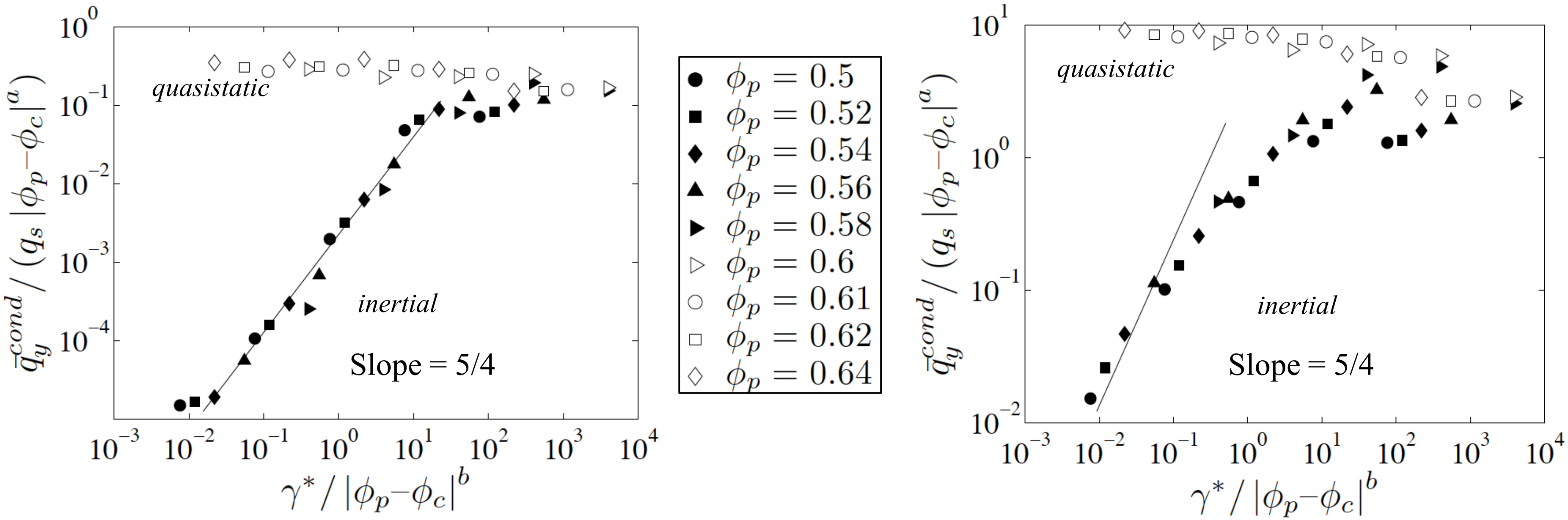
process & particle engineering

Sheared Particle Beds

TU Graz
Graz University of Technology

Summary of scaled conductive liquid flux vs dimensionless scaled shear rate

$\Gamma = 1$ $\varepsilon = 2.6 \cdot 10^{-6}$ $\Gamma = 10^{-3}$



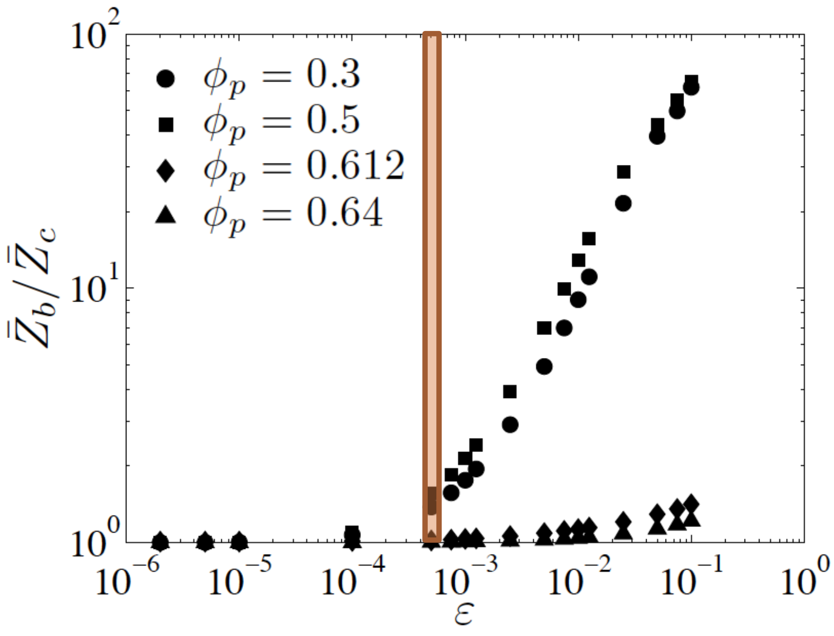
$$q_y^{cond*} / |\phi_p - \phi_c|^a = k^{inert} \left(\gamma^* / |\phi_p - \phi_c|^b \right)^{5/4}$$

Sheared Particle Beds

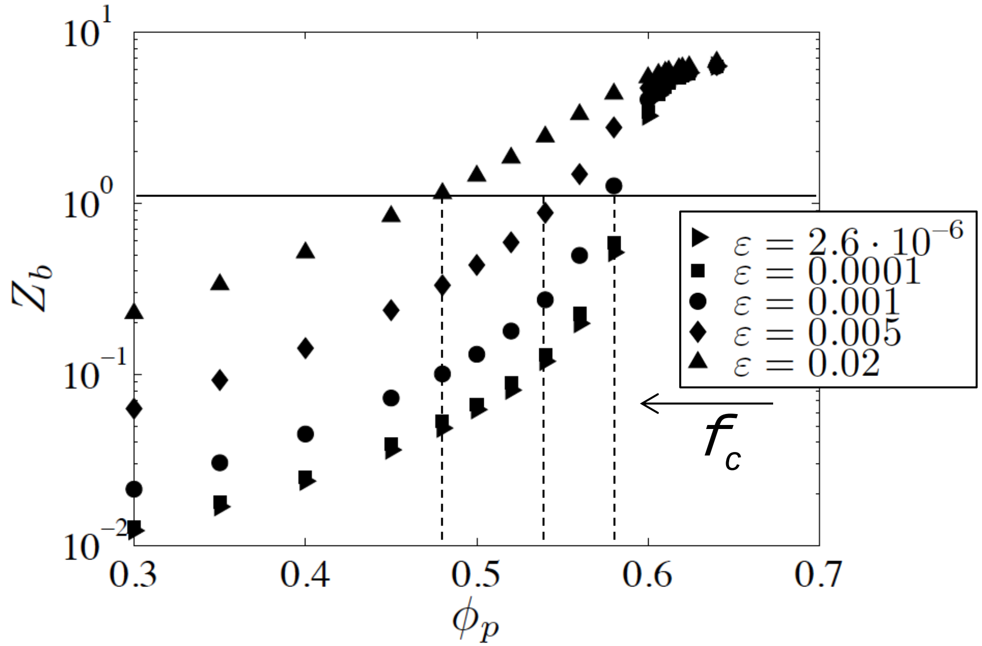
Average Coordination number (bridge and contact)

$$\overline{Z}_c = 2N_{c,tot} / N_p \qquad \overline{Z}_b = 2N_{b,tot} / N_p$$

$\Gamma = 10^{-3}$ $\gamma^* = 10^{-3}$

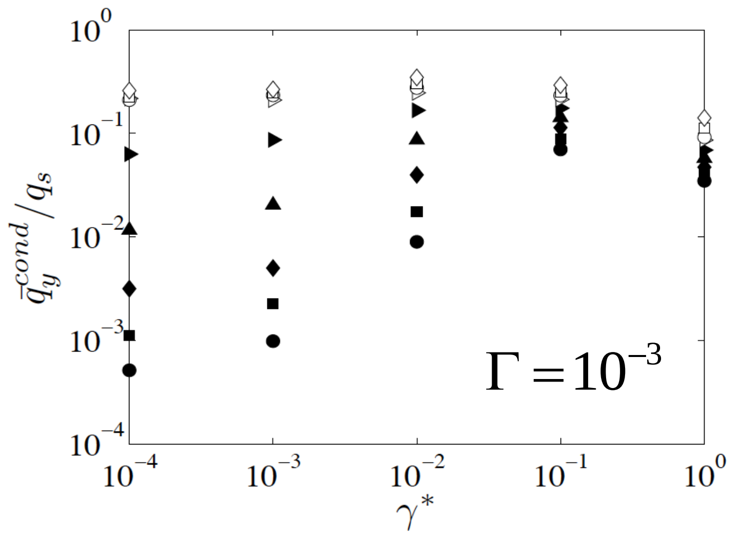


$\Gamma = 10^{-3}$ $\gamma^* = 10^{-3}$

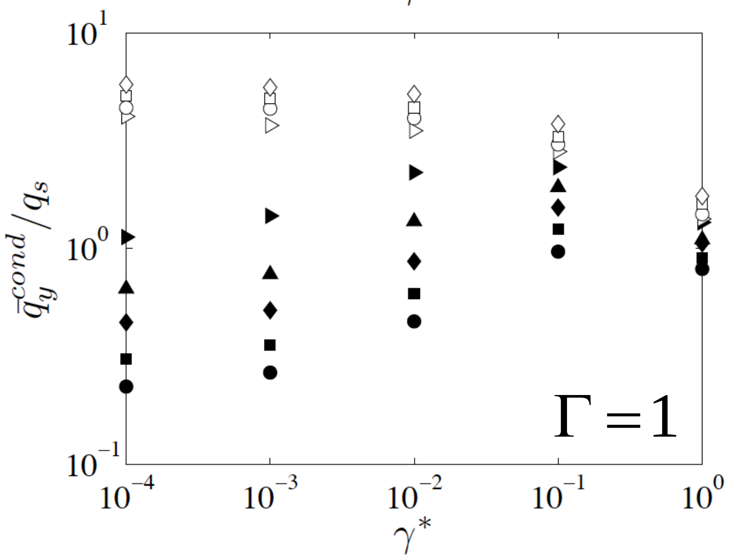


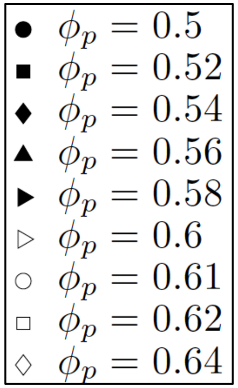
Sheared Particle Beds

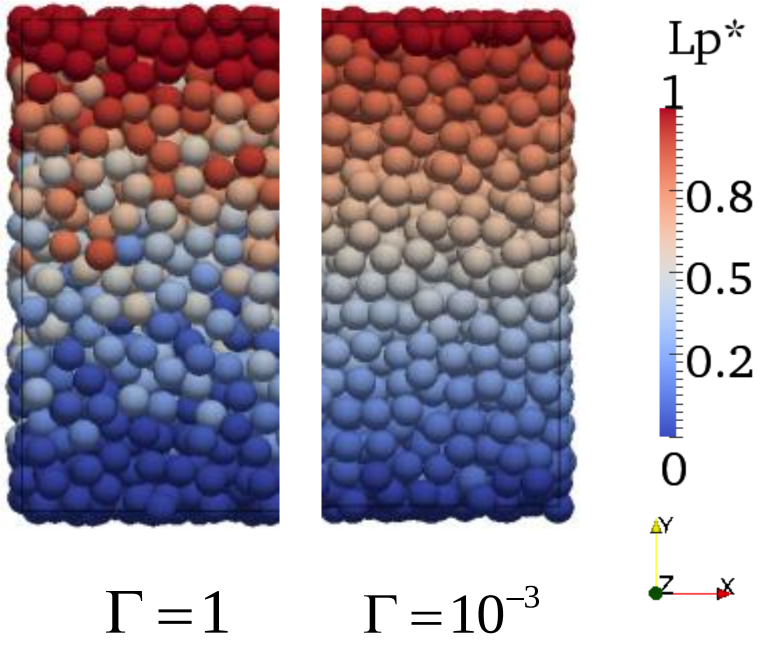
Results



$\varepsilon = 10^{-3}$



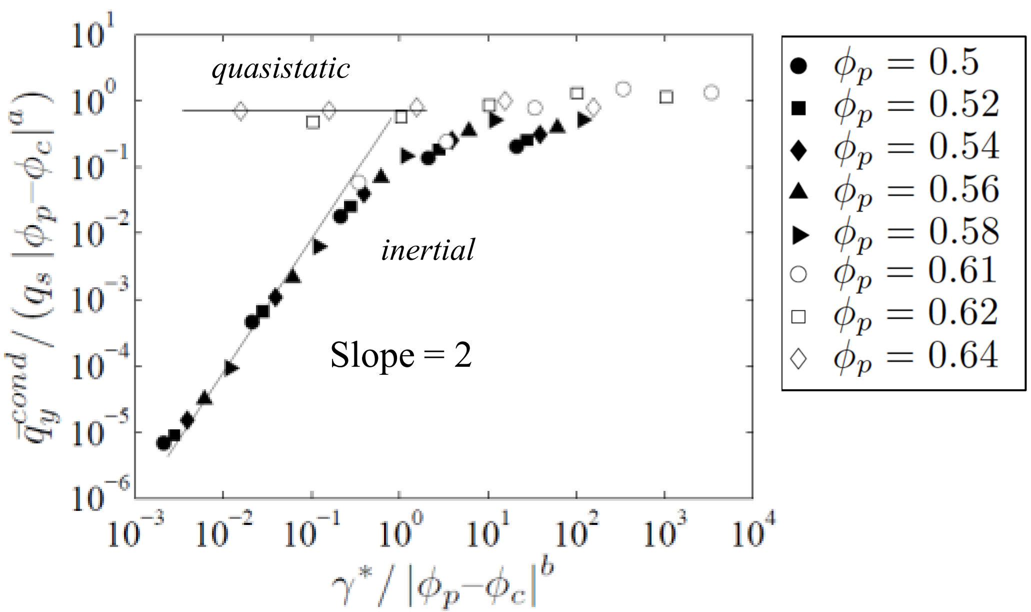




Sheared Particle Beds

Summary of scaled conductive liquid flux vs dimensionless scaled shear rate

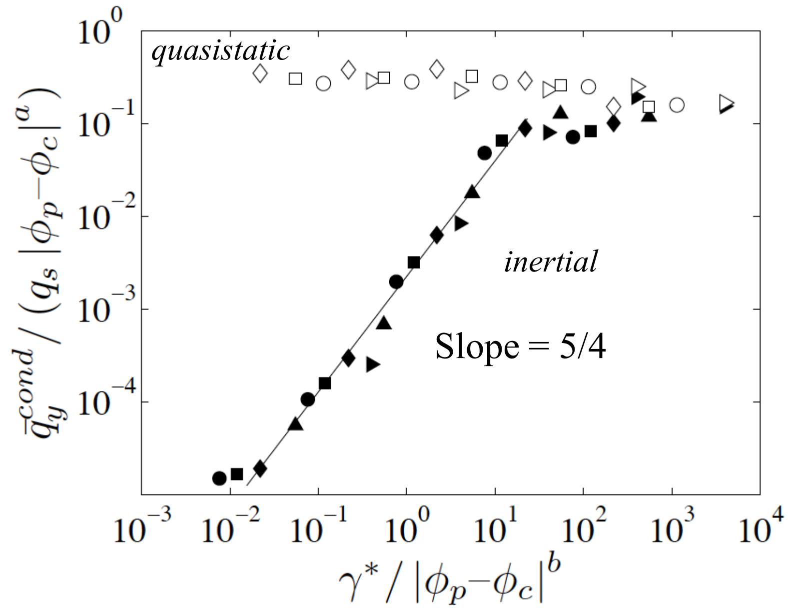
$$Pe = 10^{-2}$$



Thermal transport

$$Pe = \gamma \frac{(d_p / 2)^2}{K / \rho_p c_p}$$

$$\varepsilon = 2.6 \cdot 10^{-6} \quad \Gamma = 1$$



Liquid transport

$$\Gamma = \gamma r_{eff} \mu_l / \sigma_l$$

Conclusions

- Simplified models for liquid transfer based on different definitions of liquid transfer rates that predicts the liquid bridge formation and rupture.

- Filling rate based model for drainage of liquid into the bridge, with explicit calculation of individual liquid bridge volumes, formation and rupture.

- Effect of dimensionless liquid film thickness on the average bridge coordination number and critical particle volume fraction

- Analogy between the thermal and liquid transport

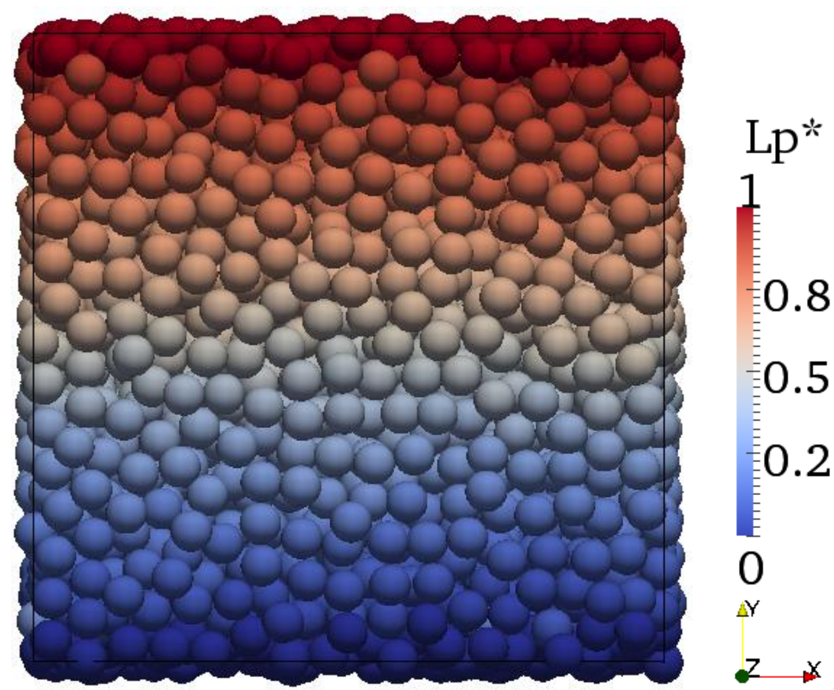
- Reference time scale for the liquid bridge filling process

$$t_{ref} = r_{eff} \cdot \frac{\mu_l}{\sigma_l}$$

process & particle engineering

TU Graz
Graz University of Technology

Predictive Capabilities of Microscopic Models for Conductive Transport in Sheared Particle Beds



Acknowledgement

Austrian Science Foundation (FWF)

FWF

(Project P23627)