Multi-level modeling of gas-fluidized beds

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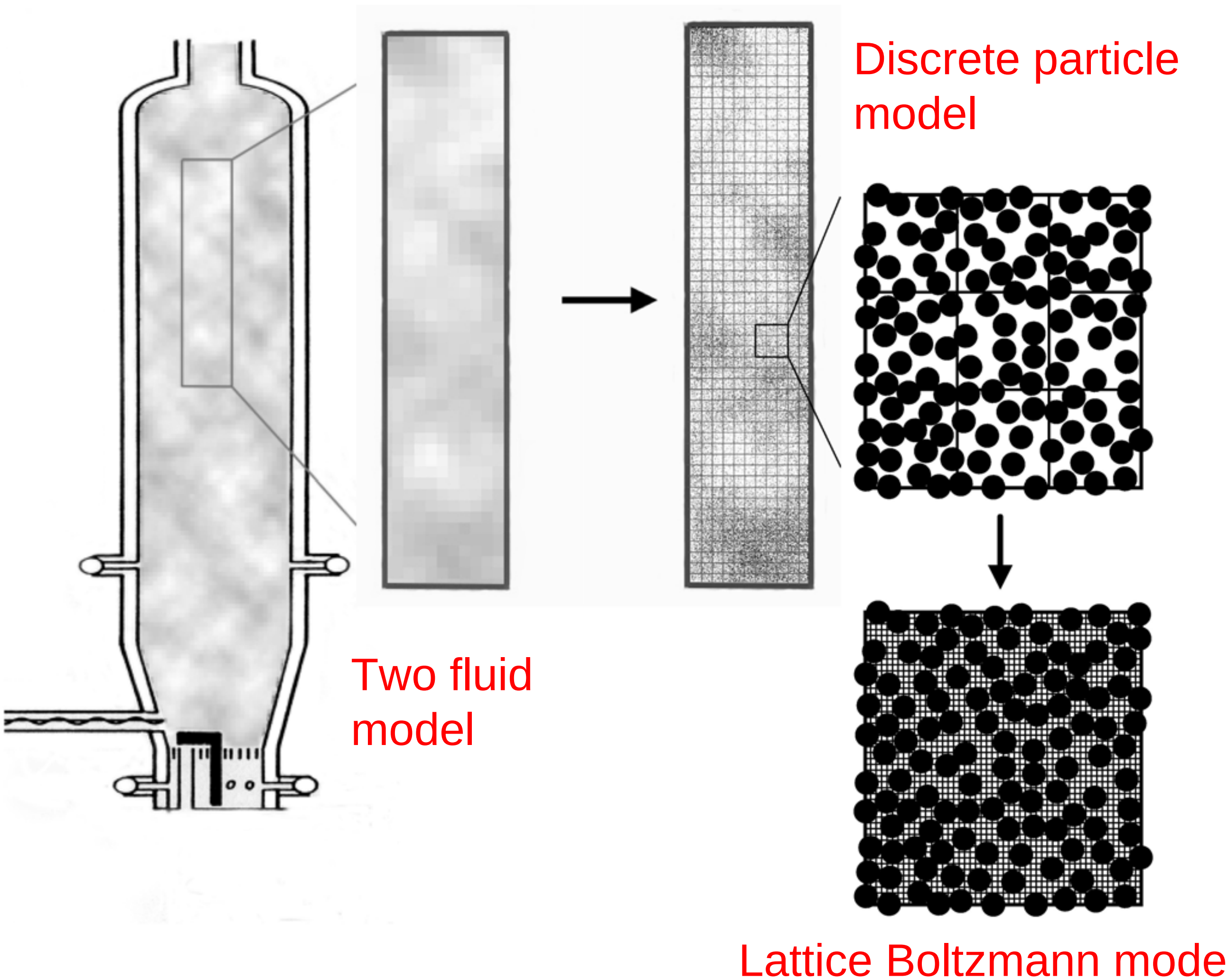
FOM

Outline

I. Overview of the models
II. Lattice Boltzmann simulations
III. Discrete particle simulations
IV. Two-fluid simulations
V. Outlook and challenges ahead

I. Overview of the models



Two Fluid Model

Gas phase:

$$\partial_t(\rho_g \vec{u}) + \vec{\nabla}\cdot(\rho_g \vec{u}\vec{u}) = -\varepsilon \vec{\nabla} P - \vec{\nabla}\cdot(\varepsilon \tau) + \beta(\vec{v} - \vec{u})$$

Solid phase:

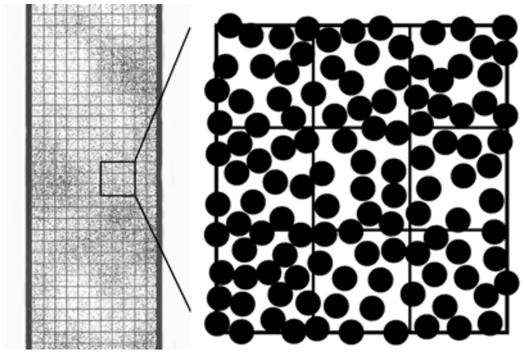
$$\partial_t(\rho_s \vec{v}) + \vec{\nabla}\cdot(\rho_s \vec{v}\vec{v}) = -\vec{\nabla} P_s - \vec{\nabla}\cdot(\varepsilon_s \tau_s) - \beta(\vec{v} - \vec{u})$$

$$\tau_s = -\mu \left[(\vec{\nabla}\vec{v}) + (\vec{\nabla}\vec{v})^T - \frac{2}{3}(\vec{\nabla} \cdot \vec{v}) I \right]$$

Gas: CFD **Solid: CFD**

Discrete Particle Model

(low resolution)



Gas phase:

$$\partial_t(\rho_g \vec{u}) + \vec{\nabla}\cdot(\rho_g \vec{u}\vec{u}) = -\varepsilon\vec{\nabla}P - \vec{\nabla}\cdot(\varepsilon\tau) + \beta(\vec{v}-\vec{u})$$

Solid phase:

$$\frac{d}{dt}m\vec{v}_i = \sum_j \vec{F}_{ij} - \frac{\beta V_i}{1-\varepsilon}(\vec{v}_i - \vec{u})$$

Particle-particle interactions (Collision forces)

Particle-gas interactions (gas-solid drag)

Gas: CFD

Solid: ***"molecular dynamics"***

Drag coefficient β : empirical relations

Most popular in chemical engineering

$$\tilde{\beta} = \frac{\beta d^2}{\mu(1-\varepsilon)} = \begin{cases} 150\,\frac{1-\varepsilon}{\varepsilon} + 1.75\,\frac{Re}{\varepsilon} & \text{Ergun (1952)} \\ 18\,(1 + 0.15\,Re^{0.687})\,\varepsilon^{-2.7} & \text{Wen \& Yu (1966)} \end{cases}$$

Other relations:

$$\tilde{\beta} = 18\,C(Re)\,\varepsilon^{-n}$$

Foscolo-Gibilaro: $C(Re) = 1 + \frac{0.44}{24}\,Re$

Schiller-Nauman: $C(Re) = \begin{cases} 1 + 0.15\,Re^{0.687} & (Re < 10^3) \\ \frac{0.44}{24}\,Re & (Re > 10^3) \end{cases}$

Turton-Levenspiel: $C(Re) = 1 + 0.173\,Re^{0.657} + \frac{0.413}{24}\left(\frac{Re}{1 + 16300 Re^{-1.09}}\right)$

Dallavalle: $C(Re) = 1 + 0.2625\,Re^{0.5} + \frac{0.413}{24}\,Re = \left(1 + \frac{0.63}{4.8}\,Re^{1/2}\right)^2$

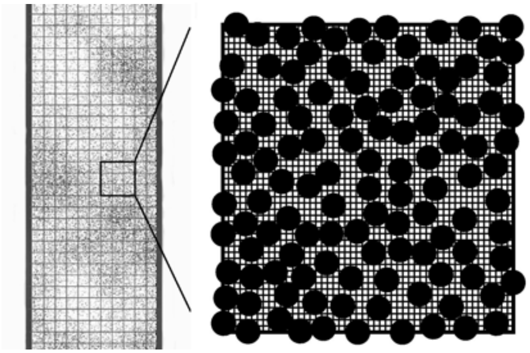
Clift-Grace-Weber: $C(Re) = \begin{cases} 1 + \frac{3}{16}\,Re & (Re < 0.01) \\ 1 + 0.1315\,Re^{0.82 - 0.05\log Re} & (0.01 < Re < 20) \\ 1 + 0.1935\,Re^{0.6305} & (20 < Re < 260) \\ 1.8335\,Re^{-0.1242 + 0.1558\log Re} & (260 < Re < 1500) \end{cases}$

Di Felice (1994):

$$2.7 - 0.65\exp\left(-\frac{1}{2}(1.5 - \log Re)^2\right)$$

Lattice Boltzmann Model

(high resolution)



Gas phase:

$$\partial_t(\rho_g \vec{u}) + \vec{\nabla}\cdot(\rho_g \vec{u}\vec{u}) = -\varepsilon \vec{\nabla} P - \vec{\nabla}\cdot(\varepsilon \tau) + \text{"boundary conditions"}$$

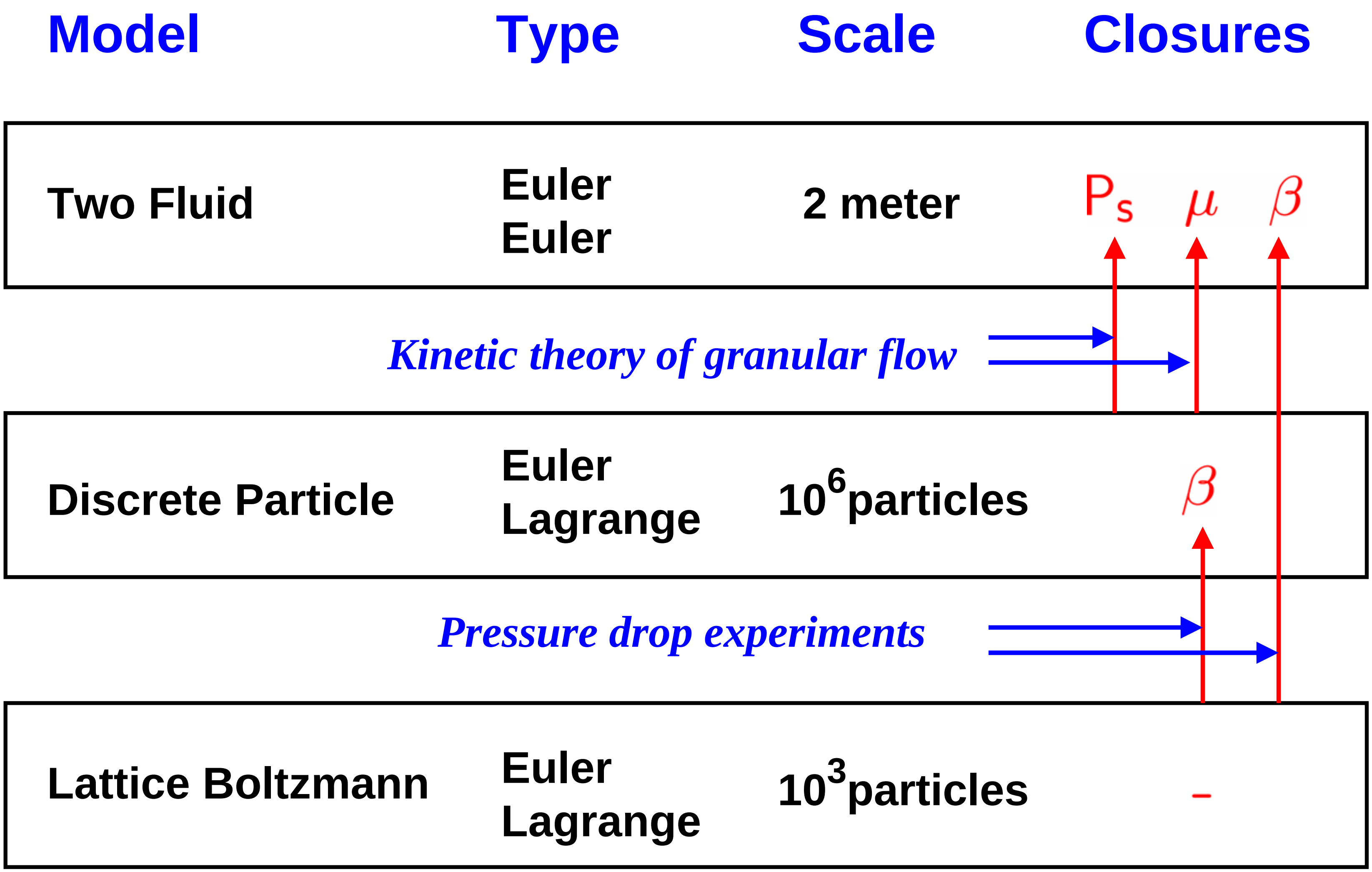
Solid phase:

$$\frac{d}{dt} m\vec{v}_i = \sum_j \vec{F}_{ij} + \vec{F}_{d,i}$$

Particle-particle interactions (Collision forces)

Particle-gas interactions (gas-solid drag)

Gas: ***Lattice Boltzmann*** **Solid:** ***"molecular dynamics"***

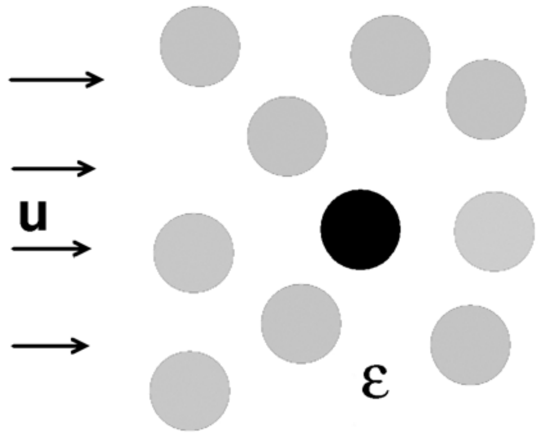

Model
Type
Scale
Closures
Two Fluid
Euler
Euler
2 meter
P_s μ β
Kinetic theory of granular flow
Discrete Particle
Euler
Lagrange
10^6particles
β
Pressure drop experiments
Lattice Boltzmann
Euler
Lagrange
10^3particles
–

II. Gas-solid drag force from lattice Boltzmann simulations

A. **Low Reynolds numbers**
B. **High Reynolds numbers**
C. **Binary systems**

A. Drag force for low Reynolds numbers

$$\tilde{\beta} = \frac{\beta d^2}{\mu(1-\varepsilon)}$$



$$\vec{F} = \frac{\tilde{\beta}}{18} 3\pi\mu d\vec{u}$$

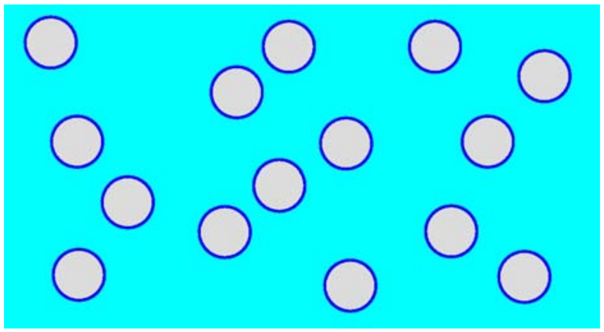
Darcy (1856): $\vec{\nabla} P = \frac{\varepsilon}{\kappa}\mu\vec{u}$

Force Balance: $\vec{\nabla} P = \frac{1-\varepsilon}{\varepsilon}\frac{\vec{F}}{V_p}$

$$\longrightarrow \tilde{\beta} = \frac{\varepsilon^2}{1-\varepsilon}\frac{d^2}{\kappa}$$

Carman-Kozeny approximation:

$$\kappa = \frac{\varepsilon}{k}\, r_h^2$$



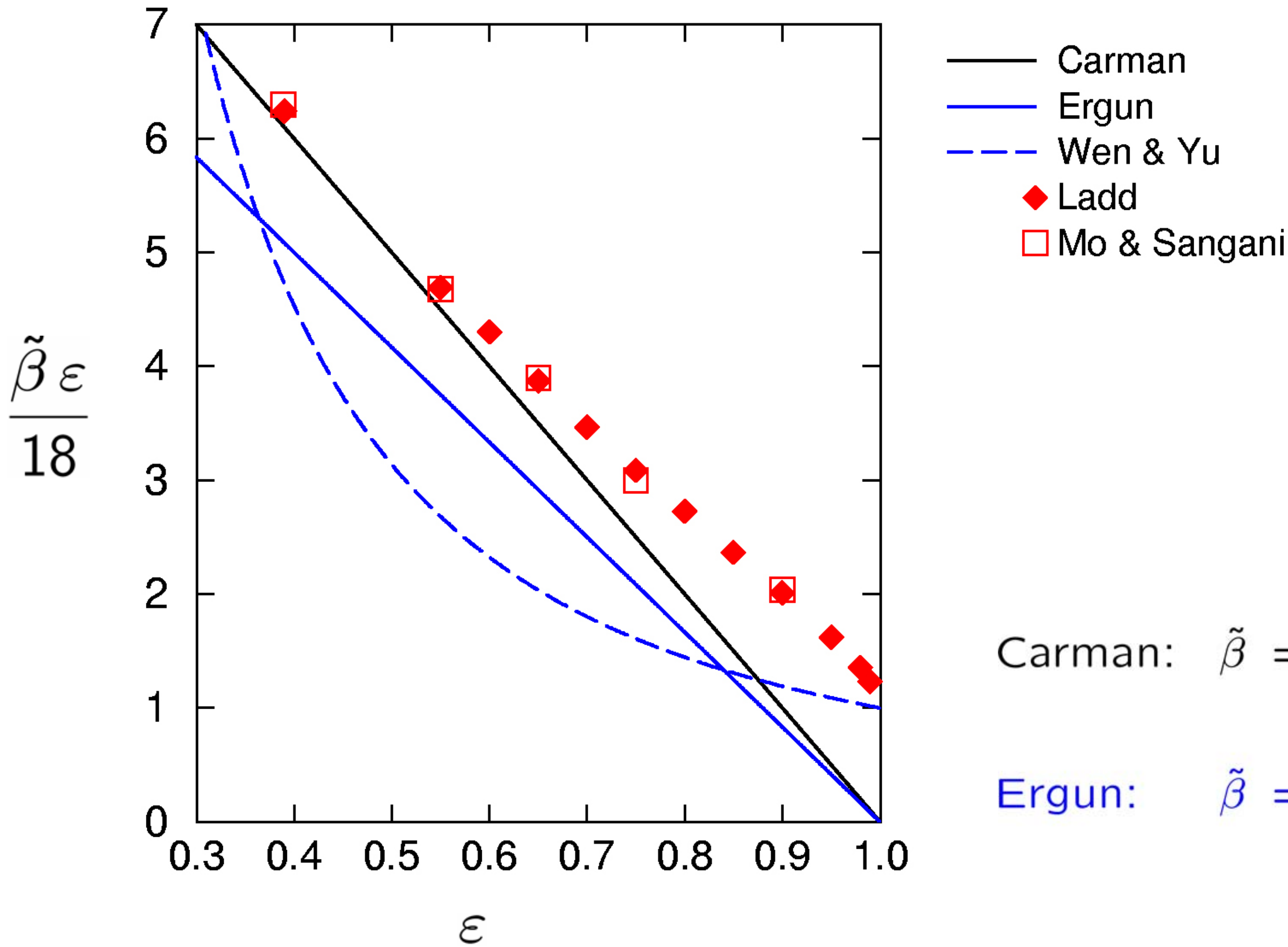
$$r_h = \quad$$  $$= \frac{\varepsilon \pi d^3/6}{(1-\varepsilon)\pi d^2} = \frac{\varepsilon d}{6(1-\varepsilon)}$$

$$k = \text{Kozeny constant} \approx 5$$

$$\downarrow$$

$$\tilde{\beta} = \frac{\varepsilon^2}{1-\varepsilon}\,\frac{d^2}{\kappa} \quad \longrightarrow \quad \boxed{\tilde{\beta} = 180\,\frac{1-\varepsilon}{\varepsilon}}$$

Carman equation



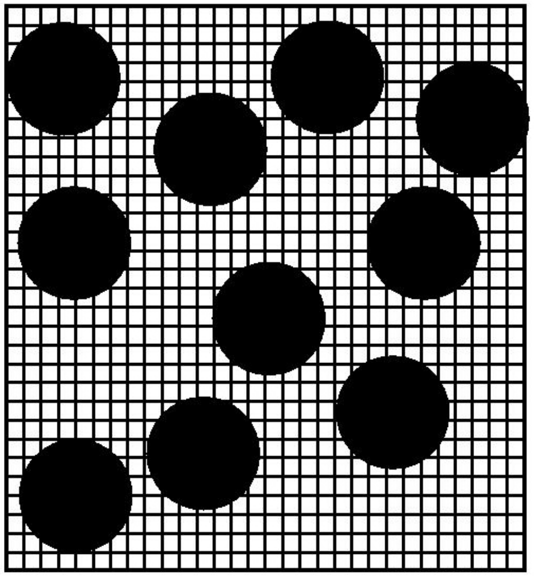
Carman: $\tilde{\beta} = 180\,\frac{1-\varepsilon}{\varepsilon}$

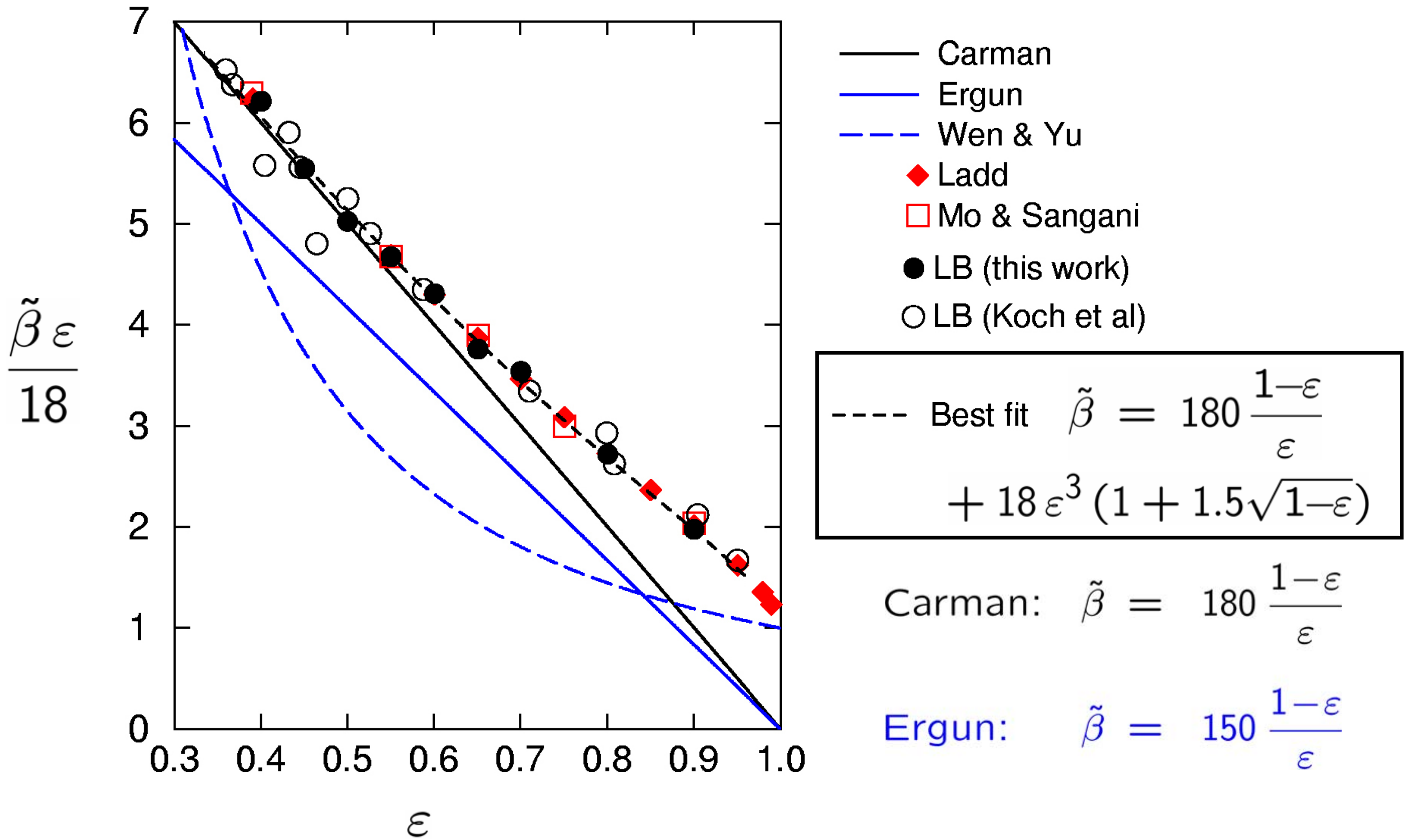
Ergun: $\tilde{\beta} = 150\,\frac{1-\varepsilon}{\varepsilon}$

Lattice Boltzmann Simulations

Simulation details:

- 54 static particles, PBC
- $\varepsilon = 0.4 - 0.9$
- d = 8, 17 and 33 lattice sites
- Results extrapolated to $d = \infty$

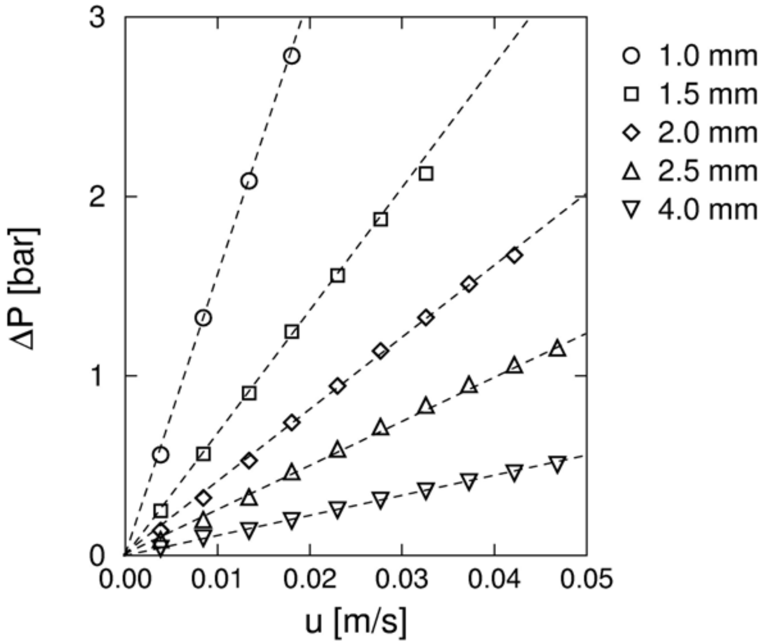



Carman
Ergun
Wen & Yu
Ladd
Mo & Sangani
LB (this work)
LB (Koch et al)
Best fit $\tilde{\beta} = 180 \frac{1-\varepsilon}{\varepsilon} + 18\,\varepsilon^3 (1 + 1.5\sqrt{1-\varepsilon})$
Carman: $\tilde{\beta} = 180 \frac{1-\varepsilon}{\varepsilon}$
Ergun: $\tilde{\beta} = 150 \frac{1-\varepsilon}{\varepsilon}$
$\frac{\tilde{\beta}\,\varepsilon}{18}$
ε
0
1
2
3
4
5
6
7
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Pressure drop measurements

Liquid: glycerine

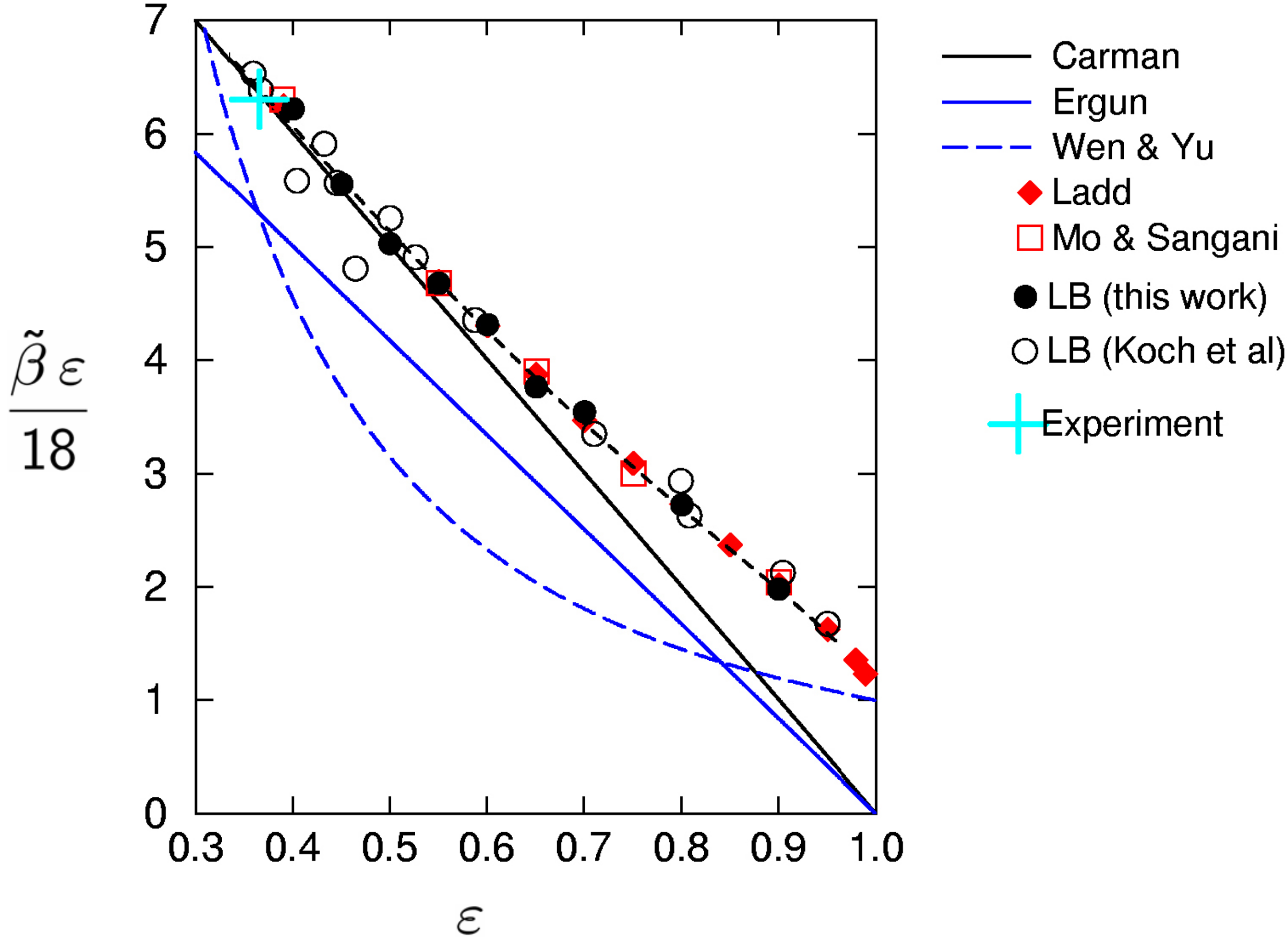
Bed: glass spheres (ε = 0.365)



$$\vec{\nabla} P = \frac{\varepsilon}{\kappa}\mu\vec{u}$$

$$\tilde{\beta} = \frac{\varepsilon^2}{1-\varepsilon}\frac{d^2}{\kappa} \quad \Rightarrow \quad \tilde{\beta}(0.365) = 41.4$$

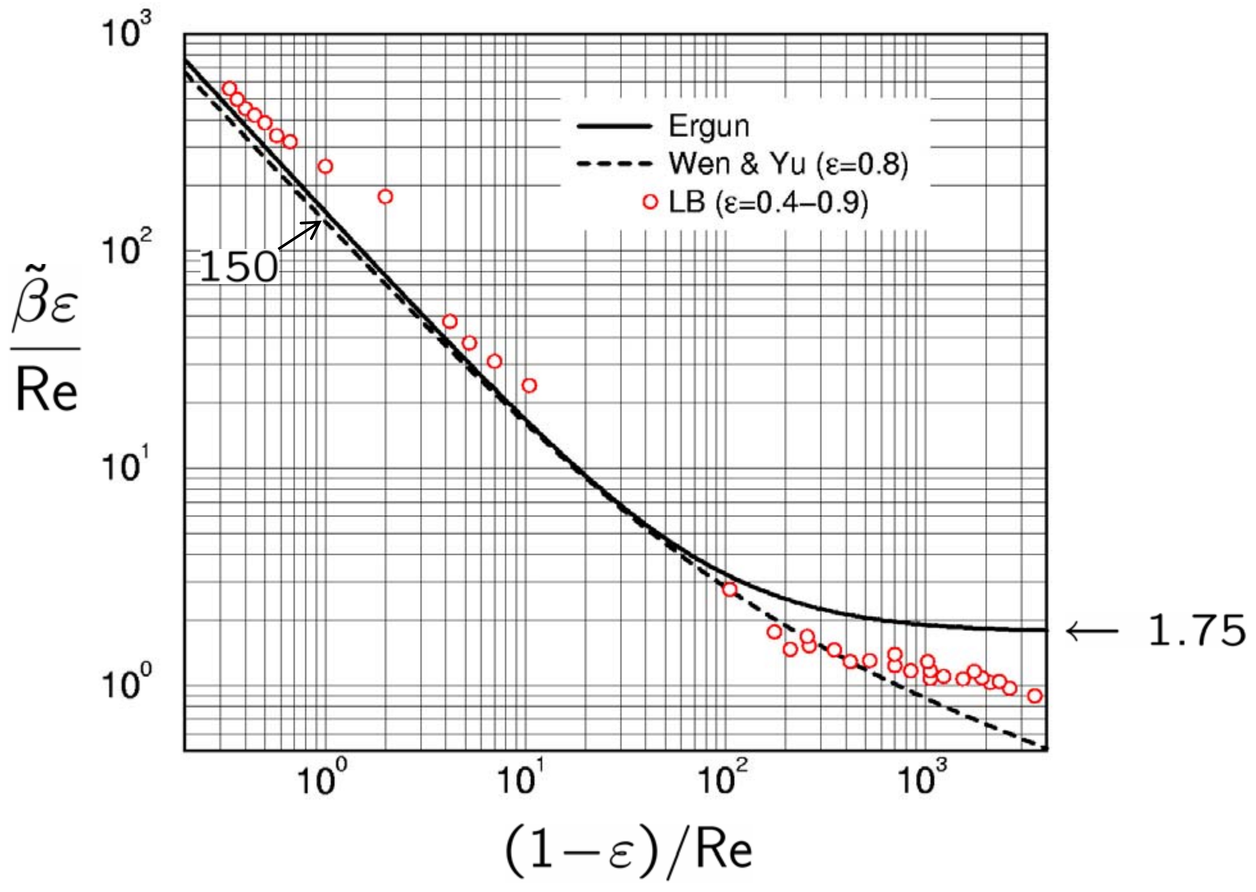
Wil Paping, Masters Thesis dec. 2004



7
6
5
4
3
2
1
0
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
$\frac{\tilde{\beta}\,\varepsilon}{18}$
ε
Carman
Ergun
Wen & Yu
Ladd
Mo & Sangani
LB (this work)
LB (Koch et al)
Experiment

B. Drag force for 10 < Re < 1000

Ergun: $\tilde{\beta} = 150\frac{1-\varepsilon}{\varepsilon} + 1.75\frac{\text{Re}}{\varepsilon} \quad \Rightarrow \quad \frac{\tilde{\beta}\varepsilon}{\text{Re}} = 150\left(\frac{1-\varepsilon}{\text{Re}}\right) + 1.75$



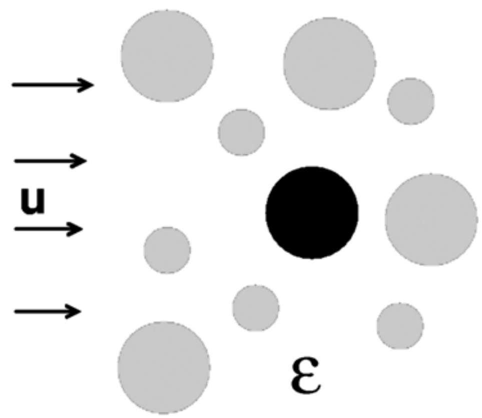
Best fit to LBM data for arbitrary Re numbers

$$\tilde{\beta} = 180\,\frac{1-\varepsilon}{\varepsilon} + 18\,\varepsilon^3\,(1 + 1.5\sqrt{1-\varepsilon})$$

$$+\ 0.31\,\frac{\mathrm{Re}}{\varepsilon}\left[\frac{\varepsilon^{-1} + 3\varepsilon(1-\varepsilon) + 8.4\,\mathrm{Re}^{-0.343}}{1 + 10^{3(1-\varepsilon)}\mathrm{Re}^{-(5-4\varepsilon)/2}}\right]\ .$$

NB: Ergun equation: $$\tilde{\beta} = 150\,\frac{1-\varepsilon}{\varepsilon} + 1.75\,\frac{\mathrm{Re}}{\varepsilon}$$

C. Drag force in binary systems



$$y_i = d_i / \langle d \rangle$$

$$\vec{F}_i = \frac{\tilde{\beta}_i}{18} 3\pi\mu d_i \vec{u}$$

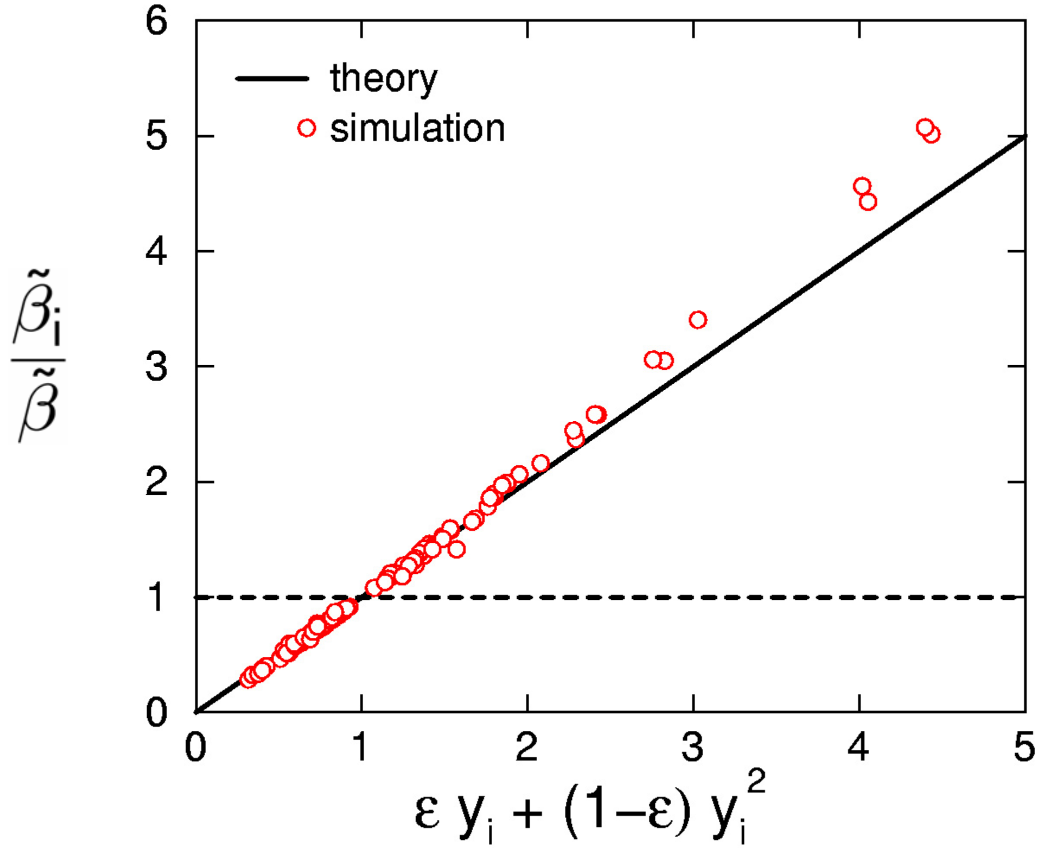
$$\downarrow$$

$$\tilde{\beta}_i = \tilde{\beta} \, ?$$

Carman-Kozeny:

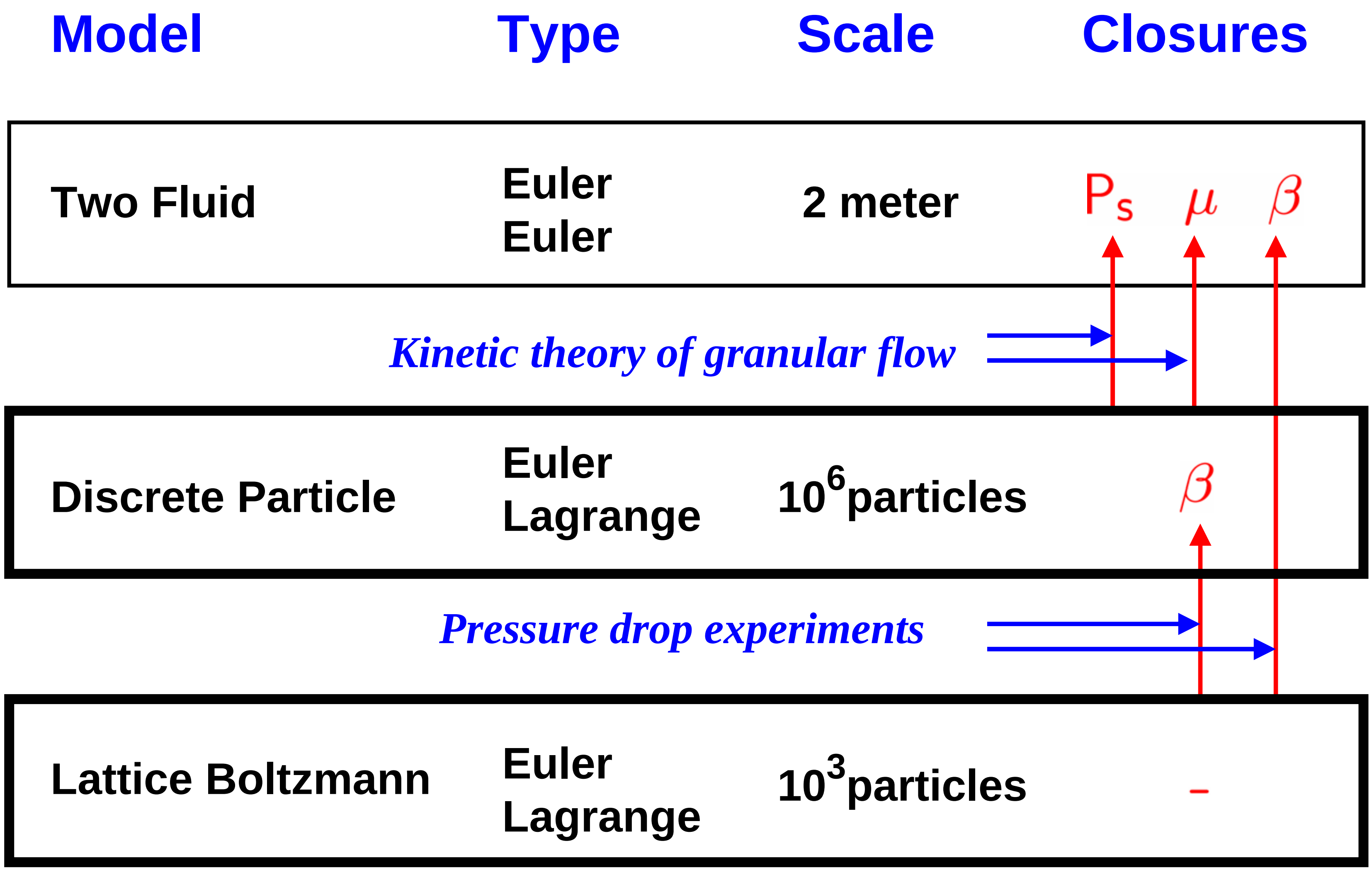
$$\tilde{\beta}_i = \left[\varepsilon\, y_i + (1-\varepsilon)\, y_i^2\right] \tilde{\beta}$$

$$\frac{\tilde{\beta}_i}{\tilde{\beta}} = \varepsilon\, y_i + (1-\varepsilon)\, y_i^2 \qquad y_i = \frac{d_i}{\langle d \rangle}$$



Re = 100

VDH, Beetstra & Kuipers,
J. Fluid Mech. 528 (2005)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Kinetic theory of granular flow
Discrete Particle
Euler
Lagrange
10^6 particles
β
Pressure drop experiments
Lattice Boltzmann
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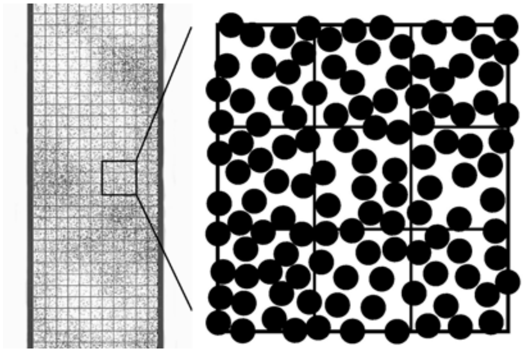
10^3 particles
–

III. Discrete particle simulations

A. Discrete particle model
B. Segregation: effect of the drag model
C. Simulation of fine powders
D. Pressure from DPM simulations

A. Discrete Particle Model



Gas phase:

$$\partial_t(\rho_g \vec{u}) + \vec{\nabla}\cdot(\rho_g \vec{u}\vec{u}) = -\varepsilon\vec{\nabla}P - \vec{\nabla}\cdot(\varepsilon\tau) + \beta(\vec{v}-\vec{u})$$

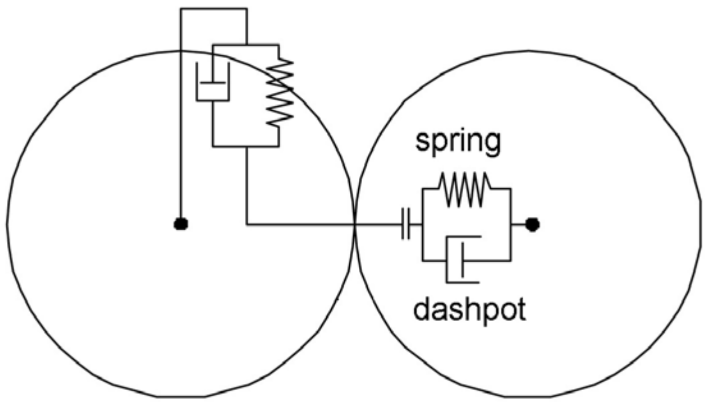
Solid phase:

$$\frac{d}{dt} m\vec{v}_i = \sum_j \vec{F}_{ij} - \frac{\beta V_i}{1-\varepsilon}(\vec{v}_i - \vec{u})$$

Particle-particle interactions

Particle-particle interaction force F_{ij}

- Collision forces : spring-dashpot model



$$\vec{F}_{ij,n} = -k\,\delta\,\vec{n}_{ij} - \eta\,\vec{v}_{ij,n}$$

spring constant (k)

damping coefficient (η)

- Electrostatic force $$\vec{F}_{ij} = -\frac{q^2}{4\pi\epsilon}\frac{\vec{n}_{ij}}{r_{ij}^2}$$

- Cohesive force $$\vec{F}_{ij} = \frac{Ad}{6}\frac{\vec{n}_{ij}}{s_{ij}^2}$$

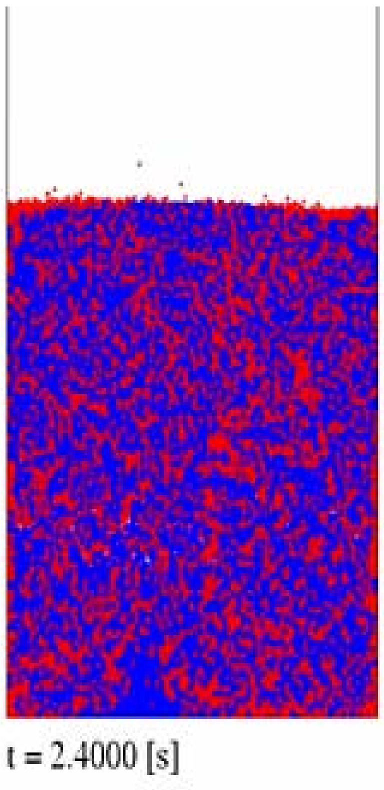
B. Effect of drag on segregation

Binary mixture of 40 000 particles:

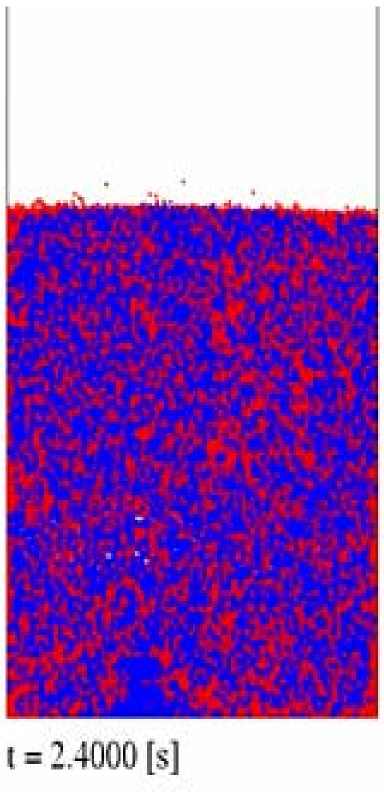
Red: 1.5 mm
U_{mf} = 0.9 m/s

Blue: 2.5 mm
U_{mf} = 1.3 m/s

Fluidized at
U = 1.3 m/s

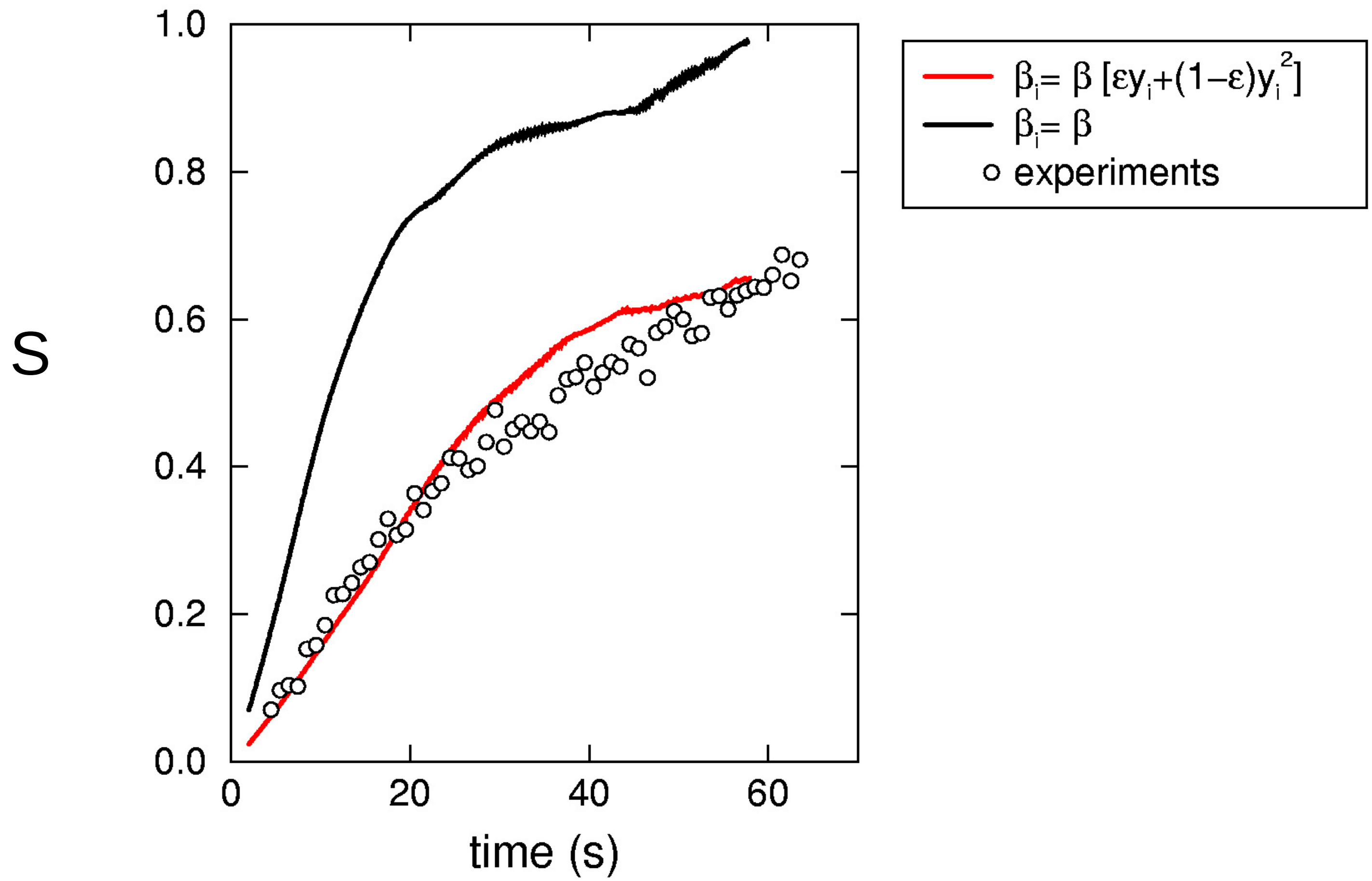


$$\beta_i = \beta$$

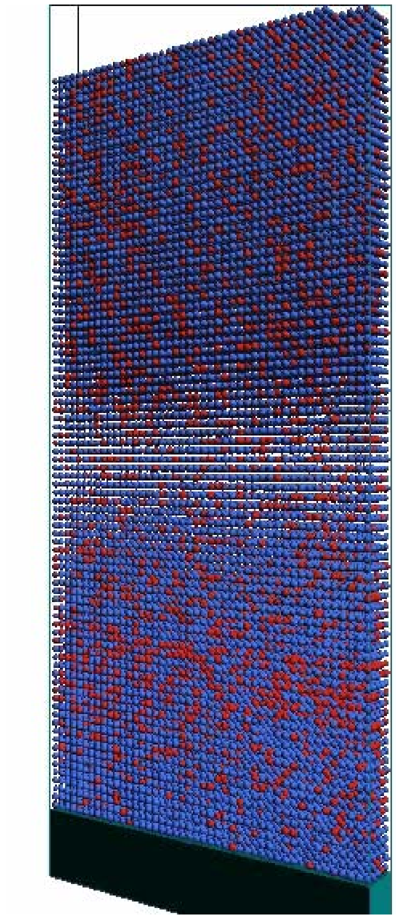


$$\beta_i = [\varepsilon y_i + (1-\varepsilon) y_i^2]\,\beta$$

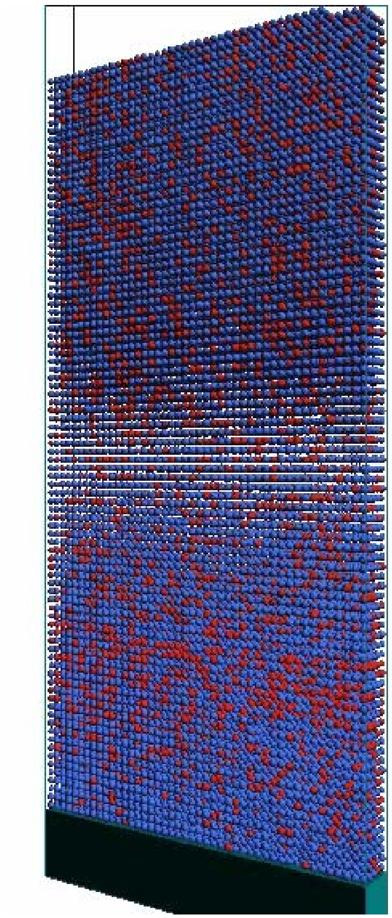
$$S = \frac{R-1}{R_{max}-1} \quad \text{with} \quad R = \frac{\langle h_1 \rangle}{\langle h_2 \rangle}$$



Intermezzo: Segregation in vibro-fluidized systems



No air



Air

N. Burtally, P.J. King
and Michael Swift

Science 2002

Bronze and glass
spheres of the
same size (100 μm)

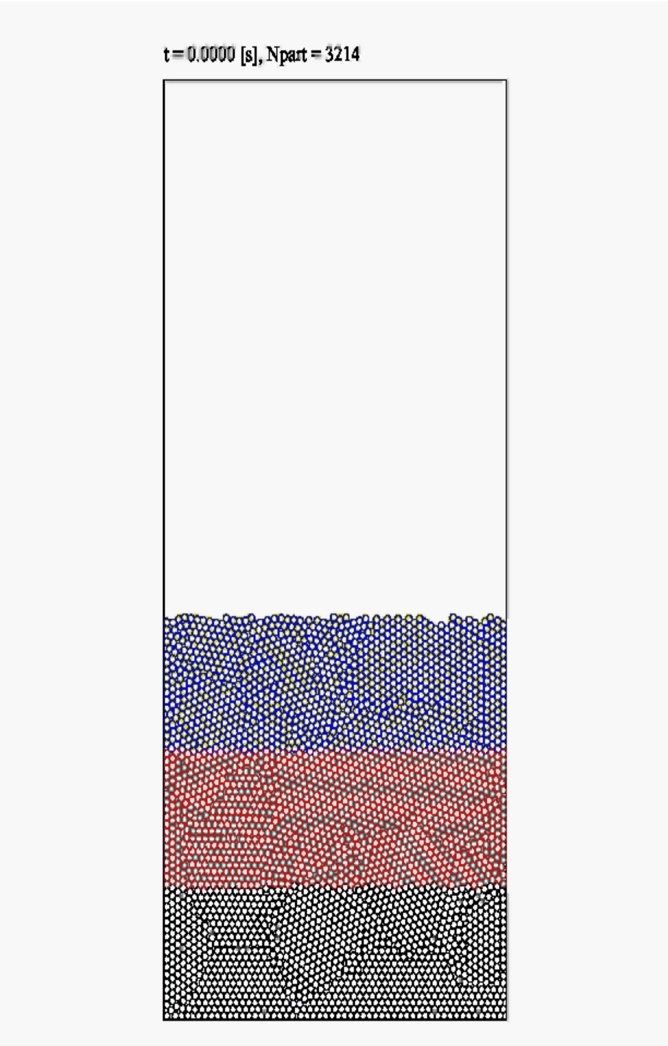
Simulation:

$$N_p = 25000$$

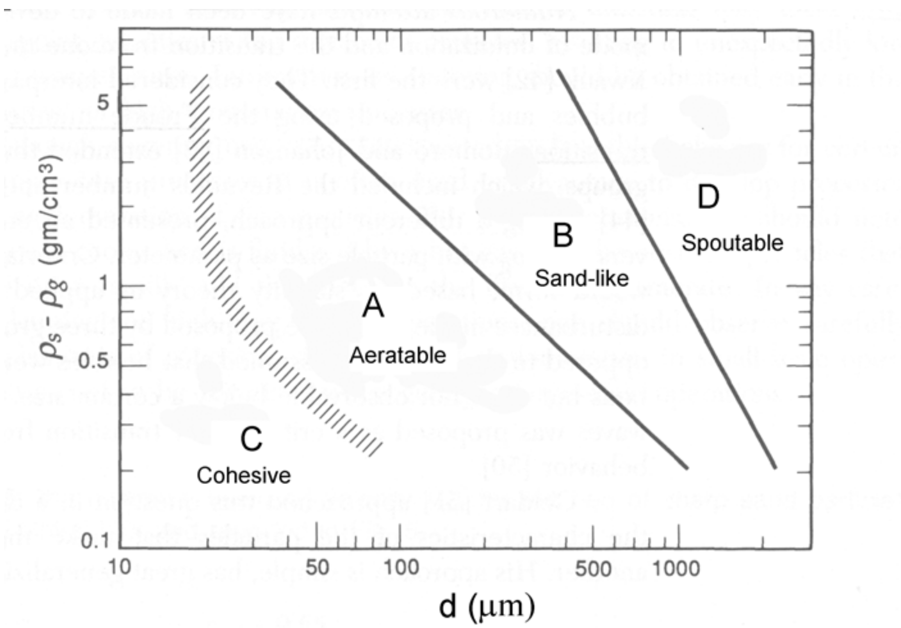
$$f = 40\text{Hz}$$

$$\Gamma = a\omega^2/g = 7$$

C. Simulation of fine powders (group A)



Geldart classification:

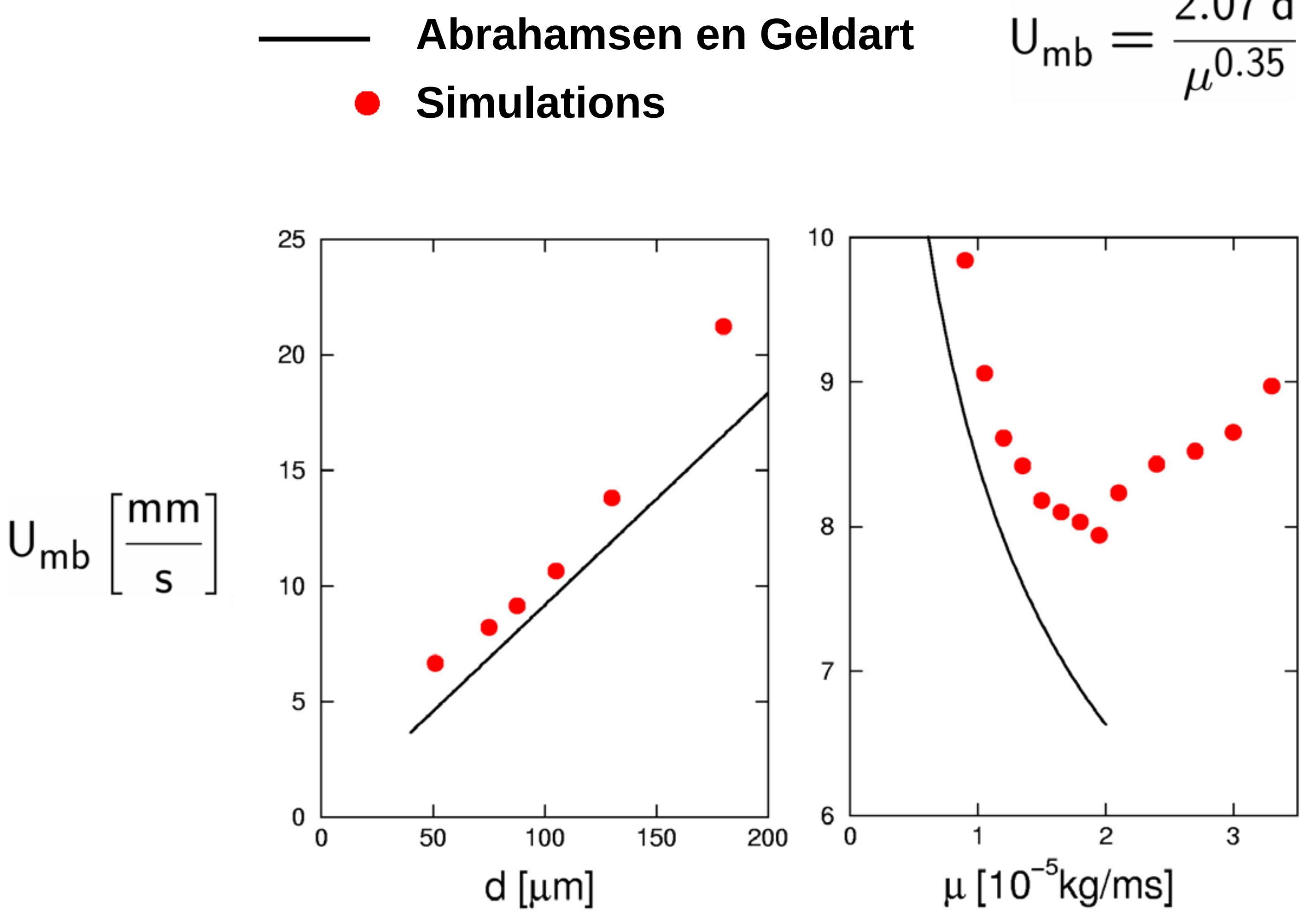


$$U_{mb} = \frac{2.07\,d}{\mu^{0.35}}$$

$$U_{mf} = \frac{(\rho_s - \rho_g)d^2}{150\mu}$$

$$\rho_s - \rho_g = \frac{310\mu^{0.65}}{d}$$

$$U_{mb} = \frac{2.07\ d}{\mu^{0.35}}$$



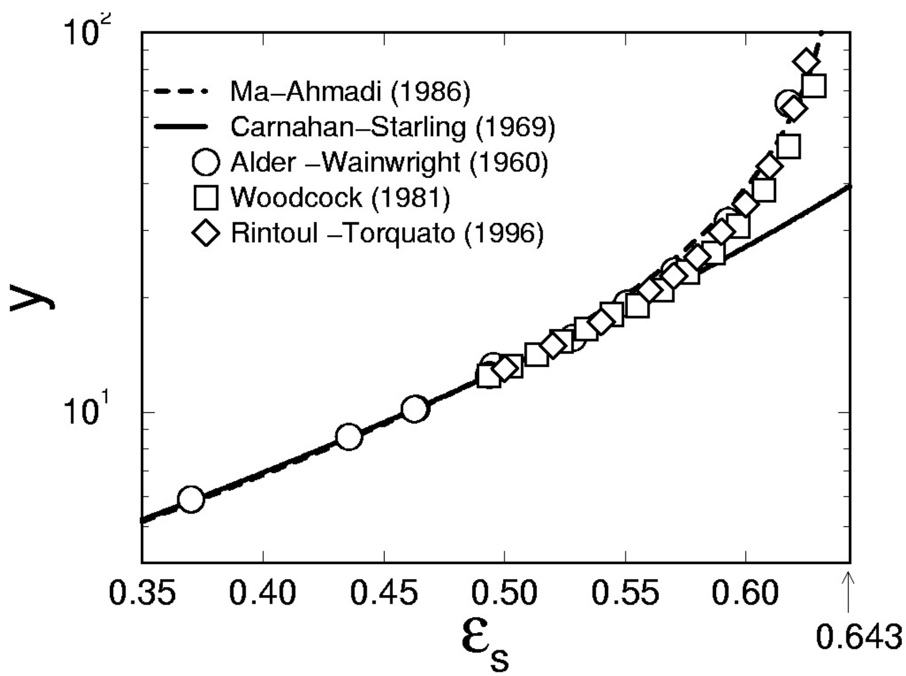
D. Solids pressure from DPM simulations

Low density: $$P_s = \rho_s \theta$$

High density: $$P_s = \rho_s \theta \,(1 + y)$$

Elastic spheres in vacuum: Carnahan & Stirling (1969)

$$y_e = \frac{\varepsilon_s (4 - 2\varepsilon_s)}{(1 - \varepsilon_s)^3}$$

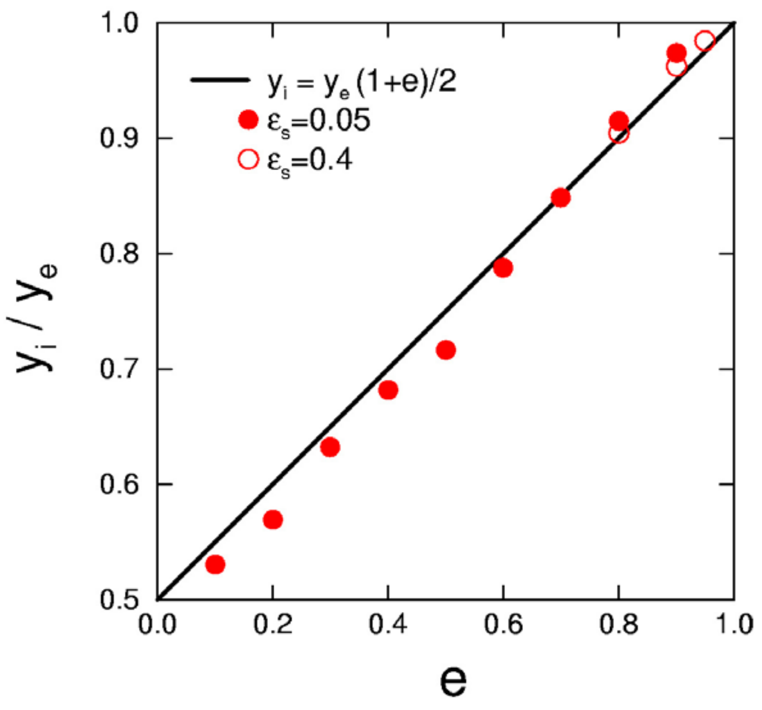


Inelastic spheres in vacuum:

$$y_i = y_e \left(\frac{1+e}{2}\right)$$

Simulations:

$$y = \frac{1}{6mN\theta} \langle \sum_{ij} \vec{F}_{ij} \cdot \vec{r}_{ij} \rangle$$



Model	Type	Scale	Closures
Two Fluid	Euler Euler	2 meter	P_s μ β
Discrete Particle	Euler Lagrange	10^6 particles	β
Lattice Boltzmann	Euler Lagrange	10^3 particles	–

Kinetic theory of granular flow → P_s, μ

Pressure drop experiments → β

Summary

Lattice Boltzmann simulations: drag force

- Monodisperse: significant deviations with Ergun & Wen/Yu
- Bidispersity has a much larger effect than currently assumed

Discrete particle simulations

- Segregation: good agreement with experiments
- A powders: qualitative agreement with the Geldart correlation
- Pressure: excellent agreement with kinetic theory

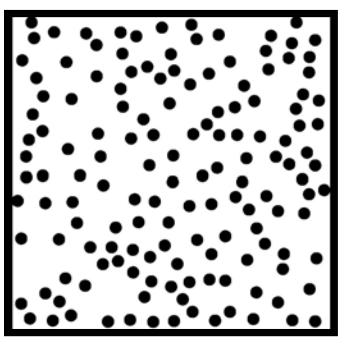
Two fluid simulations

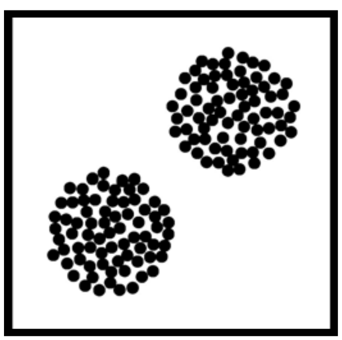
- Coefficient of restitution gives rise to heterogeneous structures
- Reasonable agreement with the experiments for the bubble size

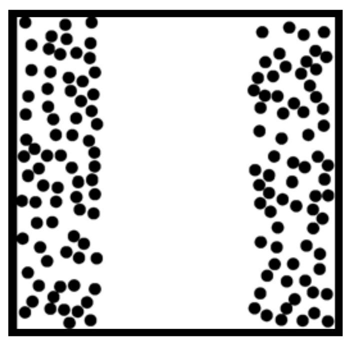
IV. Outlook & Challenges ahead

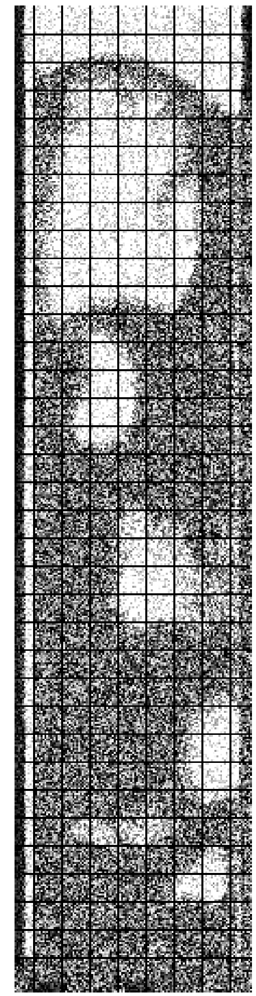
A. Drag force

- Bidisperse → polydisperse
- Mobility
- Heterogeneity









B. Closures in two-fluid model (monodisperse)

Drag coefficient β $\longrightarrow$ Lattice Boltzmann ✓

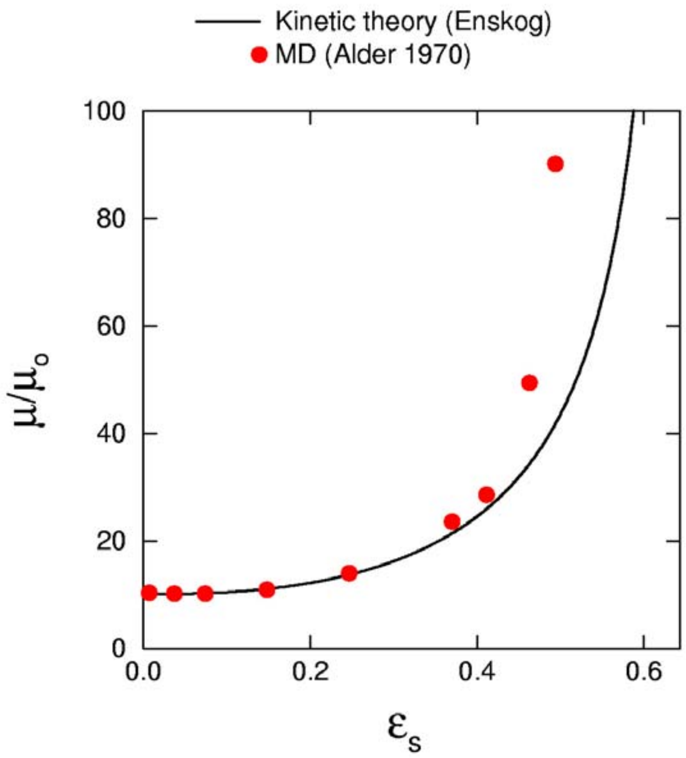
Solids pressure P_s $\longrightarrow$ $P_s = \rho_s \theta (1 + y_i)$

$$y_i = y_e \left(\frac{1+e}{2} \right)$$ ✓

Solids viscosity μ $\longrightarrow$ $\mu = \mu_o \, 4 \left(\frac{1}{y_i} + \frac{4}{5} + 0.761 \, y_i \right)$ **?**

Elastic spheres:

$$\mu = \mu_o \, 4 \left(\frac{1}{y_e} + \frac{4}{5} + 0.761 \, y_e \right)$$



Inelastic spheres:

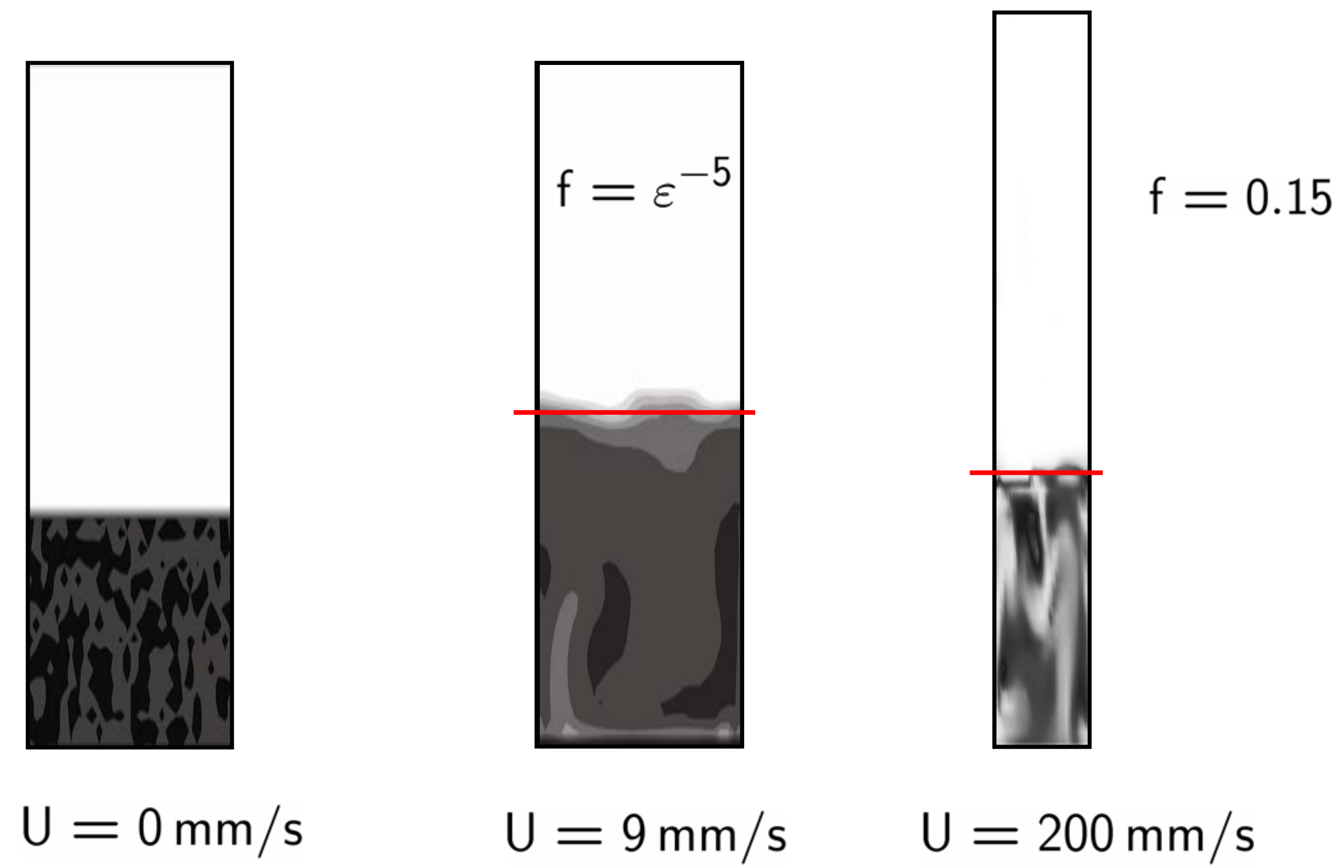
No simulation data available

$$\mu = \frac{1}{\theta V} \int_0^\infty \langle \tau_{xy}(0) \tau_{xy}(s) \rangle ds$$

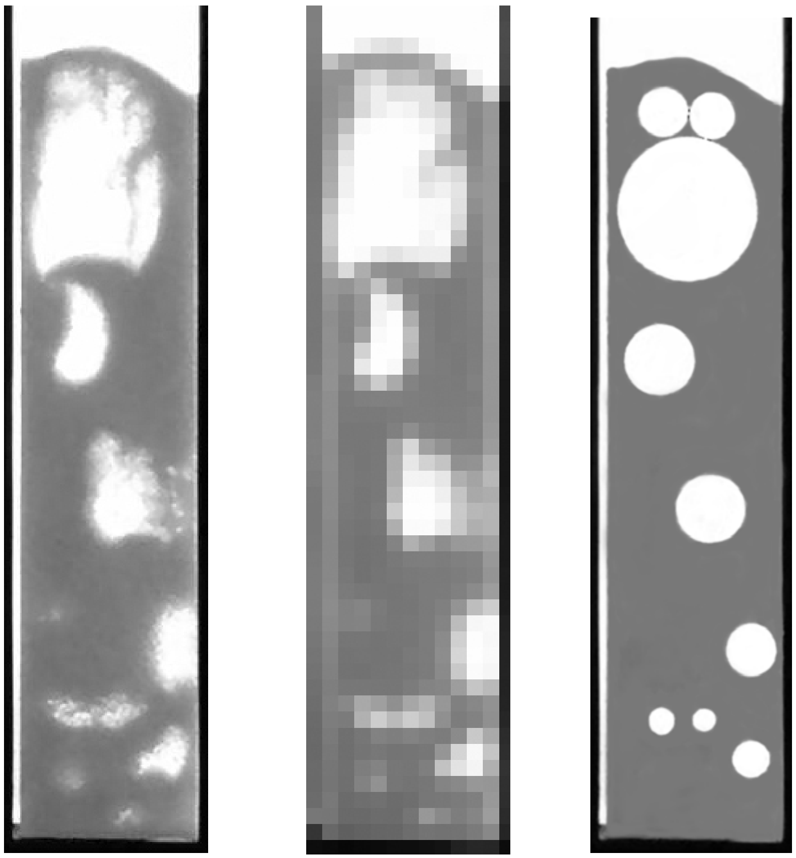
- Effect surrounding gas
- Particle friction
- Cohesive forces
- Polydispersity

C. Two-fluid simulations of Geldart A particles

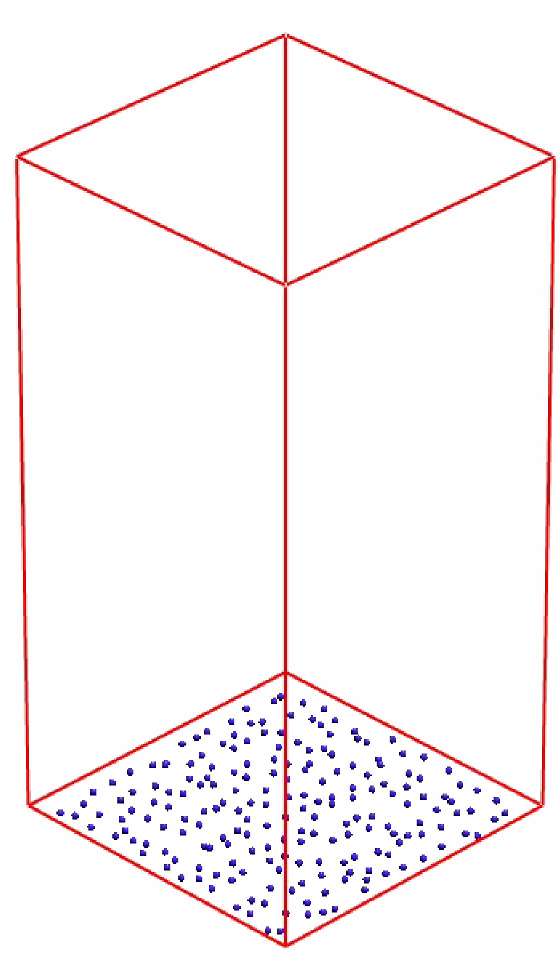
$$d = 75\,\mu\text{m}\;,\;\; \rho_s = 1500\,\text{kg/m}^3 \quad \longrightarrow \quad U_{mb} = 7\ \text{mm/s}$$



D. Simulations of industrial scale fluidized beds



real | two fluid model | discrete bubble model



Van Sint Annaland, Bokkers & Kuipers,

Industrial scale column:

- Dimensions: 4 m x 4 m x 8 m
- Gas velocity: $2.5U_{mf}$=0.25 m/s

Emulsion phase properties:

- Density: 400 kg/m^3
- Viscosity: 0.1 Pa.s

Bubble properties:

- Initial bubble size: 8 cm
- Maximum bubble size: 80 cm
- Typically ~ 5000 bubbles