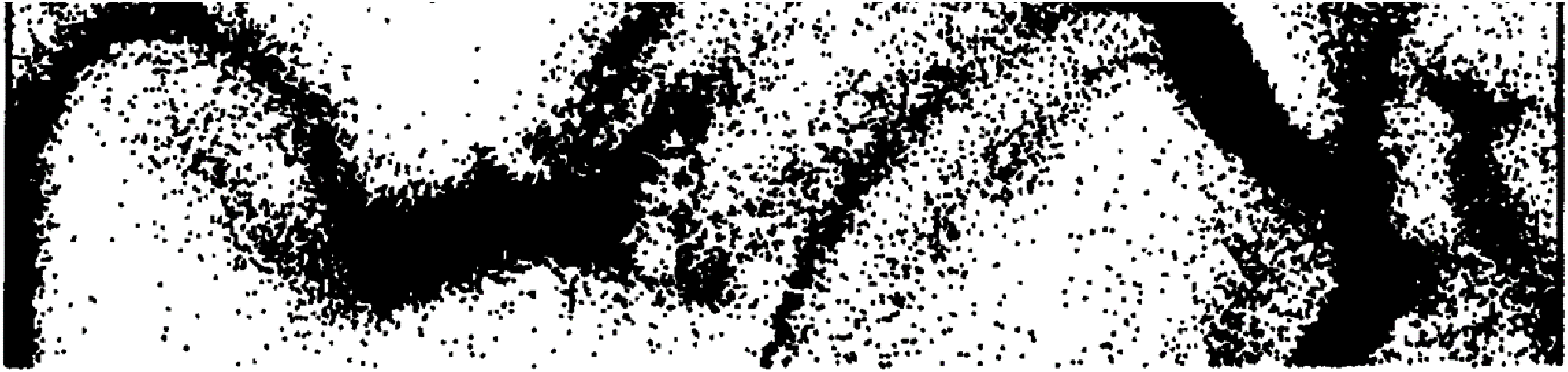
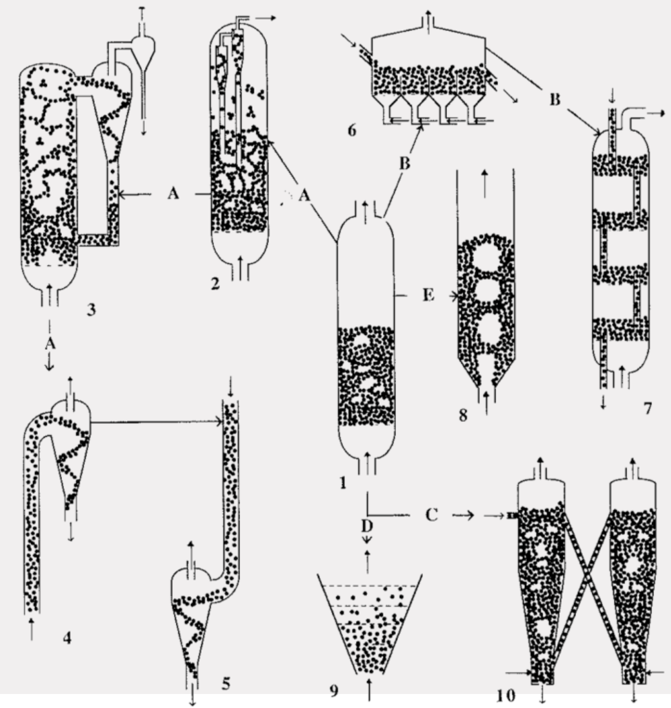


# COMPUTATIONAL FLUID MECHANICS OF GAS-SOLID SYSTEMS

Frank Peters

Chemical Engineering and Chemistry, Multiscale Modeling of Multiphase Flows

# Dense Gas-Particle Flows
# fluidized bed family of gas-solid contactors




1: bubbling bed

2: turbulent bed

3: circulating bed

4: riser

5: downer

6: lateral staged bed

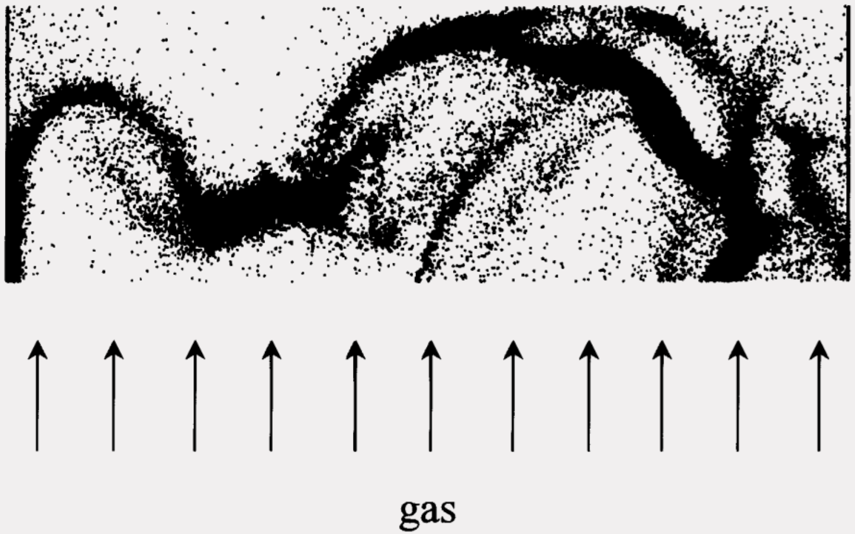
7: vertical staged bed

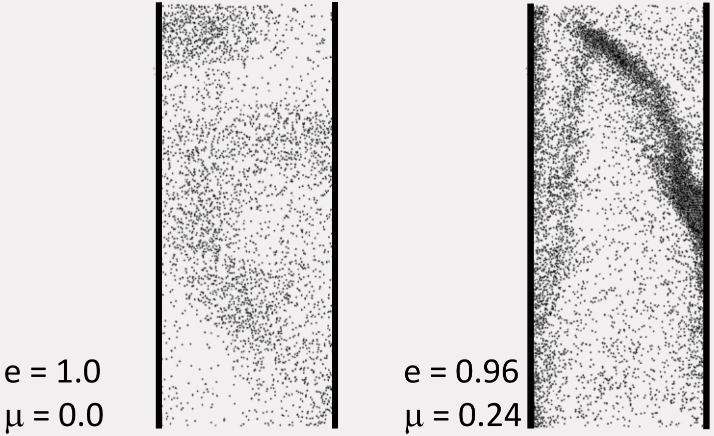
8: spouted bed

9: floating bed

10: twin bed

# Dense Gas-Particle Flows
# clusters in co-current vertical gas-solid flows



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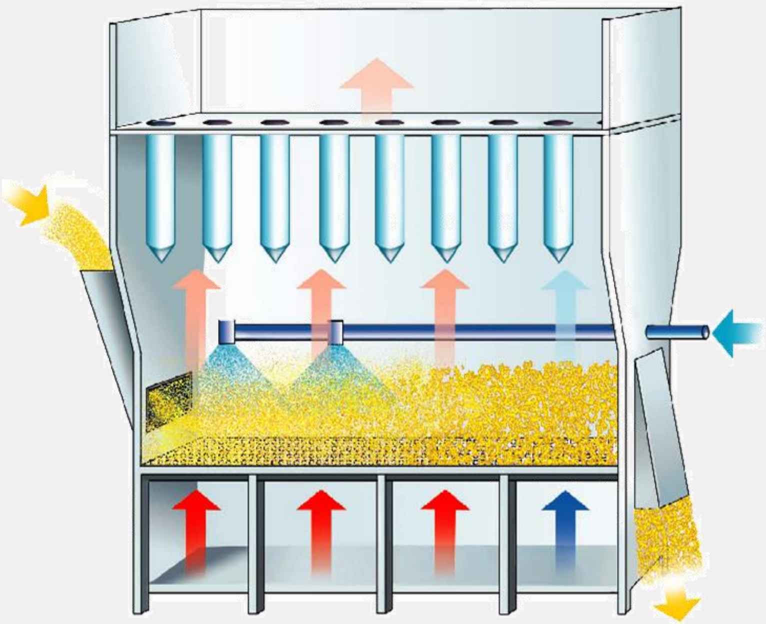
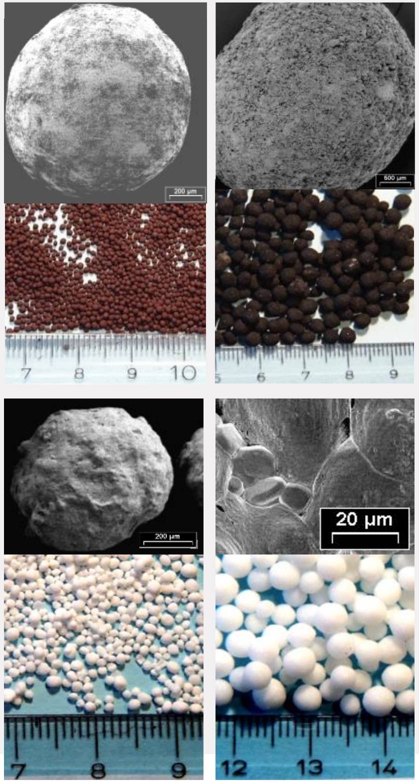
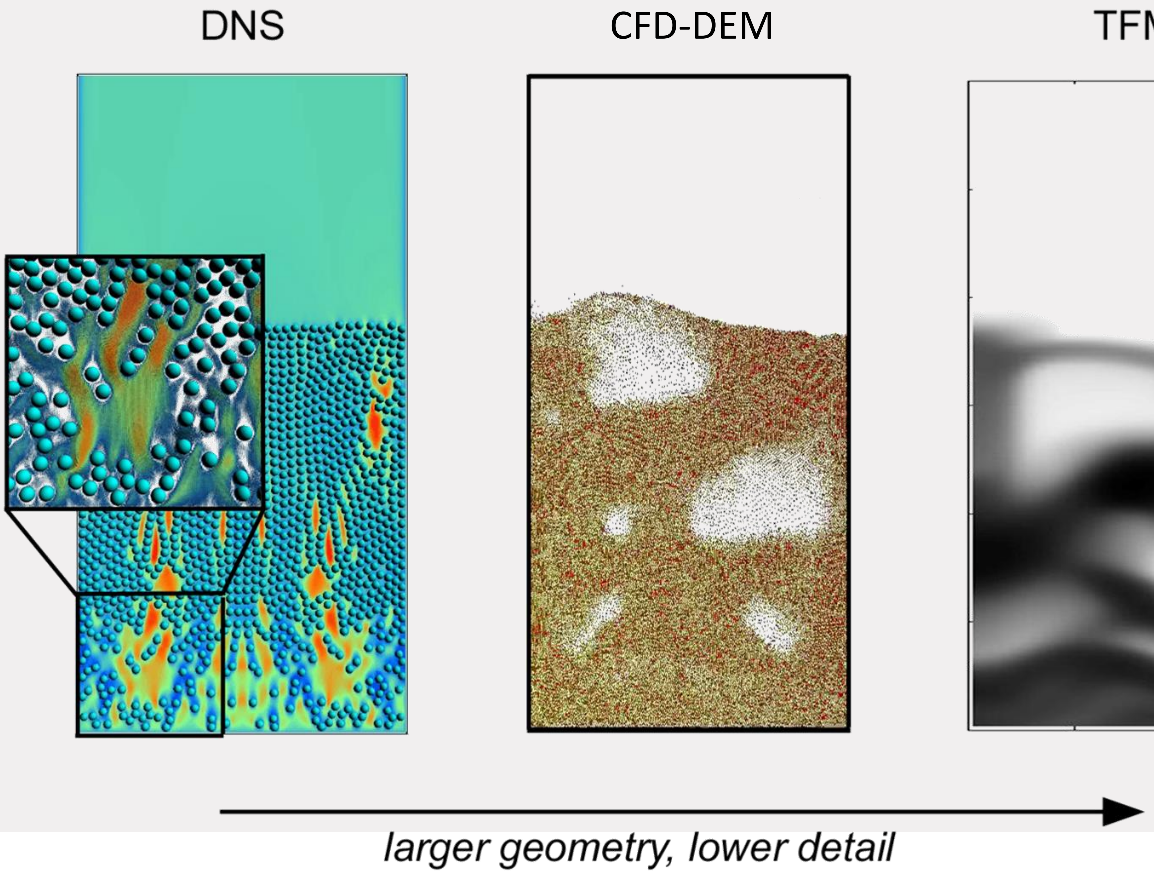
# Dense Gas-Particle Flows with Coupled Mass Momentum and Heat Transport (spray granulation)



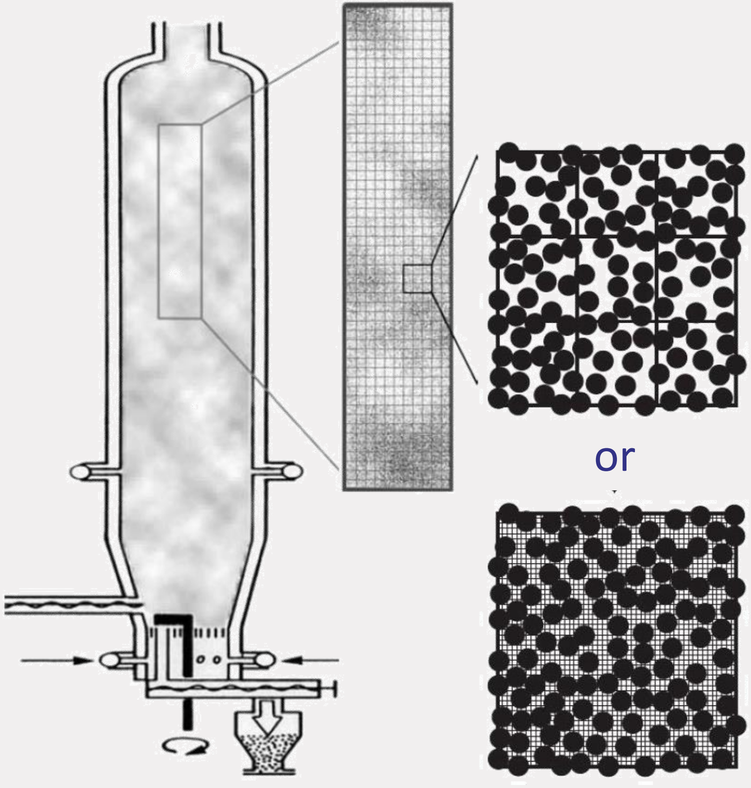



Prof. Stefan Heinrich (TUHH)

# Multiscale Modeling



# CFD-DEM vs DNS




CFD-DEM

- grid cell size $>$ particle diameter
- particle unresolved
- needs fluid-particle closure relations

DNS

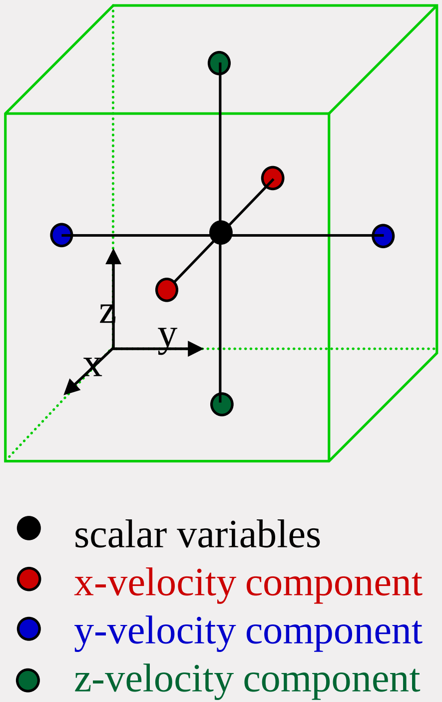
- grid cell size $\ll$ particle diameter
- particle resolved
- no-slip boundary conditions at particle surface

# Computational Fluid Dynamics

Discretize Navier-Stokes equation

Spatial discretization

- Finite difference on Cartesian staggered grid
- Viscous/diffusion terms: central differencing
- Convective term: second order total variation diminishing




Temporal discretization

- Convective terms explicit
- Viscous term and source term (semi) implicit
- Fractional step discretization: pressure correction by solving Poisson equation



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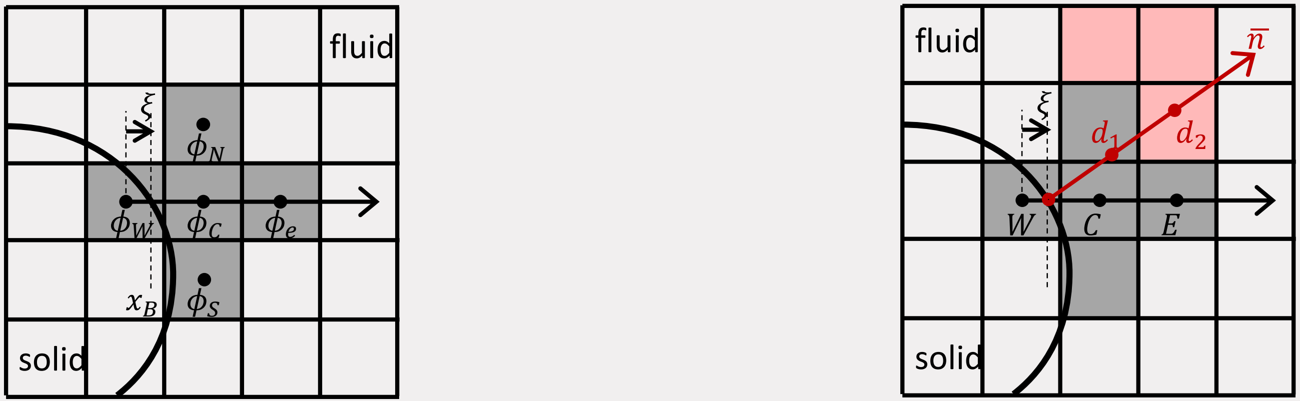
# Particle-resolved Direct Numerical Simulation

Grid size ≪ particle size

After discretization general matrix equation for unknowns $\phi_i$: $a_c\phi_c = \sum_{nb} a_{nb}\,\phi_{nb} + b_c$

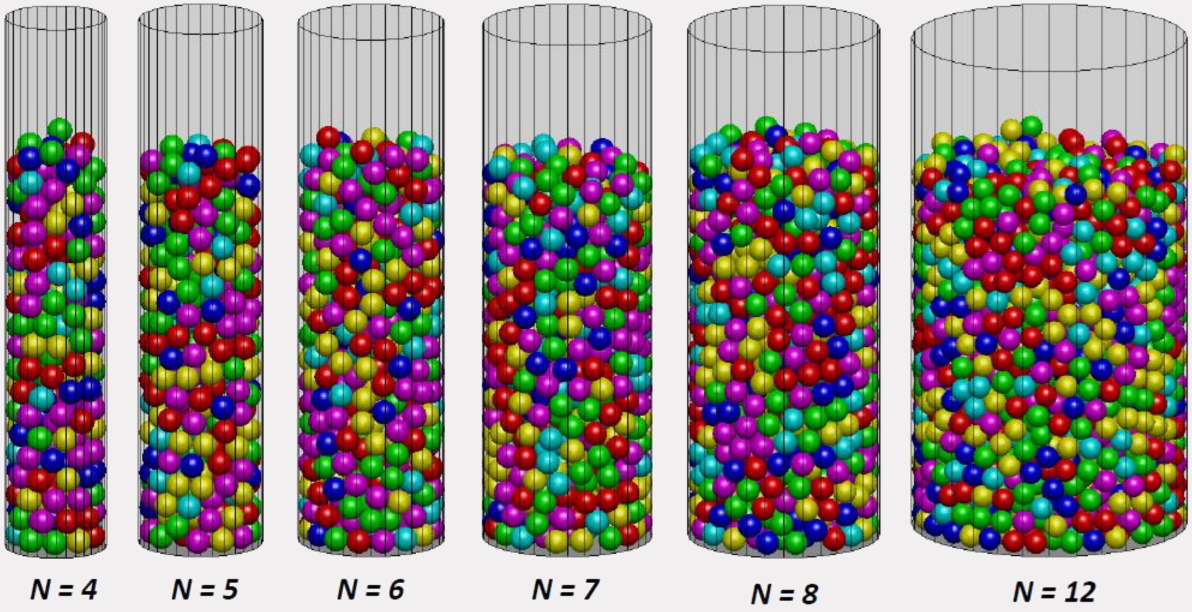
Immersed Boundary Method: eliminate nodes inside solid by extrapolation

$$\phi_w = \frac{2}{(1-\xi)(2-\xi)}\phi_B - \frac{2\xi}{1-\xi}\phi_C + \frac{\xi}{2-\xi}\phi_E$$



# Results DNS/IB Model

## transport phenomena in packed bed reactors: DEM generated beds



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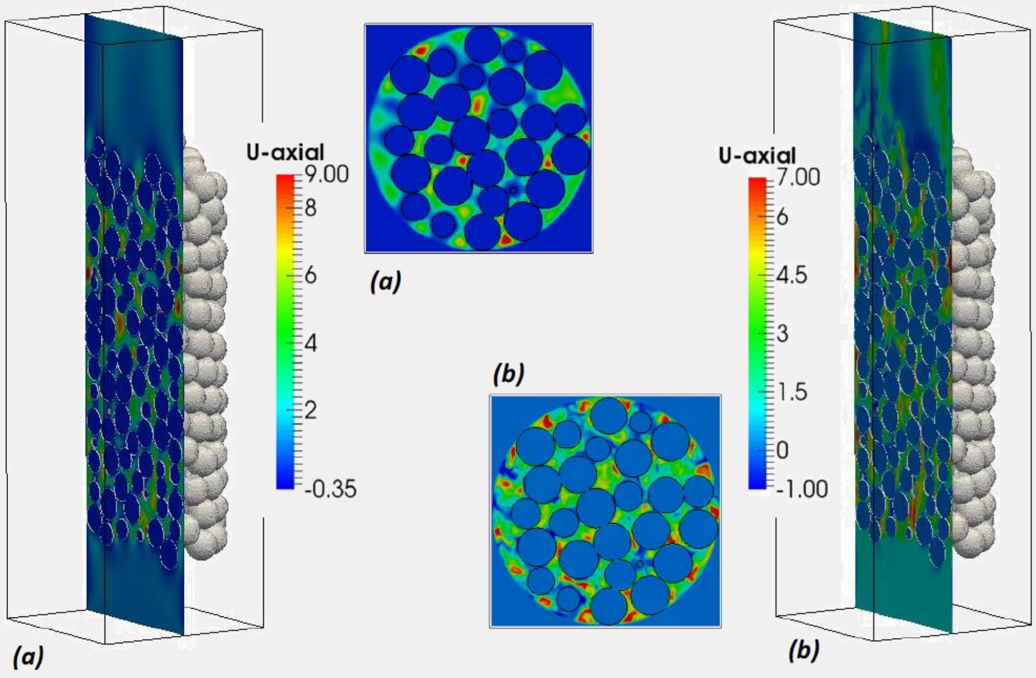
# Results DNS/IB Model

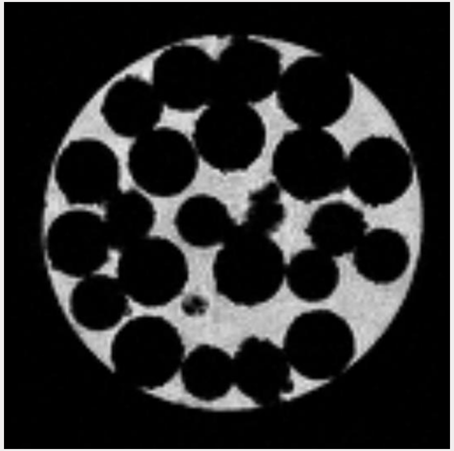
## transport phenomena in packed bed reactors: velocity profiles (N=6)

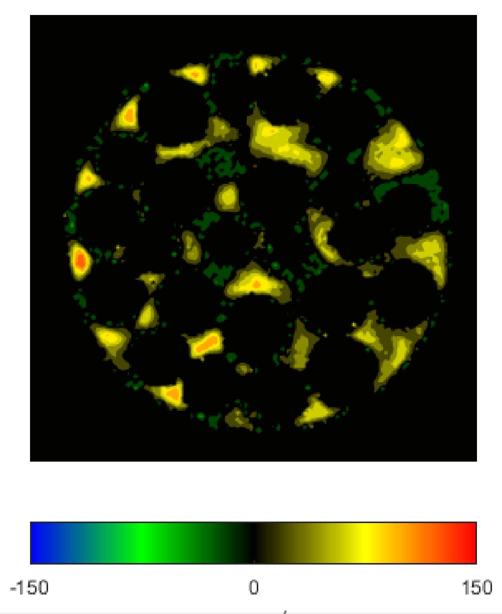



**$Re_d$=1** **$Re_d$=500**

# Results DNS/IB Model

## comparison with experiment (MRI flow imaging)

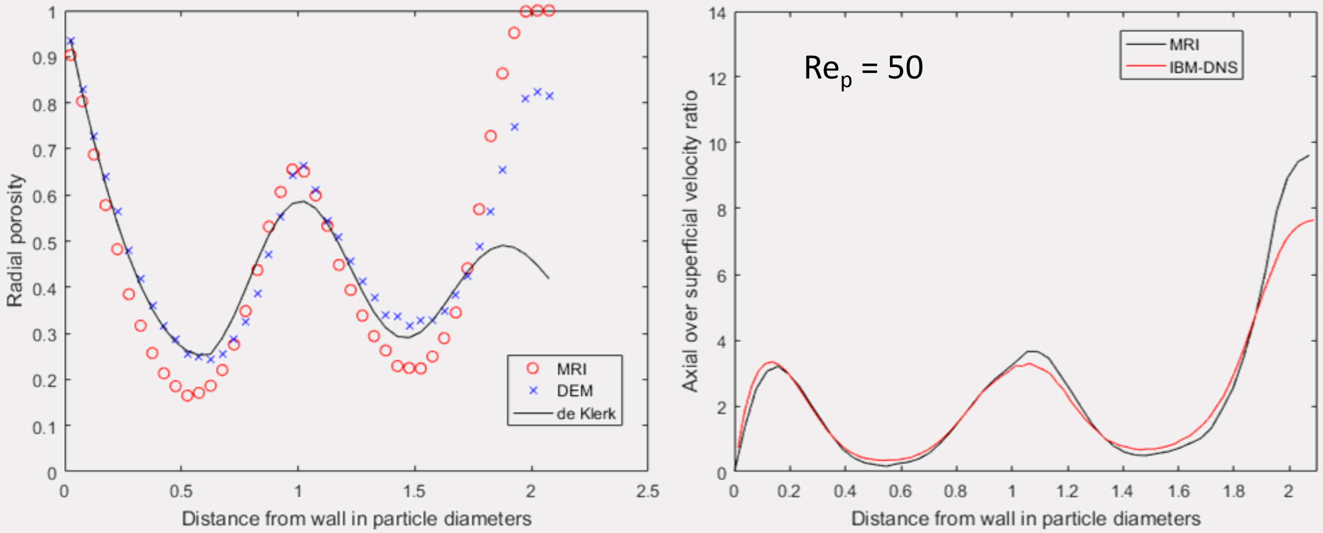





phase fractions (left) and axial velocity map (right) for a packed bed of spheres with a diameter of 4 mm

# Results DNS/IB Model

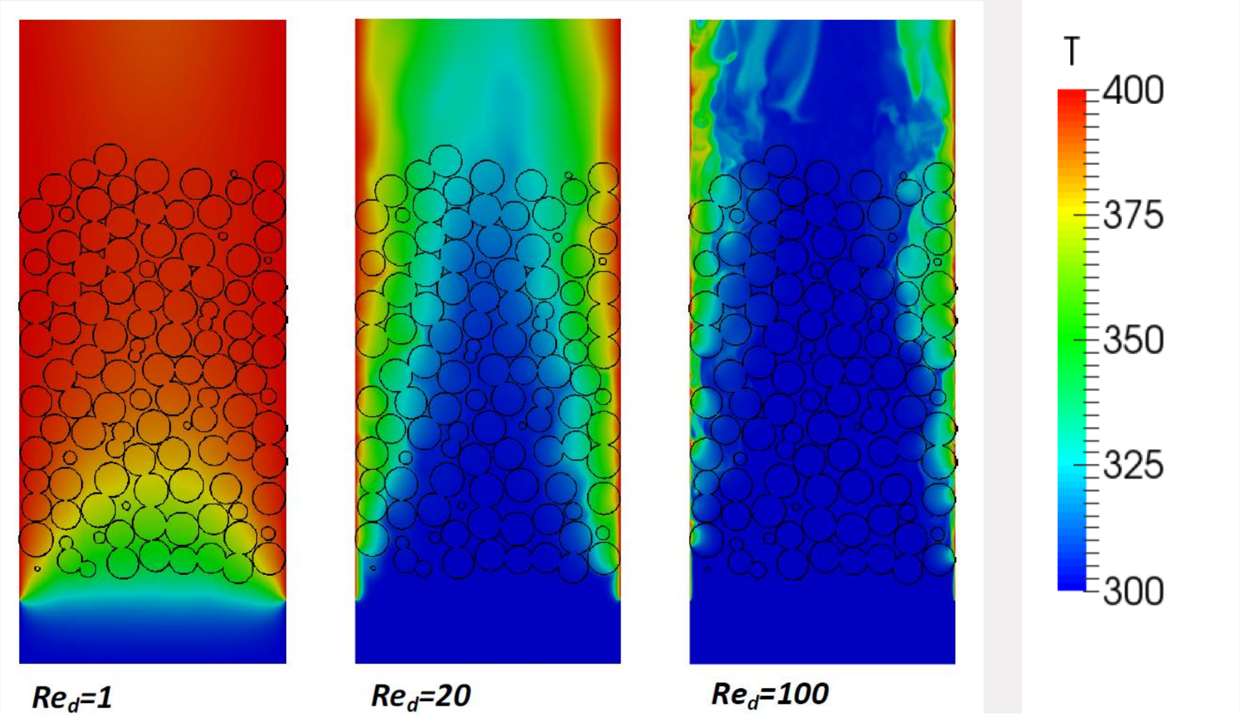
## comparison with experiment (MRI flow imaging)




radial porosity profile (left) and axial velocity profile (right)
for a packed bed of spheres with a diameter of 5 mm

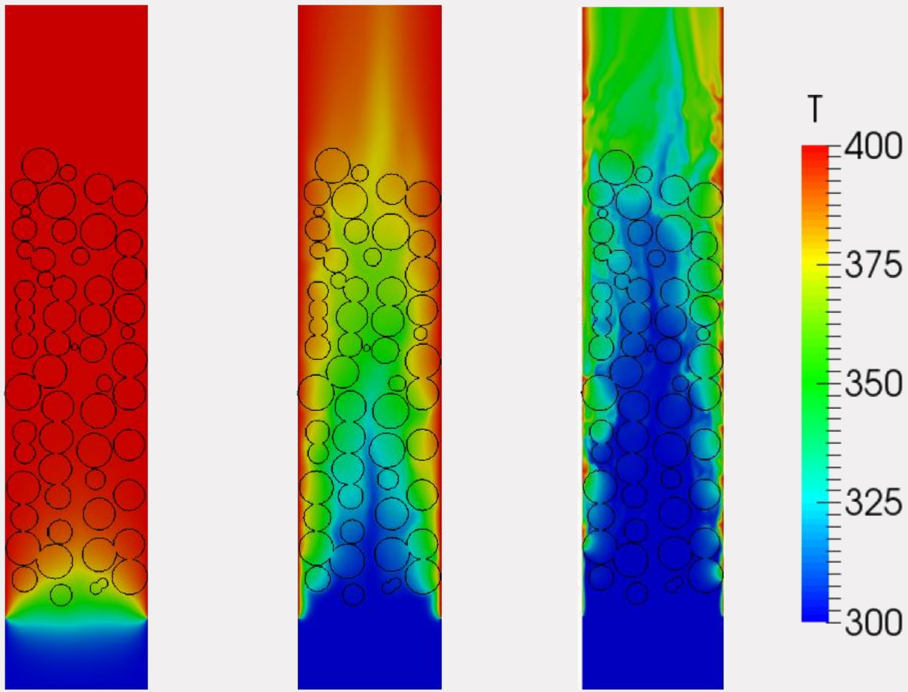
# Results DNS/IB Model

## transport phenomena in packed bed reactors: temperature profiles



# Results DNS/IB Model

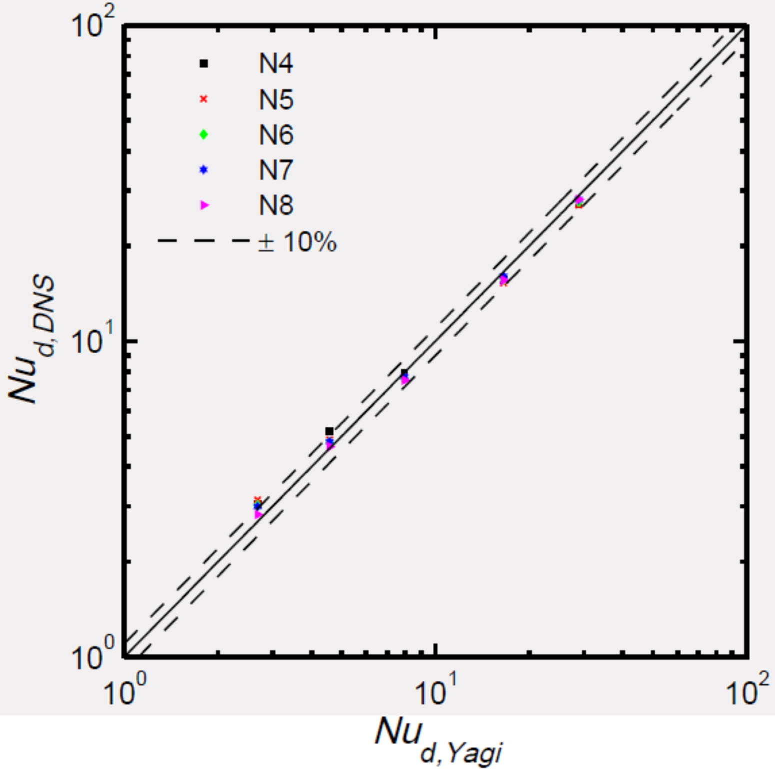
## transport phenomena in packed bed reactors: temperature profiles




$Re_d$=1 $Re_d$=20 $Re_d$=100

# Results DNS/IB Model

## transport phenomena in packed bed reactors: wall-to-bed heat transfer



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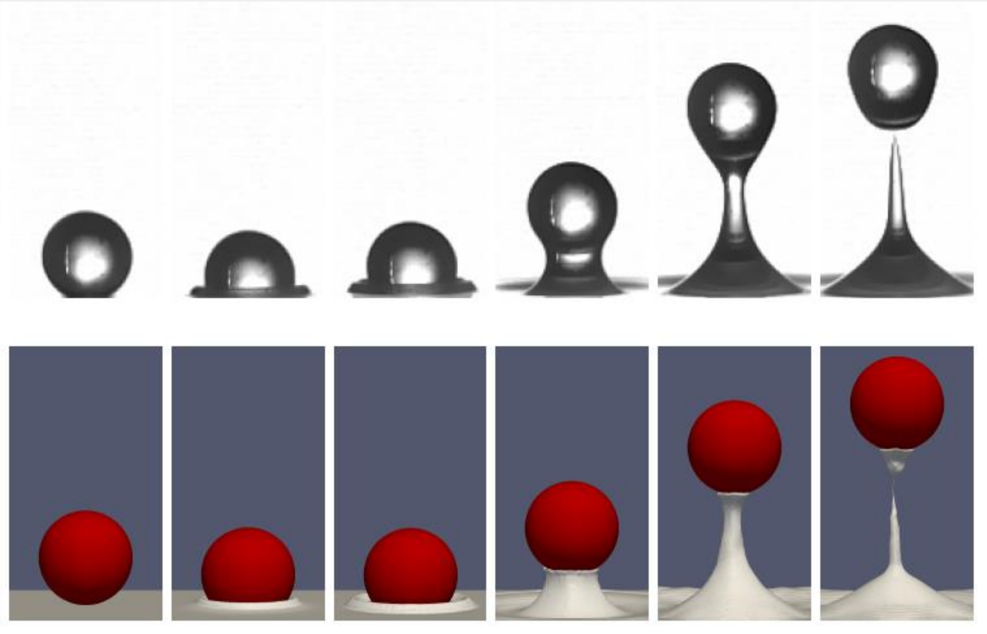
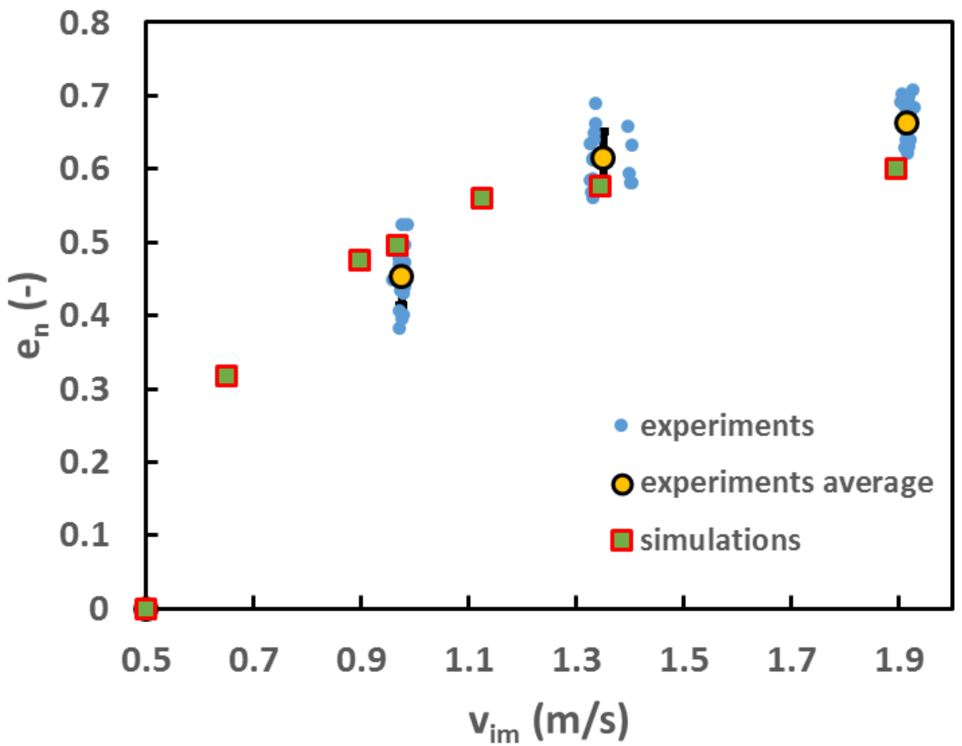
# Results: Wet collisions



Snapshot sequence of a spherical particle (1.74 mm) impacting on a wet plate with 400 µm liquid layer at an impact velocity of 1.13 m/s: experimental measurements (top) and simulation results (bottom).

# Results: Wet collisions

## collision of particle with a flat plate with thin liquid layer



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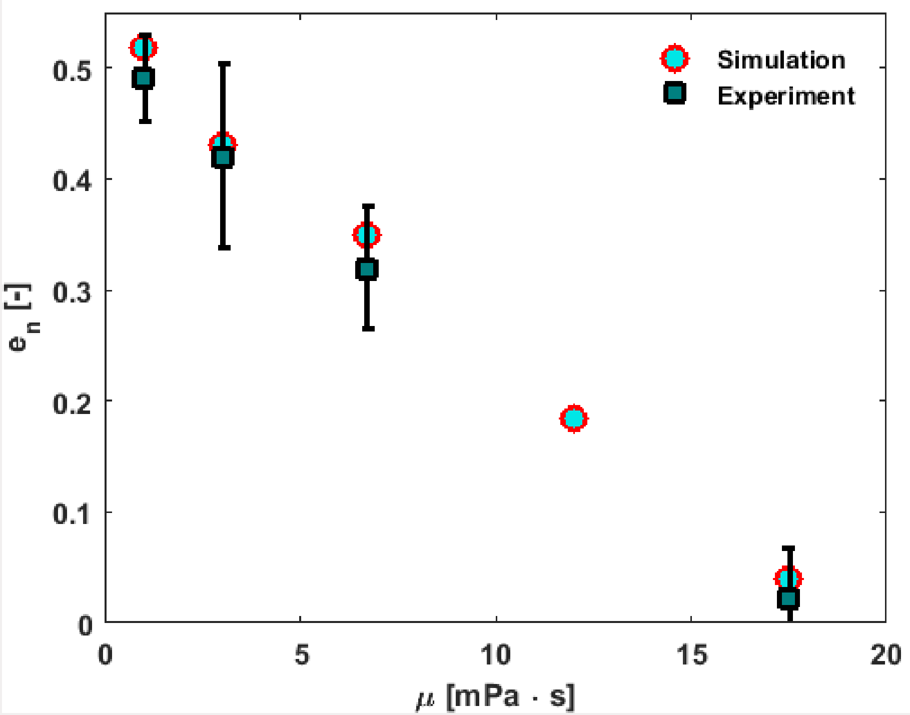
# Results: Wet collisions

## collision of particle with a flat plate with thin liquid layer



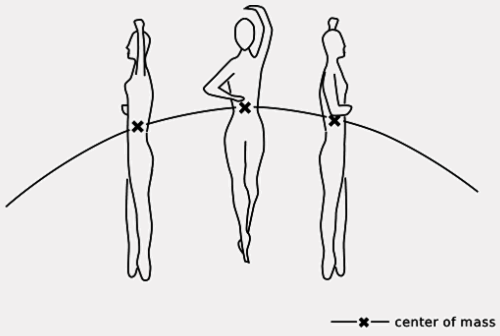
# Particle dynamics

Translation of center-of-mass

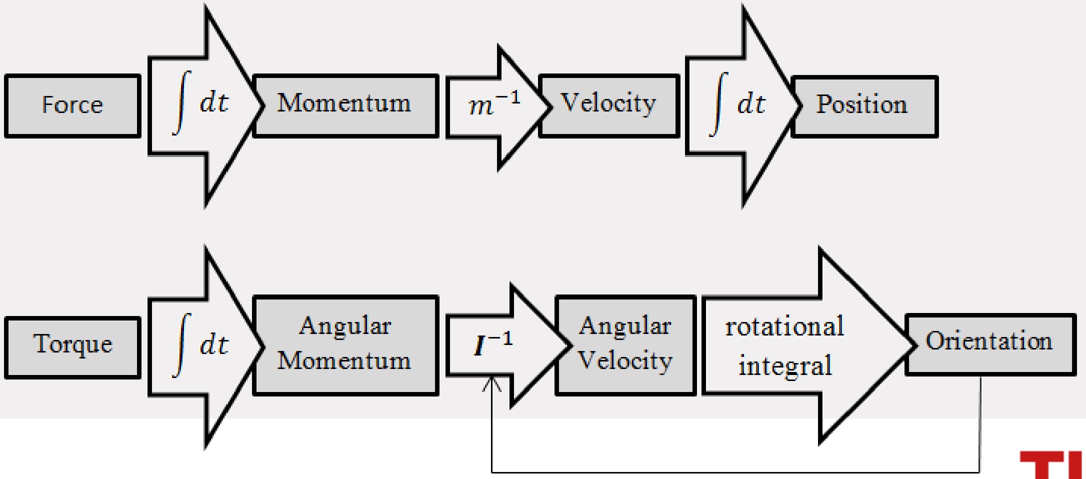
$$m_i \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = \mathbf{F}_i$$

Rotation around c.o.m.

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{I}_i \cdot \omega_i) = \mathbf{T}_i$$




generally
a complex
problem



# Forces and Torques on Particles

$$\mathbf{F}_i = \mathbf{F}_{fluid,i} + m_i\mathbf{g} + \mathbf{F}_{contact,i} + \mathbf{F}_{pp,i}$$
$$\mathbf{T}_i = \mathbf{T}_{fluid,i} + \mathbf{T}_{contact,i} + \mathbf{T}_{pp,i}.$$

Fluid-induced forces & torques

Gravity force

Direct contact forces & torques

Other particle-particle forces & torques, such as Van der Waals and charge interactions

# Contact Models

Contact model = a model specifying the forces and torques on granular particles due to direct collisions

Usually approximated as pair sums:

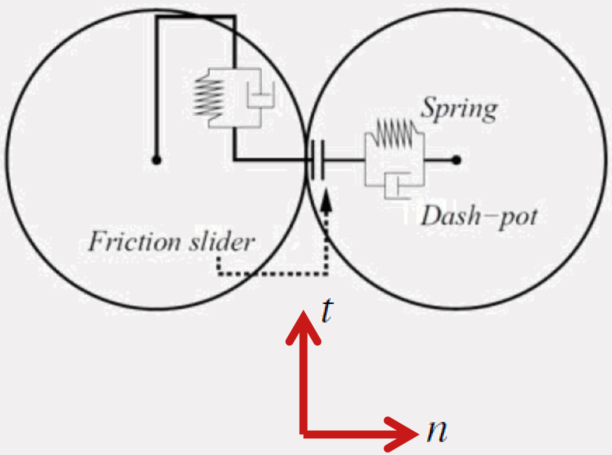
$$\mathbf{F}_{contact,i} = \sum_{j \neq i} \mathbf{F}_{ij}$$

$$\mathbf{T}_{contact,i} = \sum_{j \neq i} \mathbf{T}_{ij}$$

- Short ranged interactions
- Momentum is conserved
- Energy is not conserved (or lost as heat): dissipation

# Contact Forces: Soft Sphere Model

- Spheres can partly overlap (up to few %)
- Normal spring and dashpot
- Tangential spring and dashpot
- Friction slider for stick → slip transition




$$\mathbf{F}_{ij} = \mathbf{F}_{ij,n} + \mathbf{F}_{ij,t}$$



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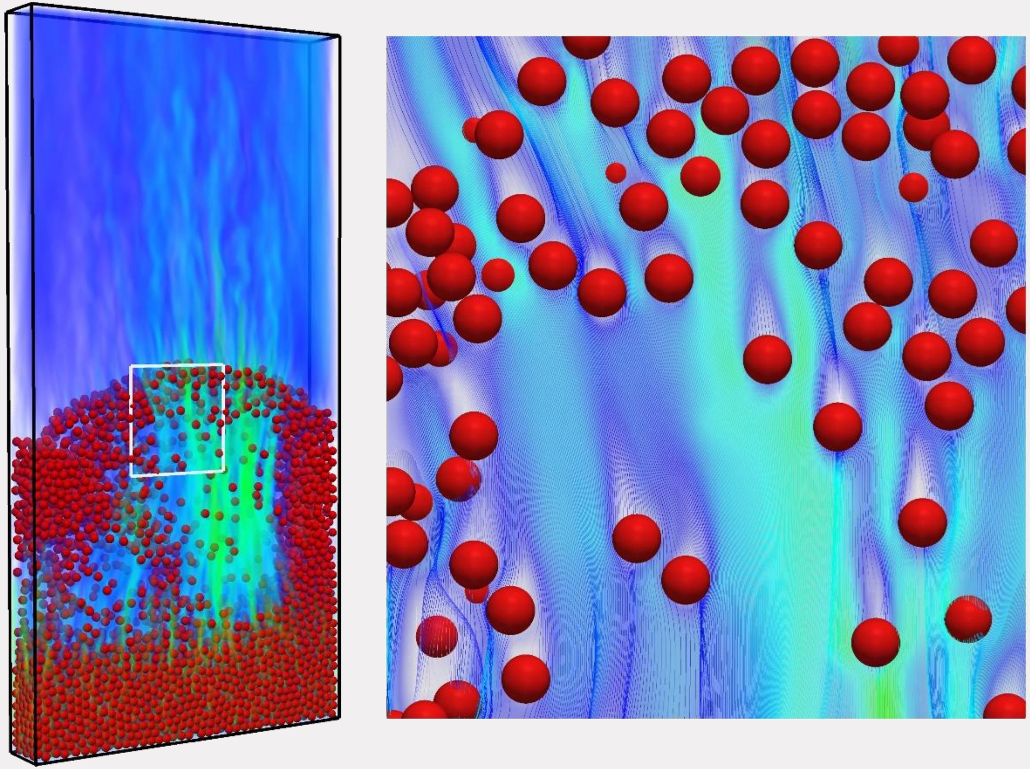
# Fluid-particle Forces in DNS

- Forces exerted on particle by fluid
- Integrate computed stresses and pressure on particle surface

$$\mathbf{F}_{fluid,i} = \oiint (\boldsymbol{\tau} \cdot \mathbf{n} - p\,\mathbf{n})\, dA$$

- Use values defined on staggered grid to approximate this integral

# Results: Particle-resolved DNS Fluidized Bed



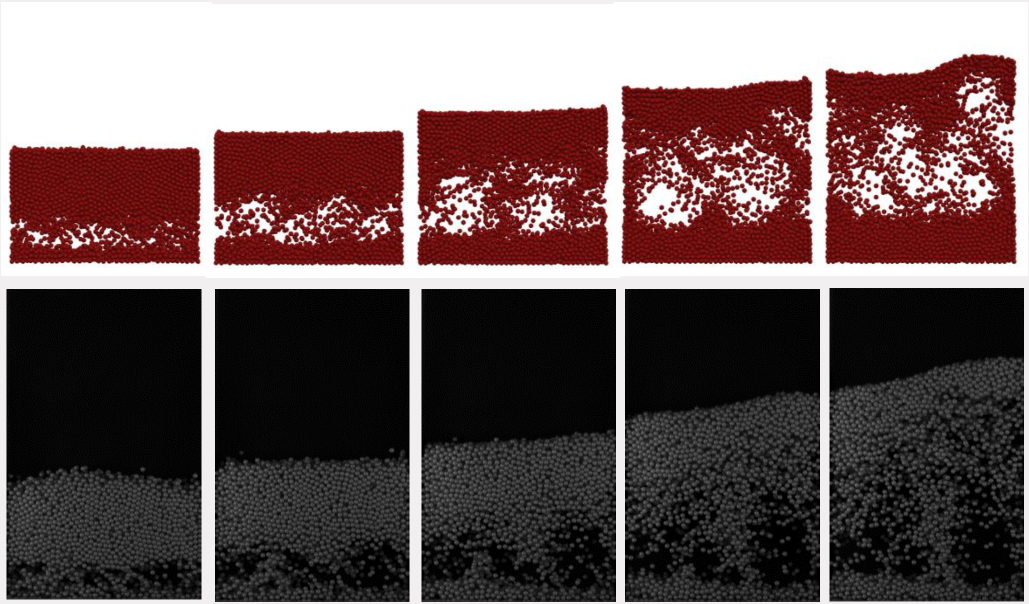
Pseudo-2D fluidized bed with 3000 particles

# Dynamics in a Small Pseudo-2d Fluidized Bed

## Flow regime

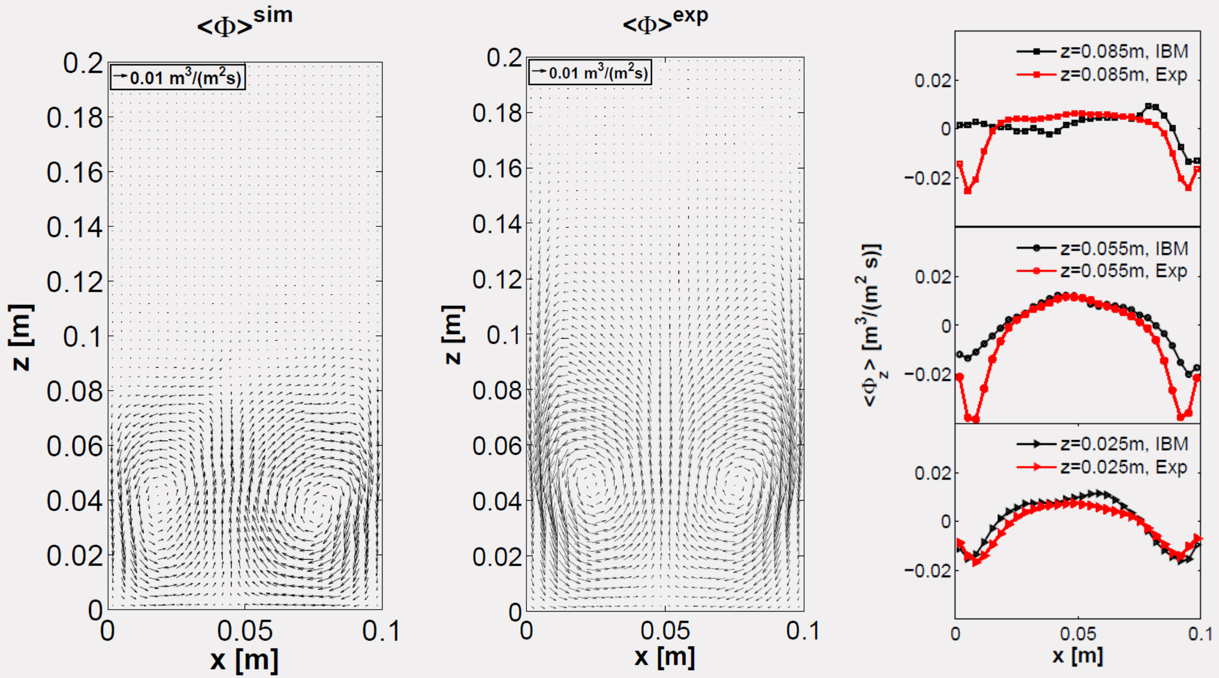
Sim.

Exp.



# Dynamics in a small pseudo-2D fluidized bed

## Time-averaged solids flux

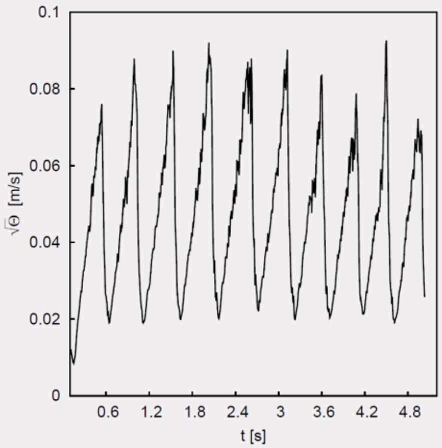


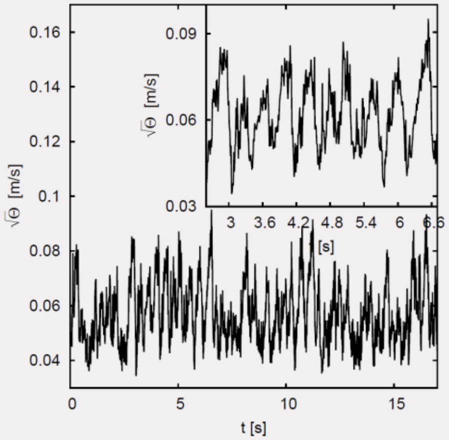

IBM　　　　PIV/DIA

# Dynamics in a small pseudo-2D fluidized bed

## Granular temperature

IBM

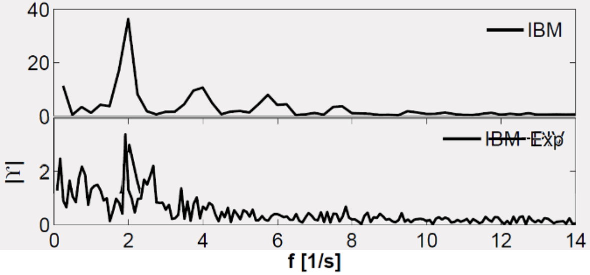


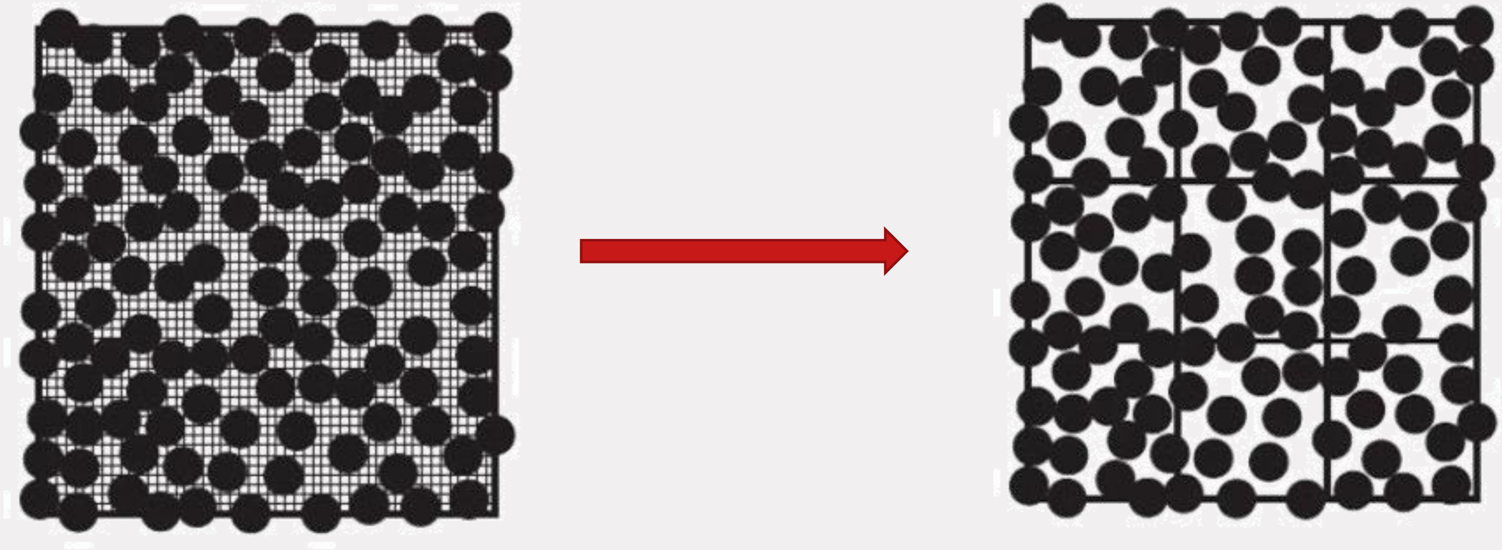

PIV

Characteristic frequency

$f = 2 \pm 0.3\ s^{-1}$



# Multiscale approach: DNS to CFD-DEM



Clossure relations obtained from DNS

# Drag Correlations

DNS: measure average drag force as a function of

solids volume fraction f

particle Reynolds number Re

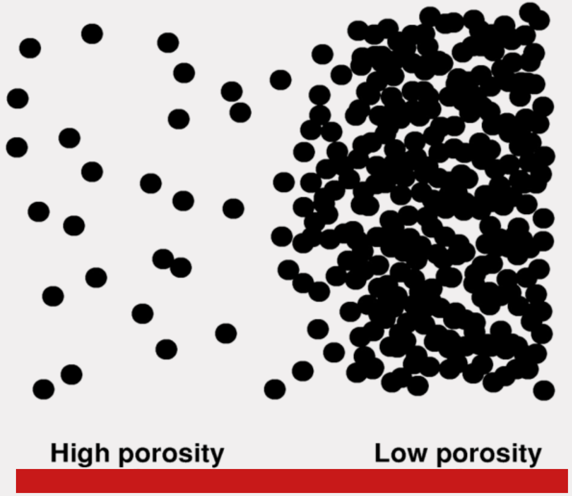
$$\mathrm{Re} = \frac{(1-\phi)\rho_g\,|\mathbf{u}-\mathbf{v}_i|\,d}{\mu}$$

non-dimensionalize with Stokes drag in dilute limit

$$\frac{F_{drag}}{3\pi\mu d\,|\mathbf{u}-\mathbf{v}_i|} = \frac{1}{18\phi}\frac{\beta d^2}{\mu}$$

$$F(\mathrm{Re},\phi) \equiv \frac{\beta d^2}{\mu}$$

$$\epsilon = 1-\phi$$



# Drag correlation from DNS/IBM

$$F_d(\phi, \mathrm{Re}) = 10\phi(1-\phi)^{-2} + (1-\phi)^2\left(1+1.5\sqrt{\phi}\right)$$ low-Re flow

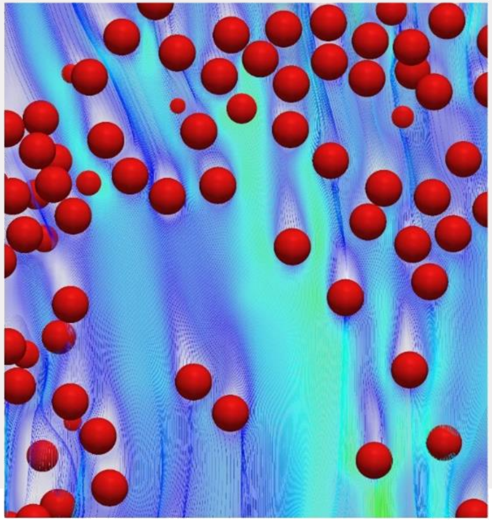
$$+\mathrm{Re}\cdot\{0.11\phi(1+\phi) - 0.00456(1-\phi)^{-4} + [0.169(1-\phi) + 0.0644(1-\phi)^{-4}]\cdot \mathrm{Re}^{-0.343}\}$$ inertial effects

$$+2.98\mathrm{Re}_T\phi(1-\phi)^{-2}$$ mobility effect

with

$\phi$: solids volume fraction

$$\mathrm{Re} = \frac{\rho_g d_p U}{\mu_g}, \mathrm{Re}_T = \frac{\rho_g d_p \sqrt{\Theta}}{\mu_g}$$





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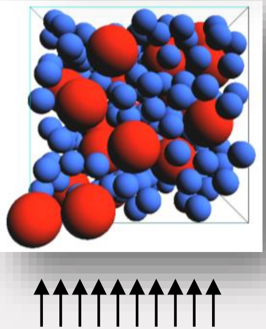
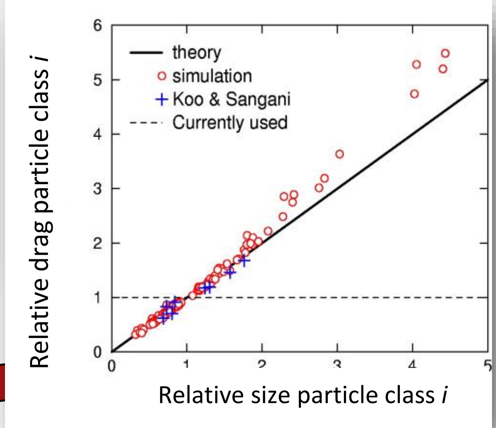
# Drag in Binary Mixtures of Particles

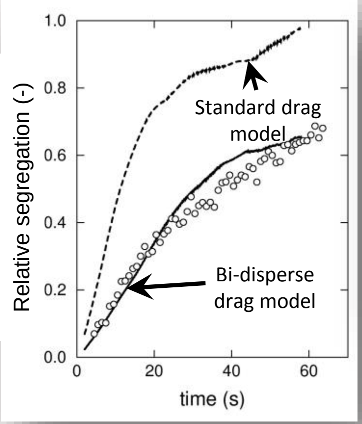
## multiscale approach to segregation in binary system

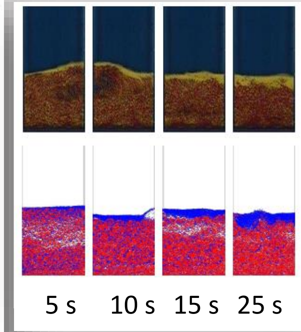
O($10^2$) particles






O($10^5$) particles

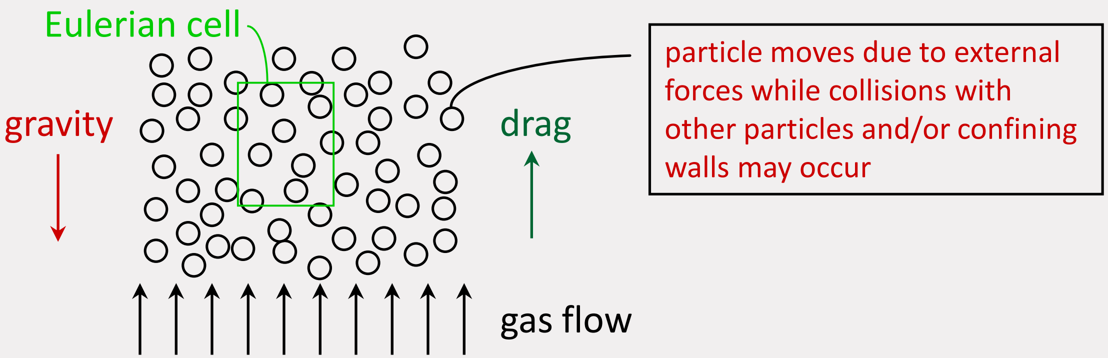



$$F_i = \left(\varepsilon_g y_i + \varepsilon_s y_i^2 + 0.064\varepsilon_g y_i^3\right) F(\varepsilon_s, \mathrm{Re}) \qquad \text{with} \qquad y_i = \frac{d_i}{\langle d \rangle}$$

$$F(\varepsilon_s, \mathrm{Re}) = \frac{10\varepsilon_s}{\varepsilon_g^2} + \varepsilon_g^2\left(1 + 1.5\varepsilon_s^{1/2}\right) + \frac{0.413}{24\varepsilon_g^2}\left[\frac{\varepsilon_g^{-1} + 3\varepsilon_s\varepsilon_g + 8.4\,\mathrm{Re}^{-0.343}}{1 + 10^{3\varepsilon_s}\,\mathrm{Re}^{-(1+4\varepsilon_s)/2}}\right]$$

# CFD-DEM: Key Ingredients




**+ particle collision dynamics**

**+ gas phase flow field**

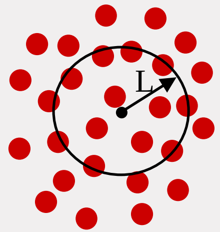
**+ drag force on particles**

**+ bed voidage and source terms in momentum equation gas phase**

# CFD-DEM: Gas phase Hydrodynamics

- Gas phase conservation equations

  equations formulated and solved at length scale which is large compare to the particle size but small compared to the macroscopic system size




- Volume-averaged Navier-Stokes equations

  + continuity equation

$$\frac{\partial}{\partial t}\left((1-\phi)\rho_g\right) + \nabla \cdot \left((1-\phi)\rho_g\,\mathbf{u}\right) = 0$$

  + momentum equation

$$\frac{\partial}{\partial t}\left((1-\phi)\rho_g\mathbf{u}\right) + \nabla \cdot \left((1-\phi)\rho_g\mathbf{u}\mathbf{u}\right) = -(1-\phi)\nabla P - \nabla \cdot \left((1-\phi)\bar{\mathbf{S}}\right) - \mathbf{S}_p + (1-\phi)\rho_g\mathbf{g}$$

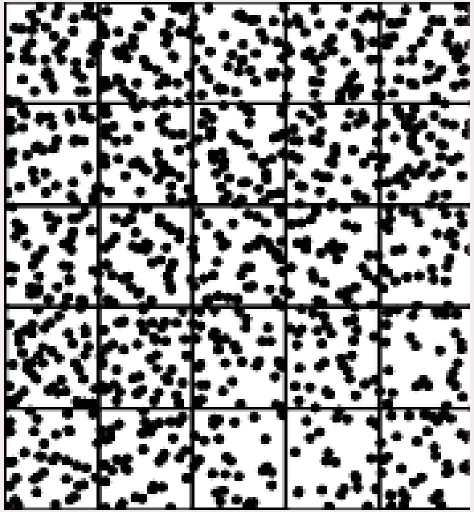
  + interaction with solids phase

$\phi$: solids volume fraction, $\mathbf{S}_p$: - drag of solids on fluid

# CFD-DEM: Fluid-particle interactions

fluid-induced force on particle:

- buoyant force
- effective drag force:
- $\mathbf{F}_{fluid,i} = -V_i \boldsymbol{\nabla} \mathrm{P} + \frac{V_i \beta_i}{\phi} (\mathbf{u} - \mathbf{v}_i)$
- local gas velocity, $\mathbf{u}$
- local solid volume fraction, $\phi$
- local inter-phase momentum transfer coefficient, $\beta$



solids-induced force on fluid (action = - reaction)

$$\phi = \sum_{i=1}^{N} V_i \, \delta_h(\mathbf{r} - \mathbf{r}_i)$$

$$\boldsymbol{S}_p = \sum_{i=1}^{N} \frac{V_i \beta_i}{\phi} (\mathbf{u} - \mathbf{v}_i) \, \delta_h(\mathbf{r} - \mathbf{r}_i) \stackrel{\text{def}}{=} \beta \mathbf{u} - \boldsymbol{\alpha}$$

regularized delta function

$$\iiint \delta_h(\mathbf{r} - \mathbf{r}_i) \, dV = 1$$



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# CFD-DEM: Force Distribution & Velocity Interpolation

Exchange information between Lagrangian points, $\mathbf{r}_i$, and Eulerian mesh, $\mathbf{r}_k$

$$\delta_h(\mathbf{r}-\mathbf{r}_i) \rightarrow \frac{1}{V_{cell}} D(\mathbf{r}_k-\mathbf{r}_i), \qquad \sum_k D(\mathbf{r}_k-\mathbf{r}_i) = 1$$

Particle-fluid forces at Lagrangian points,$\mathbf{r}_i$, distributed to Eulerian grid positions, $\mathbf{r}_k$

$$\mathbf{S}_p(\mathbf{r}_k) = \frac{\mathbf{1}}{V_{cell}} \sum_{i=1}^{N} \frac{V_i \beta_i}{\phi} (\mathbf{u}-\mathbf{v}_i)\, D(\mathbf{r}_k-\mathbf{r}_i)$$

Velocities known at Eulerian positions needed at Langrangian points

$$\boldsymbol{u}(\mathbf{r}_i) = \sum_{i=1}^{N} \boldsymbol{u}(\mathbf{r}_k)\, D(\mathbf{r}_k-\mathbf{r}_i)$$



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# CFD-DEM: Volume Weighing

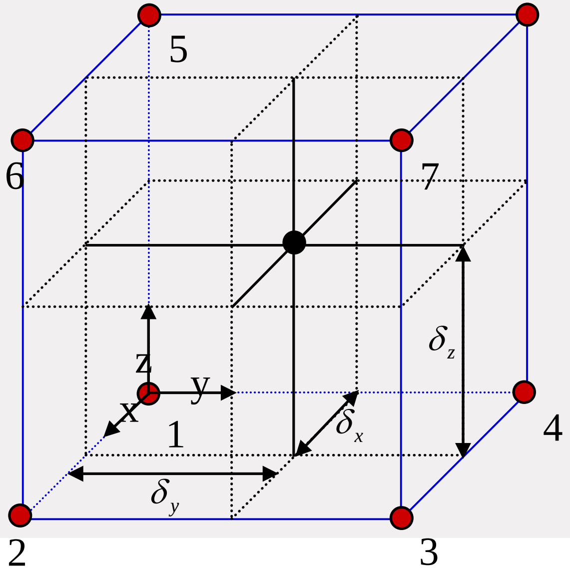
Simplest approach: volume weighing = tri-linear interpolation

- ● particle
- ● velocity nodes

$$\lambda_x = \frac{\delta_x}{\Delta x}$$

$$\lambda_y = \frac{\delta_y}{\Delta y}$$

$$\lambda_z = \frac{\delta_z}{\Delta z}$$




$$D(\mathbf{r}_1 - \mathbf{r}_p) = (1-\lambda_x)(1-\lambda_y)(1-\lambda_z)$$

$$D(\mathbf{r}_2 - \mathbf{r}_p) = \lambda_x(1-\lambda_y)(1-\lambda_z)$$

$$D(\mathbf{r}_3 - \mathbf{r}_p) = \lambda_x\lambda_y(1-\lambda_z)$$

$$D(\mathbf{r}_4 - \mathbf{r}_p) = (1-\lambda_x)\lambda_y(1-\lambda_z)$$

$$D(\mathbf{r}_5 - \mathbf{r}_p) = (1-\lambda_x)(1-\lambda_y)\lambda_z$$

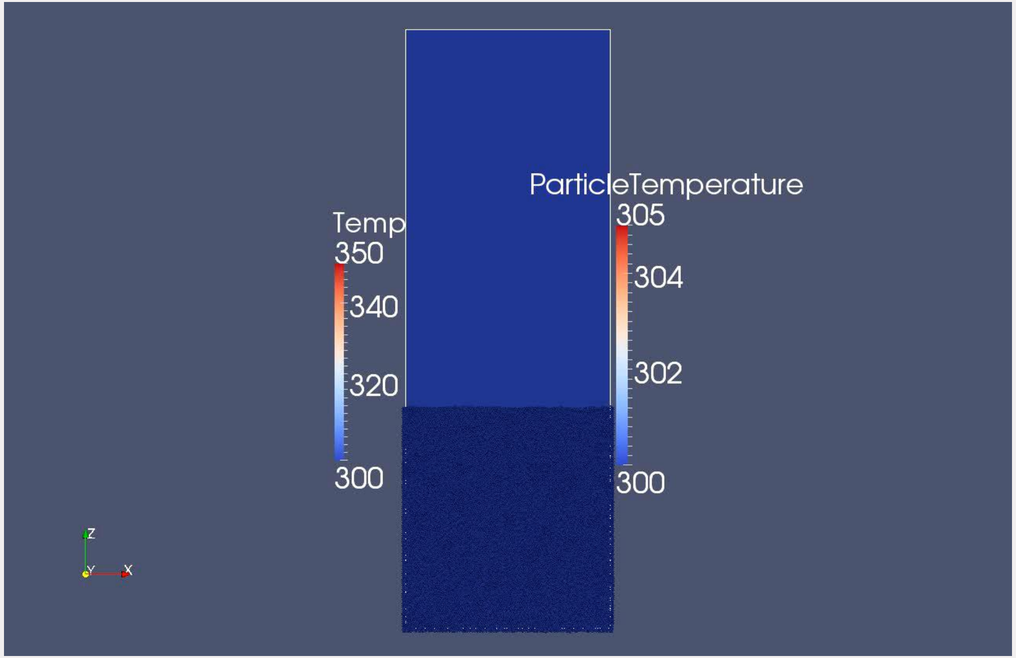
$$D(\mathbf{r}_6 - \mathbf{r}_p) = \lambda_x(1-\lambda_y)\lambda_z$$

$$D(\mathbf{r}_7 - \mathbf{r}_p) = \lambda_x\lambda_y\lambda_z$$

$$D(\mathbf{r}_8 - \mathbf{r}_p) = (1-\lambda_x)\lambda_y\lambda_z$$

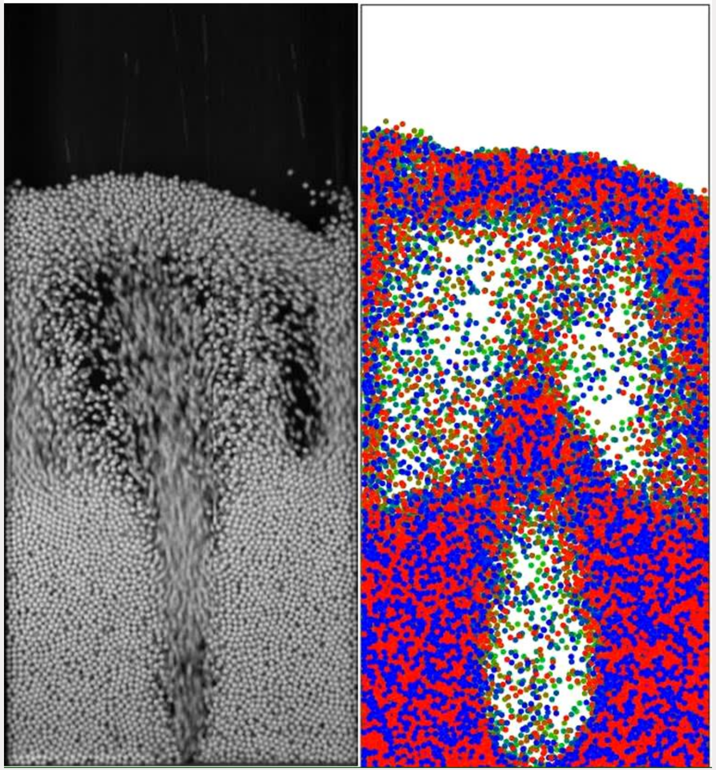
# Larger scale CFD-DEM simulations

Uses correlations from DNS



# Results CFD-DEM

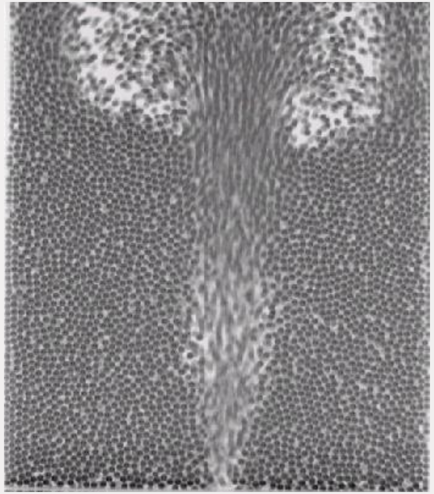
## spouted bed



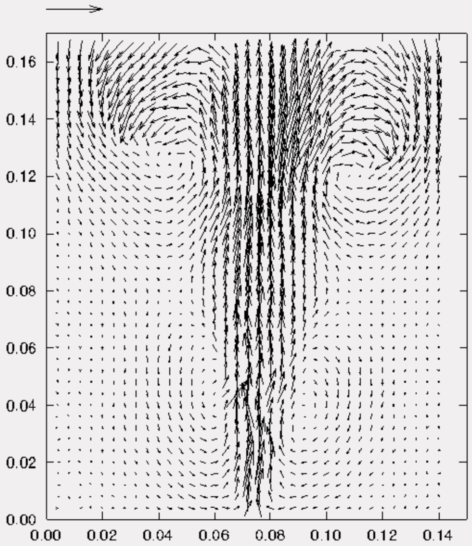
# Results CFD-DEM

## spouted bed

$$u_{sf} / u_{mf} = 16.0 \leftrightarrow u_{bf} / u_{mf} = 1.2$$



particle configuration

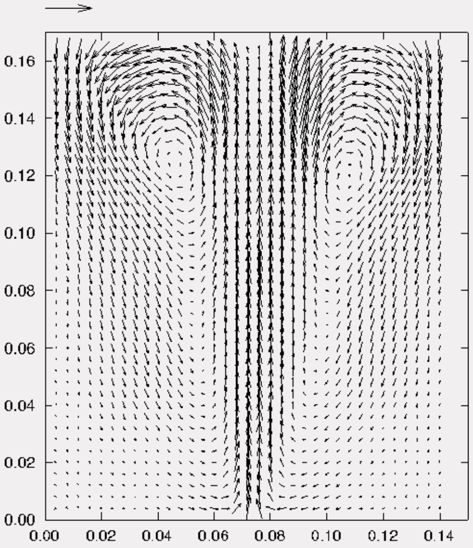



particle velocity map

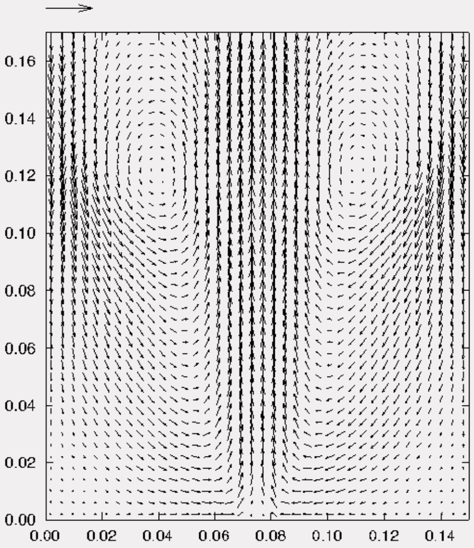
# Results CFD-DEM

## spouted bed

$$u_{sf} / u_{mf} = 16.0 \leftrightarrow u_{bf} / u_{mf} = 1.2$$




experimental




simulated



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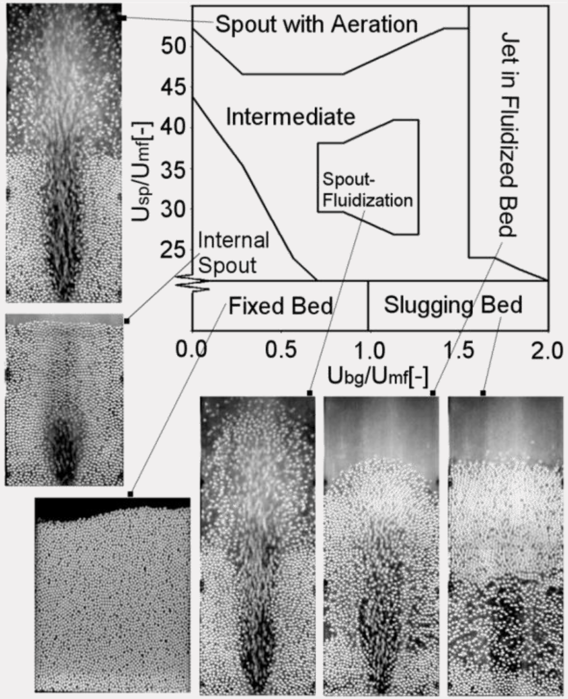
# Results CFD-DEM

## spouted bed




“CAPABILITIES” OF CFD-DEM
(COLLISION PARAMETERS!!!)
(Link et al., CES, 2005)

REGIME PREDICTION

GAS BUBBLES BEHAVIOUR

PRESSURE FLUCTUATIONS

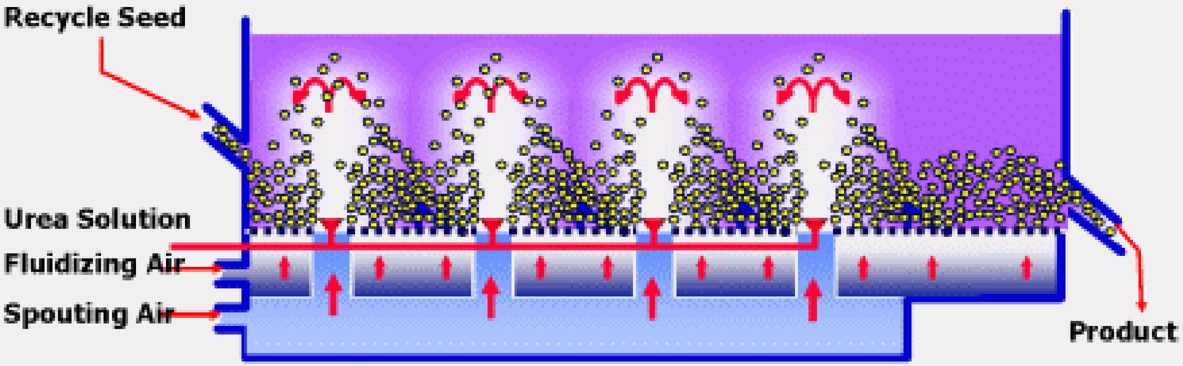
SOLIDS MOTION

# Results CFD-DEM

## multiple spouts with interaction

RATIONAL DESIGN OF FLUID BED GRANULATORS:

OPTIMAL DISTANCE BETWEEN SPOUTS ?

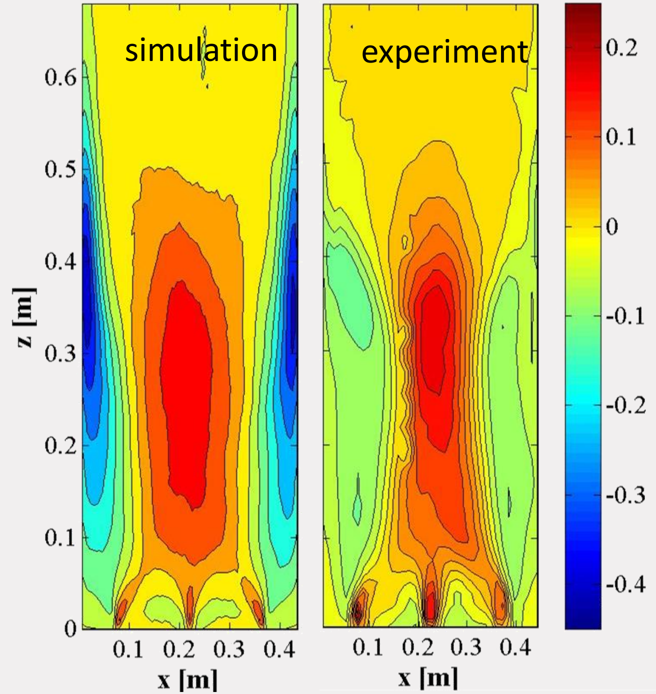



***Optimal Arrangement of Multi-stage Spouted Bed***

- Round and Uniform Product
- High Drying Efficiency

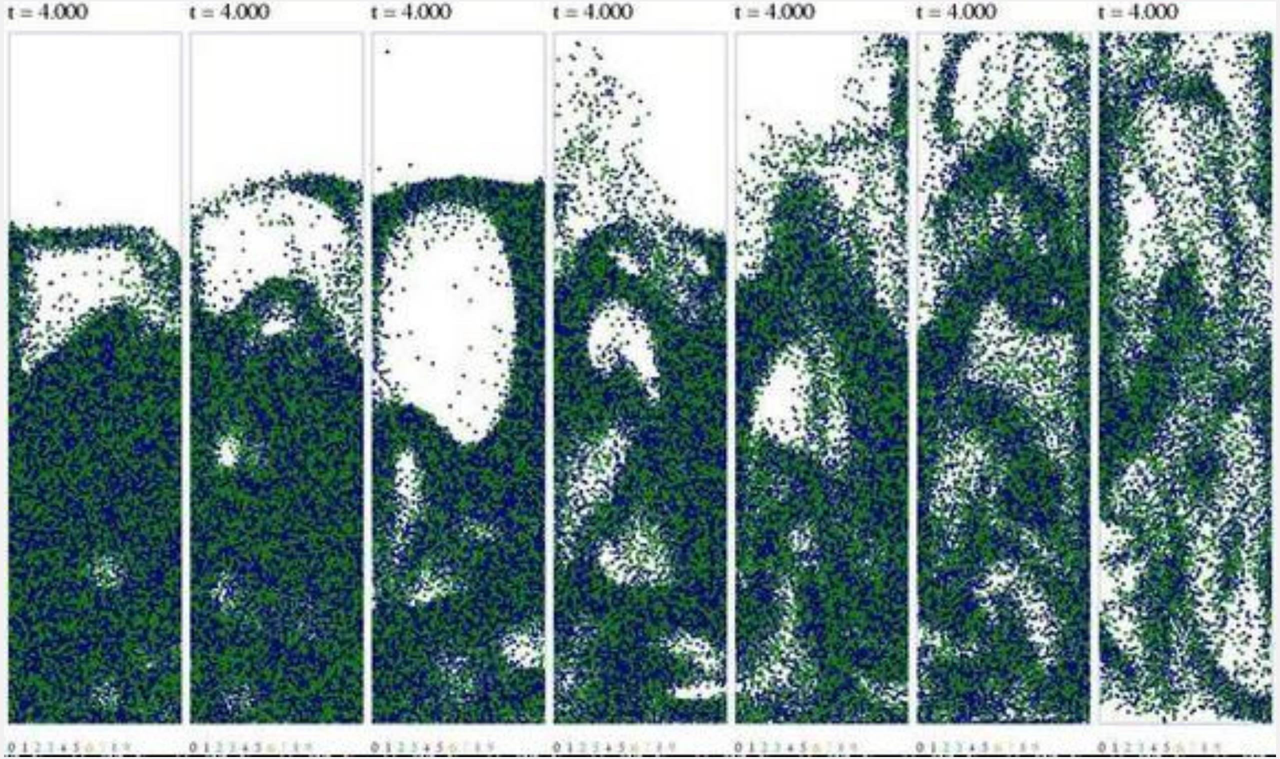
# Results CFD-DEM

## multiple spouts with interaction (?)

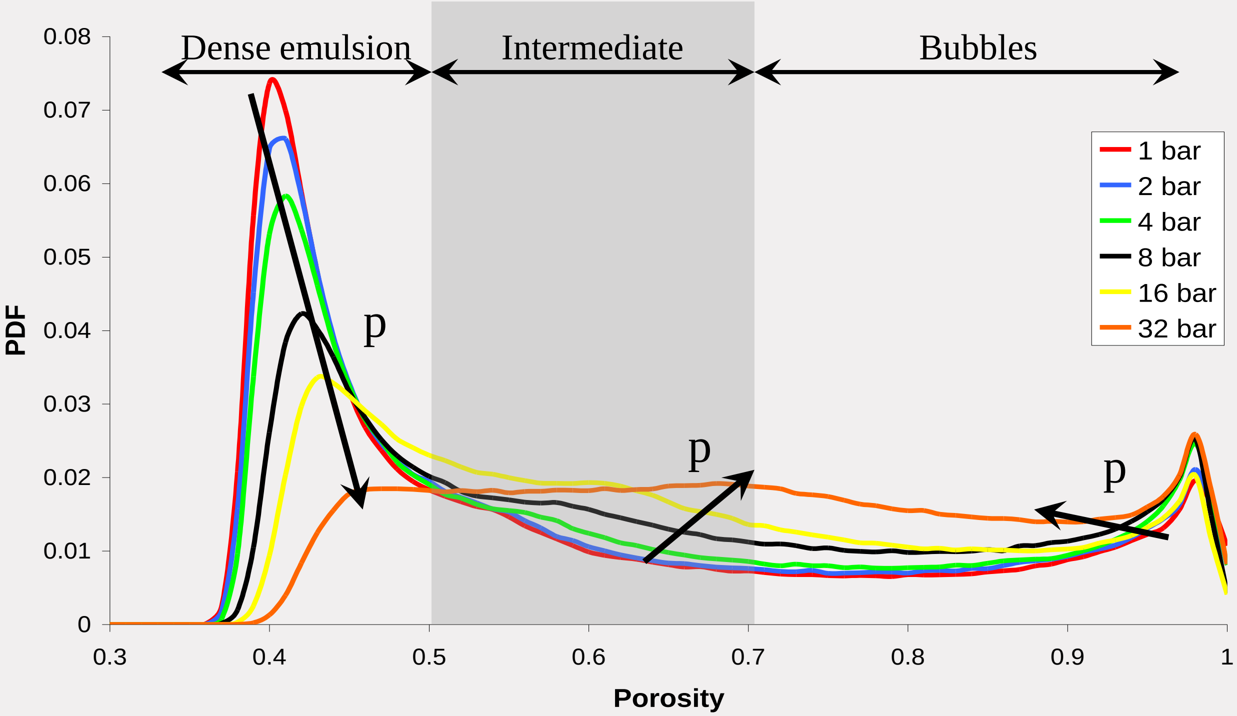
# Results CFD-DEM

## effect of operating pressure



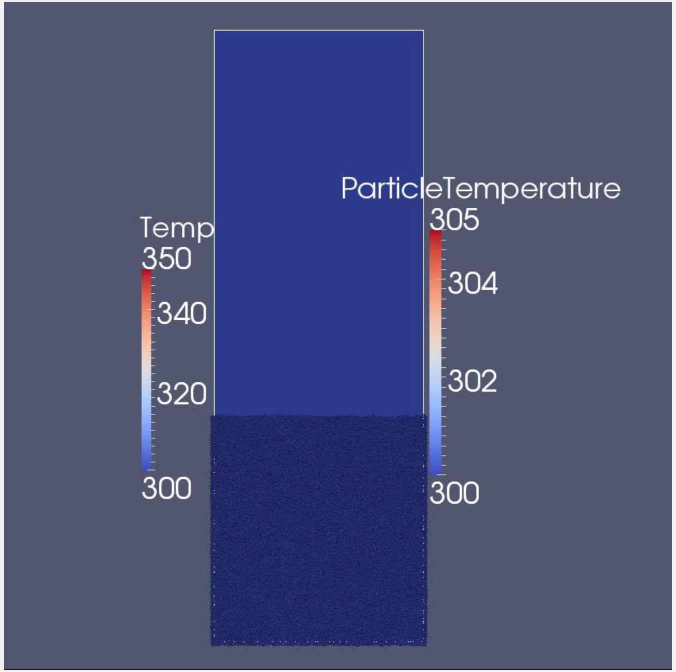
# Results CFD-DEM

## effect of operating pressure



# CFD-DEM: Extension To Heat Transfer

Relevance: in many fluidized beds particles catalytic with large heat effects

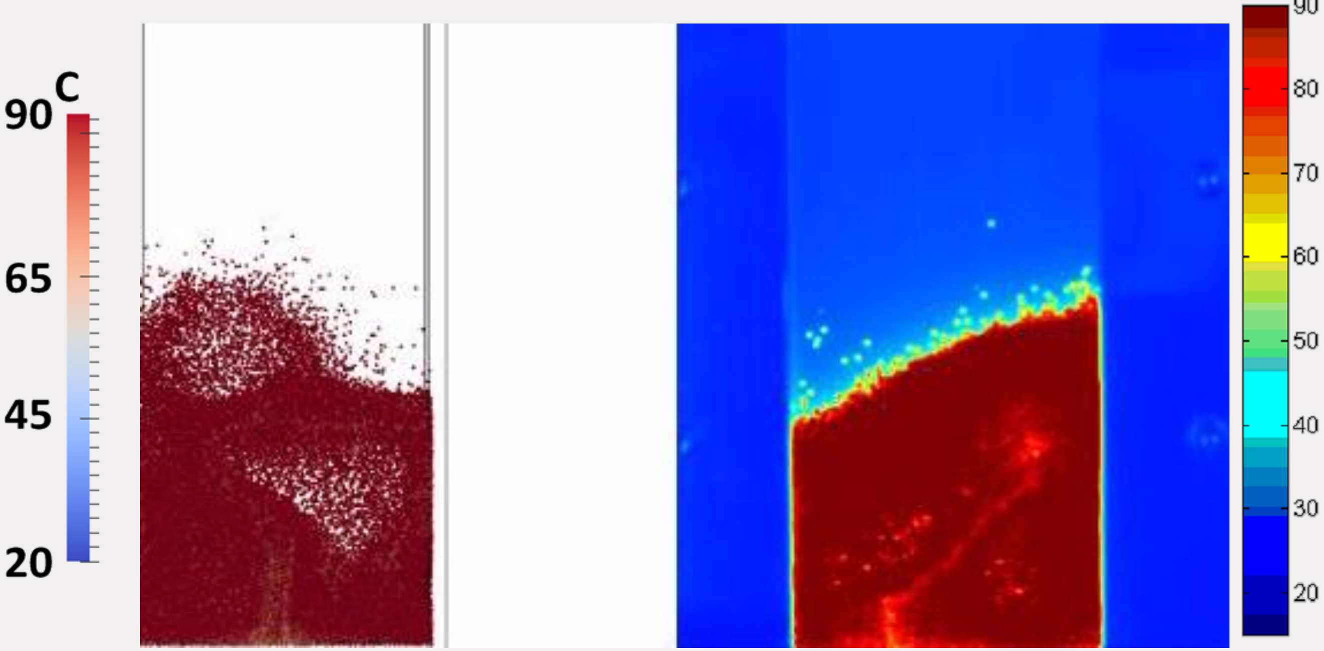


# CFD-DEM: Extension To Heat Transfer

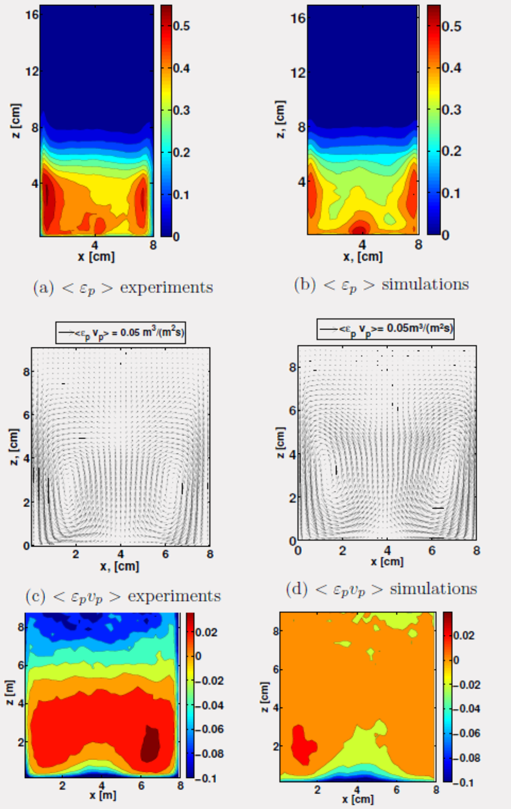
## lab-scale experiments for validation

Cooling of a hot fluidized bed by injection of a cold gas

Simulations Experiments



# Quantitative Comparison




(a) $<\varepsilon_p>$ experiments

(b) $<\varepsilon_p>$ simulations

(c) $<\varepsilon_p v_p>$ experiments

(d) $<\varepsilon_p v_p>$ simulations

(e) Temperature distribution $\Gamma$ experiments

(f) Temperature distribution $\Gamma$ simulations

$$\overline{\varepsilon_p(i,j)} = \frac{1}{N_t}\sum_t \varepsilon_p(t,i,j)$$

$$\overline{\mathbf{\Phi}_p(i,j)} = \frac{1}{N_t}\sum_t \varepsilon_p(t,i,j)\,\mathbf{v}_p(t,i,j)$$

$$\overline{\Gamma_p(i,j)} = \frac{1}{\sum_t \varepsilon_p(t,i,j)} \sum_t \varepsilon_p(t,i,j)\,\frac{T_p(t,i,j)-\langle T_p(t)\rangle_\varepsilon}{\langle T_p(t)\rangle_\varepsilon - T_{g,\mathrm{in}}(t)}$$



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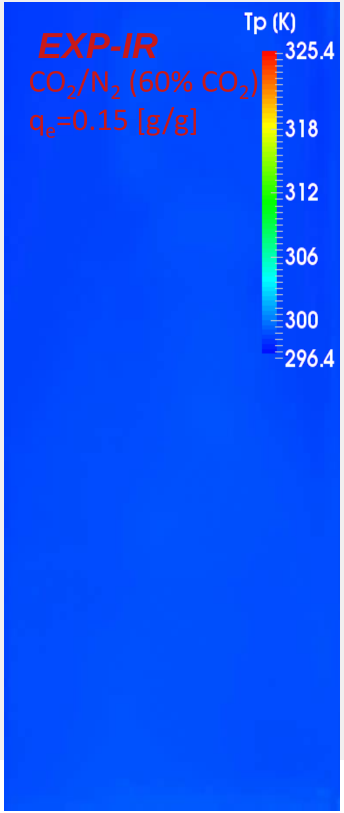
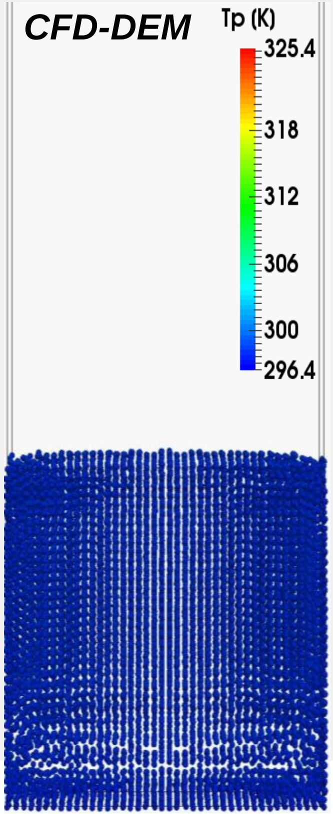
# CFD-DEM Modelling of Heat Transfer in Gas-fluidized Beds

## experiment (l) versus simulation (r)




**experimental system**

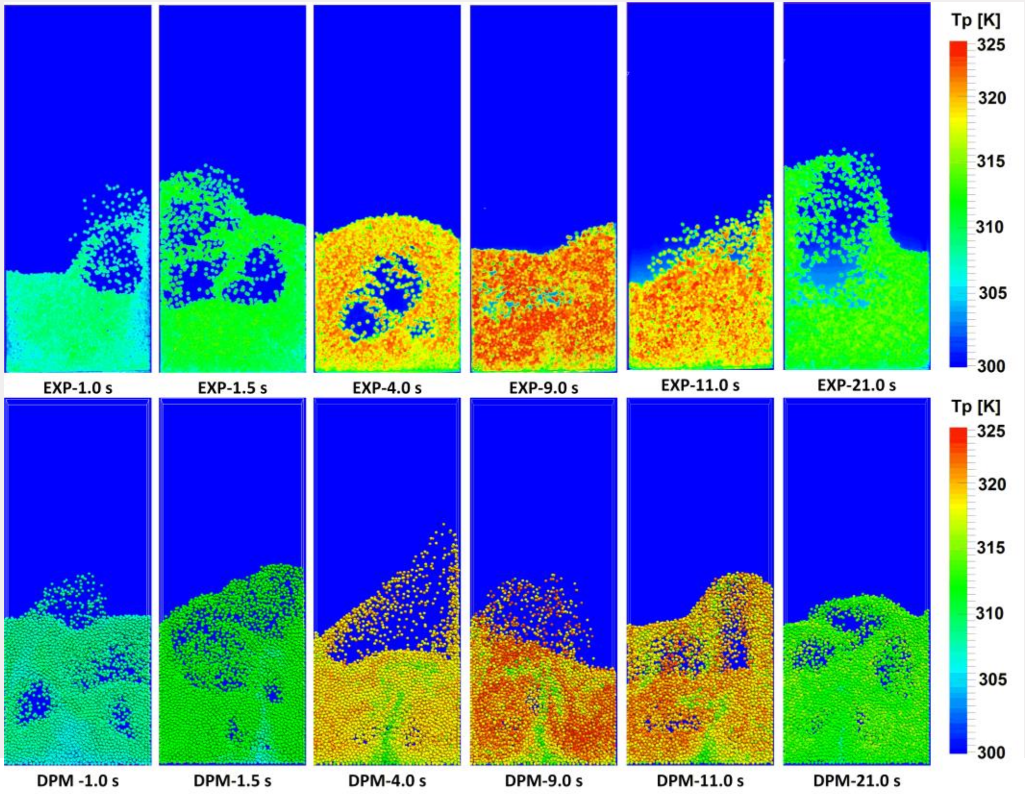
**$CO_2$ absorption on Zeolite particles in pseudo 2D gas-fluidized bed to represent heat liberation due to exothermic chemical reaction**

**PIV +DIA**

**IR-thermography for temperature distribution in particulate phase**

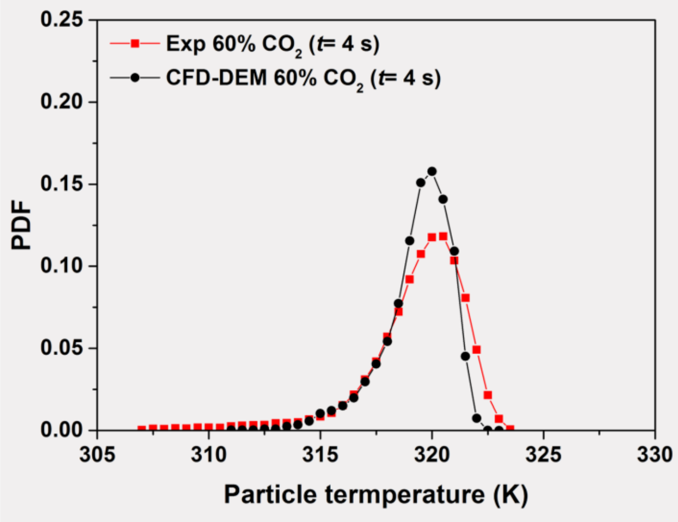
# CFD-DEM Modelling of Heat Transfer in Gas-fluidized Beds

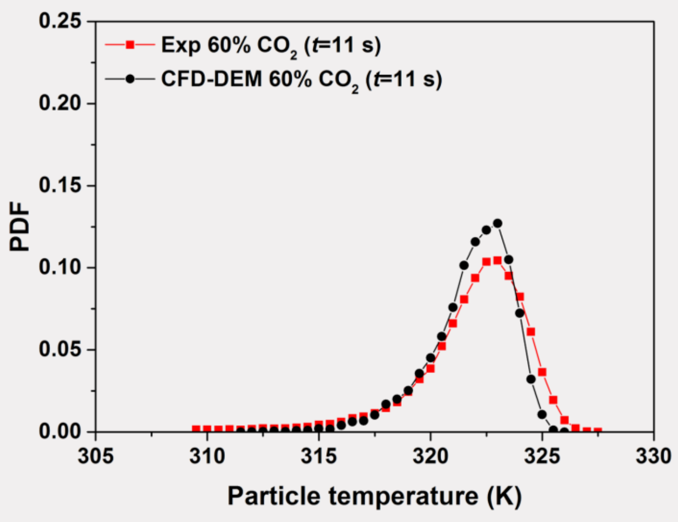
## experiment (top) versus simulation (bottom)



# CFD-DEM Modelling of Heat Transfer in Gas-fluidized Beds

## PDF of particle temperature

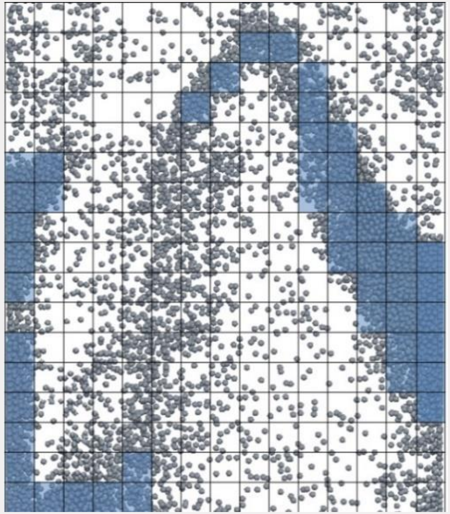


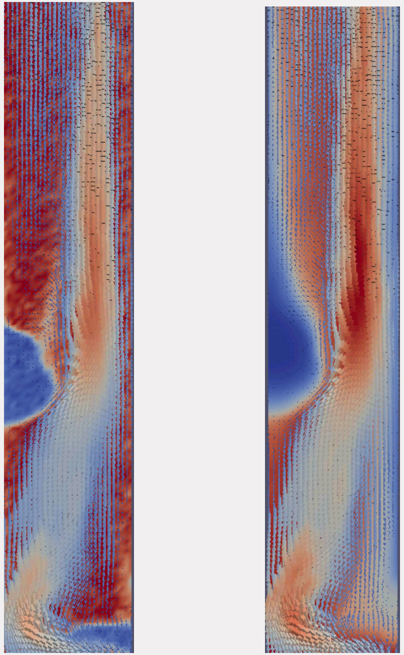



# Riser Flow

## influence of particle clusters on mass transfer

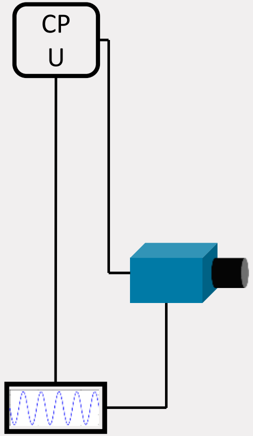
CFD-DEM simulations of riser flow



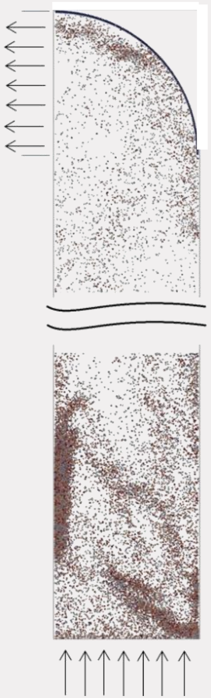


porosity mass fraction

# Experimental Validation of Lab-scale CFB



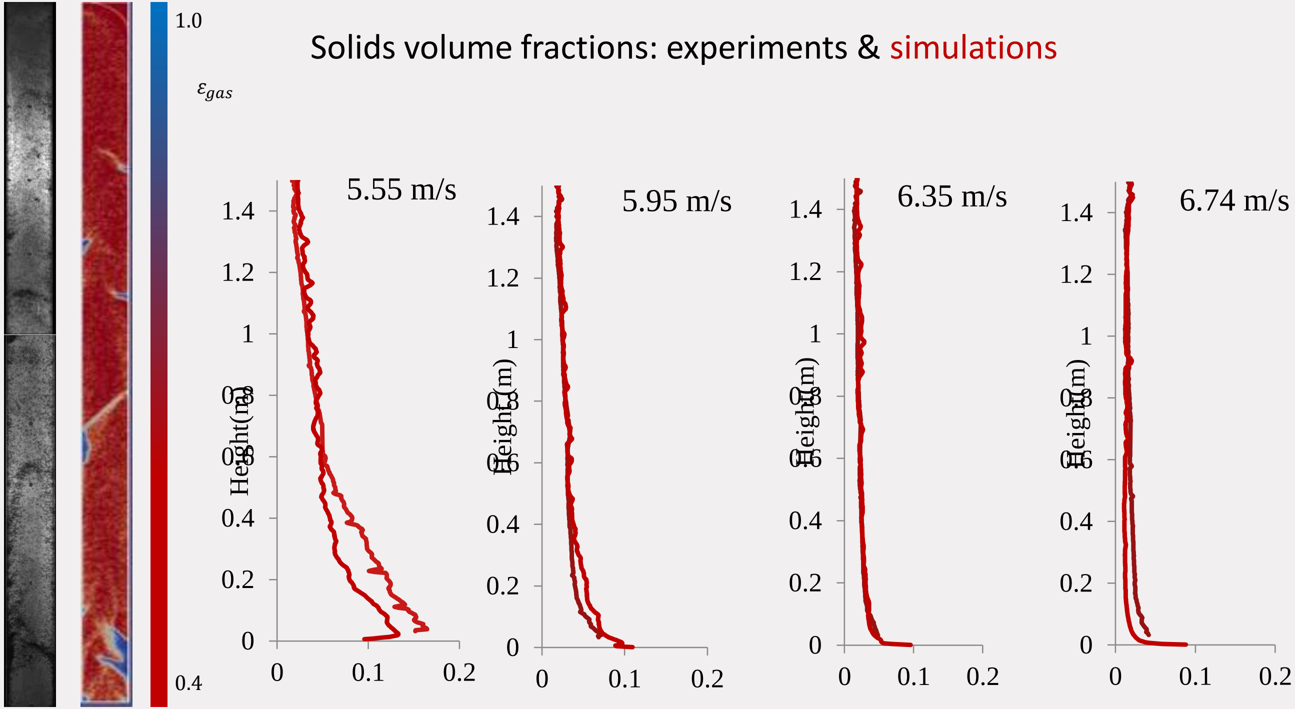

experimental setup



computational domain

# Experimental Validation of Lab-scale CFB

## time-averaged results



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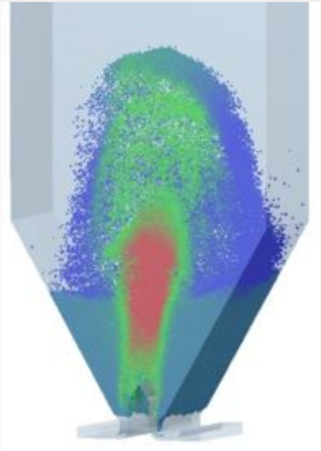
# Wet Collisions In Fluid Bed Granulation Processes

CFD-DEM

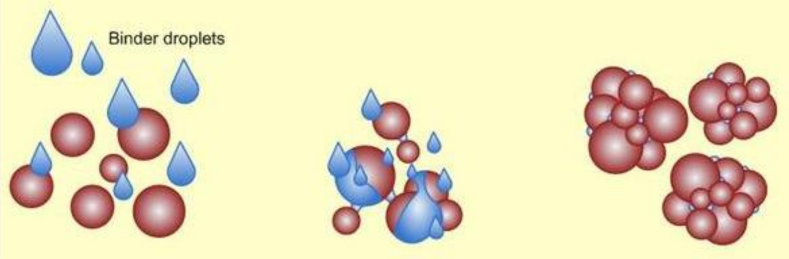


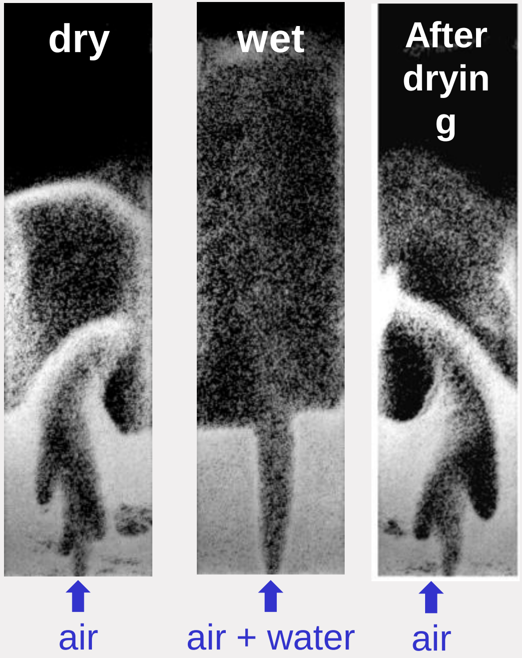
Particulate flows involving liquid:

- Granulation
- Agglomeration
- Coating

Particle interactions:

- Different from dry particles
- Liquid bridge formation




Antonyuk et al., 2009
Particuology

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Yali Tang
Alvaro Carlos Varas
Junwu Wang
Mao Ye

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DSM
ERC
FOM
NWO-CW
Sabic
Shell
STW
Unilever
Yara




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# Take home messages

Multi-scale approach fruitful

Experimental validation of numerical models important

Particle-resolved DNS can simulate small fluid-particle systems

Provides closure relation for coarser models

CFD-DEM numerical laboratory for fluidized systems

Can simulate lab-scale gas-solid systems

Suited for investigating influence meso-scale structures (bubbles, particle clusters)

Developments: towards realistic (reactor) systems

Heat & mass transfer, wet collisions