Karlsruhe Institute of Technology

31. Deutscher Flammentag

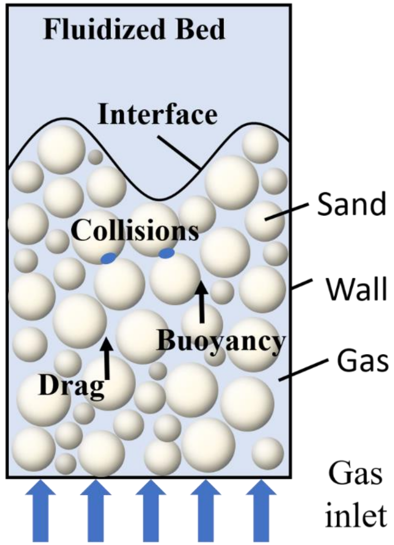
27.-28. Sept. 2023

TU Berlin

An assessment of fluidized bed dynamics with CPFD simulations

F. Zhang, S. Tavakkol, S. Dercho, L. Bohlender, T. Zirwes, M. Zeller, J. Vogt, D. Stapf

Institute for Technical Chemistry (ITC)



Multiphysics

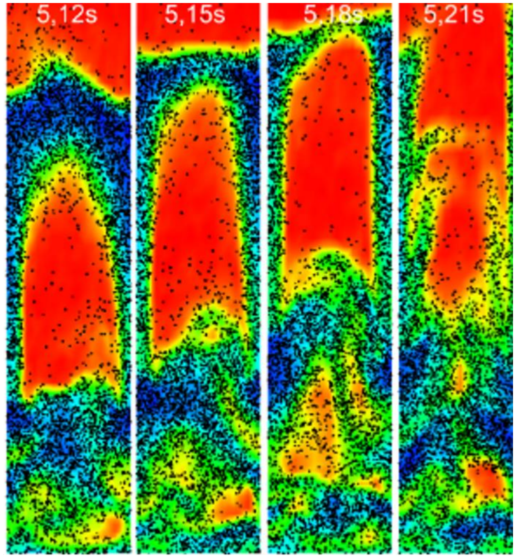
Multiphase

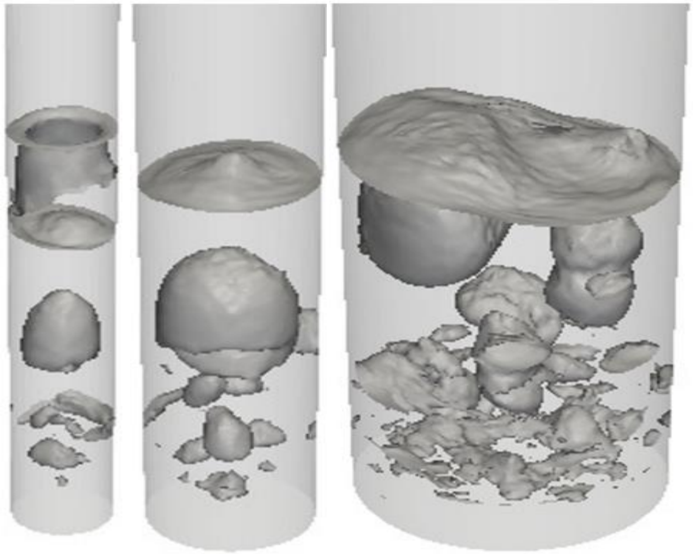
Multiscale

Hydrodynamics

Heat-/mass transfer

Reaction kinetics





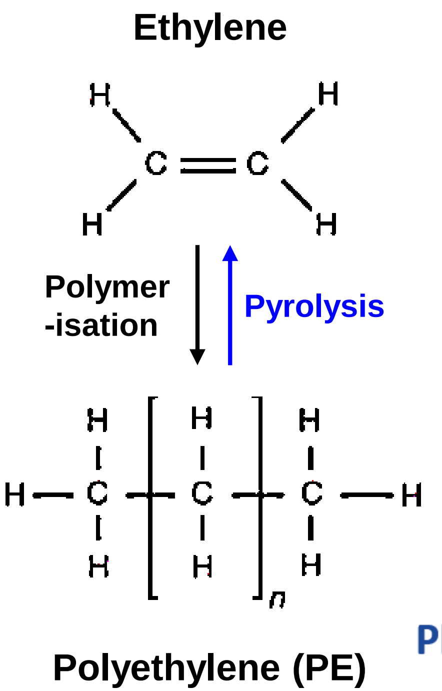
Outline

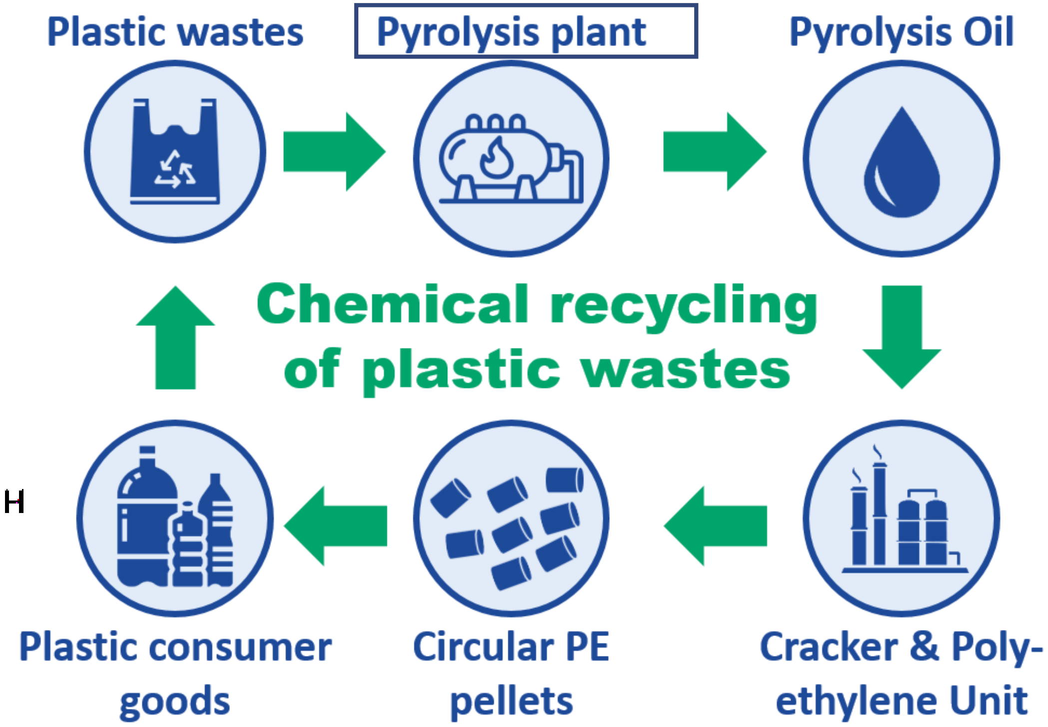
- ☐ Motivation
- ☐ Simulation method
- ☐ Numerical setups
- ☐ Results
    - ☐ Fluidization behavior
    - ☐ Effect of gas temperature
    - ☐ Effect of up-scaling
- ☐ Summary

Chemical recycling of plastic wastes

- ~350 Mt plastic waste per year worldwide
  - 22% mismanaged, 9% recycled
- Chemical recycling of plastic wastes
  - Contaminated/mixed plastics
- Challenges
  - Process design, efficiency, product yield, scale-up, economic viability
- Fluidized bed technology
  - Enhanced, homogeneous heating
  - Potential for scale-up
- Simulation of lab-scale fludized bed
  - Model validation, hydrodynamics

Pyrolysis: Degradation of polymers at high temperature and oxygen-free environment into short-chain hydrocarbons





https://www.oecd.org/environment/plastic-pollution-is-growing-relentlessly-as-waste-management-and-recycling-fall-short.htm

Mismanaged 22%	Landfilled 49%	incinerated 19%	recycled

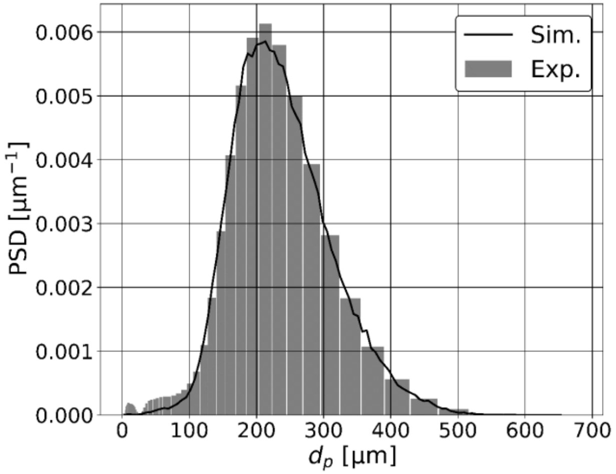
3D simulations of cold-mode fluidized bed

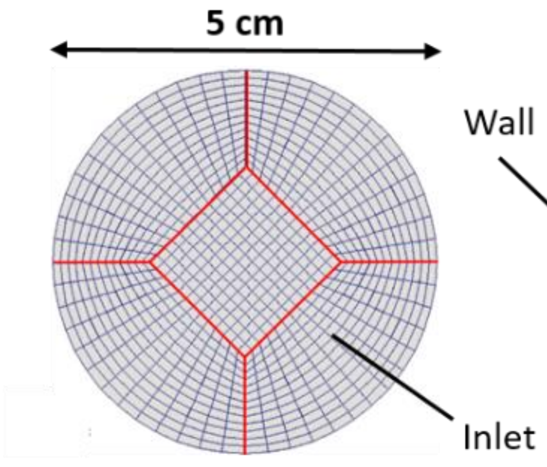
☐ Numerical setups

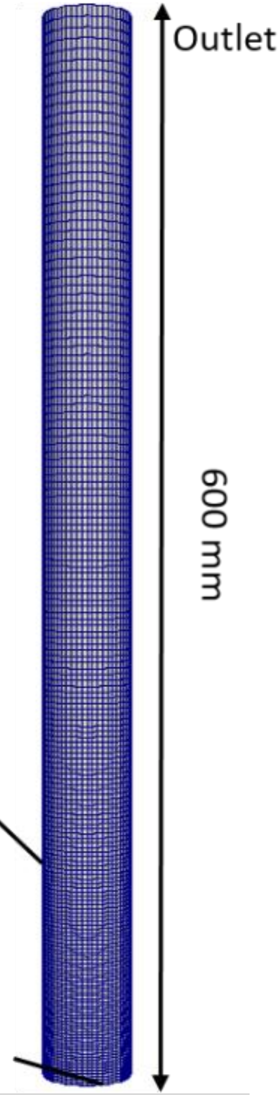
- Cylindrical reactor
- Bed material: quartz sand
- Fluidizing agent: N_2
- PSD: $d_{\mathrm{mean}} = 2.3\ \mathrm{mm}$
- Diameter: $\underline{d_R = 3, 5, 10\ \mathrm{cm}}$
- Gas temperature: $\underline{T_G = 25 \text{ and } 500\ ^{\circ}\mathrm{C}}$
- OpenFOAM-v2206
- Grid resolution: 1 mm
- No. parcels: up to 32 mil.

$d_R = 5\ \mathrm{cm}$

m_S [g]	u_G [cm/s]
195	13.6
293	16.9
390	21.2
488	25.4
586	29.7

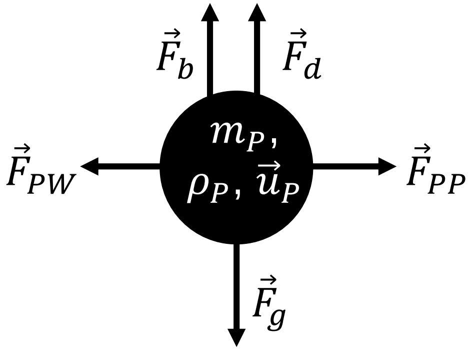






Computational particle fluid dynamics (CPFD)

- ❑ **Euler-Lagrange modeling (4-way coupling)**
- ❑ **Multiphase particle-in-cell (MPPIC) for modeling collisional force**



Continuous phase – gas

Balance of momentum

(Navier-Stokes equations)

$$\overset{\vec{S}_u}{\underset{\vec{F}_d}{\Longleftrightarrow}}$$

Disperse phase – particle

Conservation of momentum

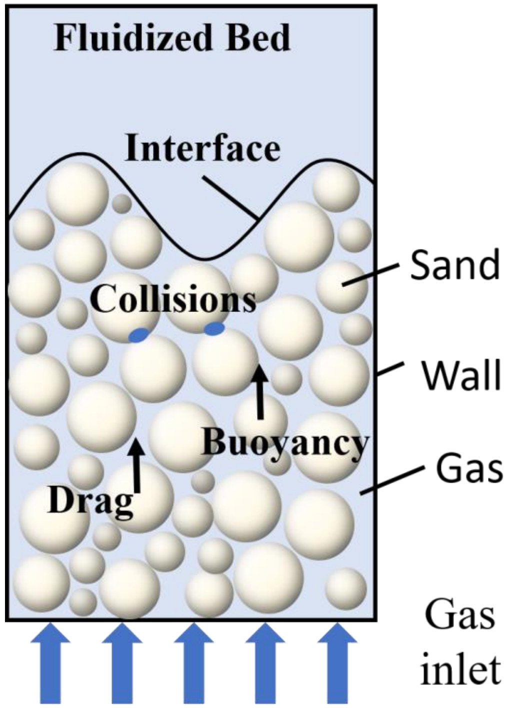
(Newton‘s 2nd law)

$$\frac{\partial(\alpha_g\rho_g\vec{u}_g)}{\partial t} + \nabla\left(\alpha_g\rho_g\vec{u}_g\vec{u}_g\right)$$
$$= -\nabla p + \nabla\left(\alpha_g\vec{\tau}_{eff}\right) + \alpha_g\rho_g\vec{g} + \boxed{\vec{S}_u}$$

$$\vec{S}_u = -\frac{1}{V_{cell}}\sum_{i=1}^{n_{p,cell}}\boxed{\vec{F}_d}$$

$$m_p\frac{d\vec{u}_p}{dt} = \sum\vec{F}_{external}$$
$$= \boxed{\vec{F}_d} + \vec{F}_g + \boxed{\vec{F}_c} + \vec{F}_i$$

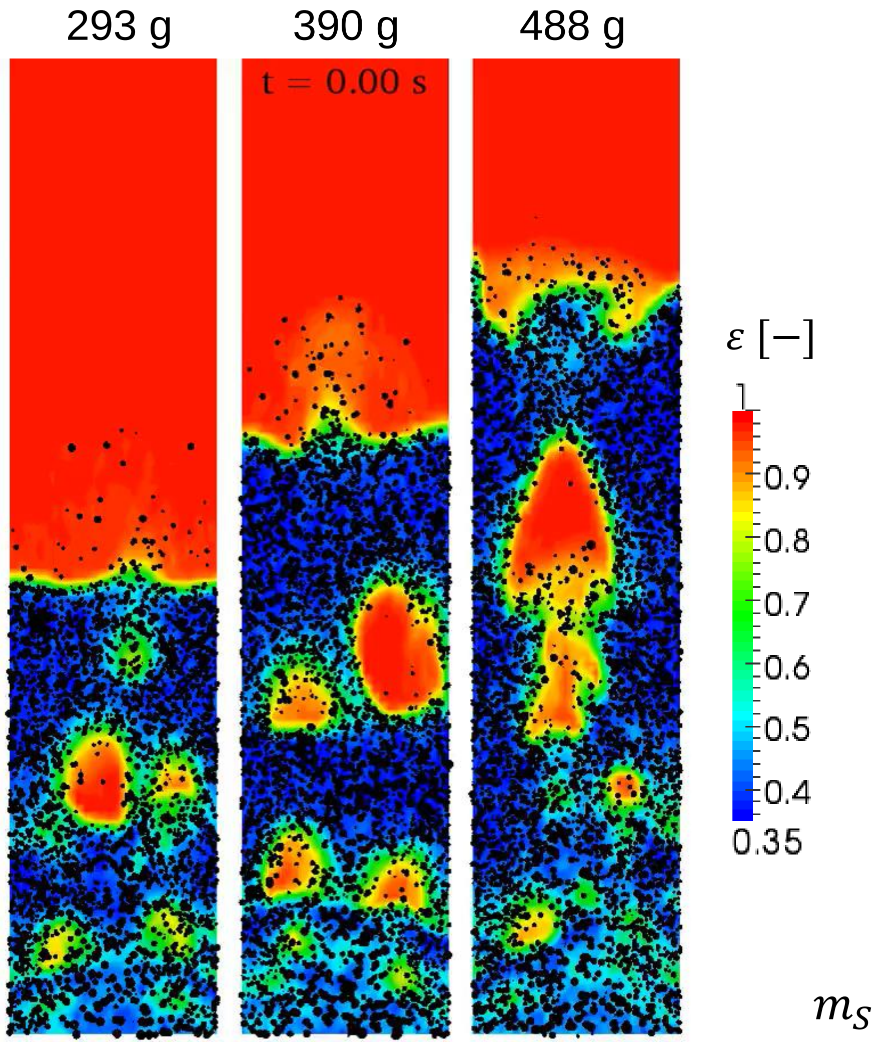
$$\boxed{\vec{F}_c} \propto \nabla\tau_p \qquad \tau_p = \frac{p_s * \alpha_p^{\beta}}{\alpha_{packed} - \alpha_p}$$



Results

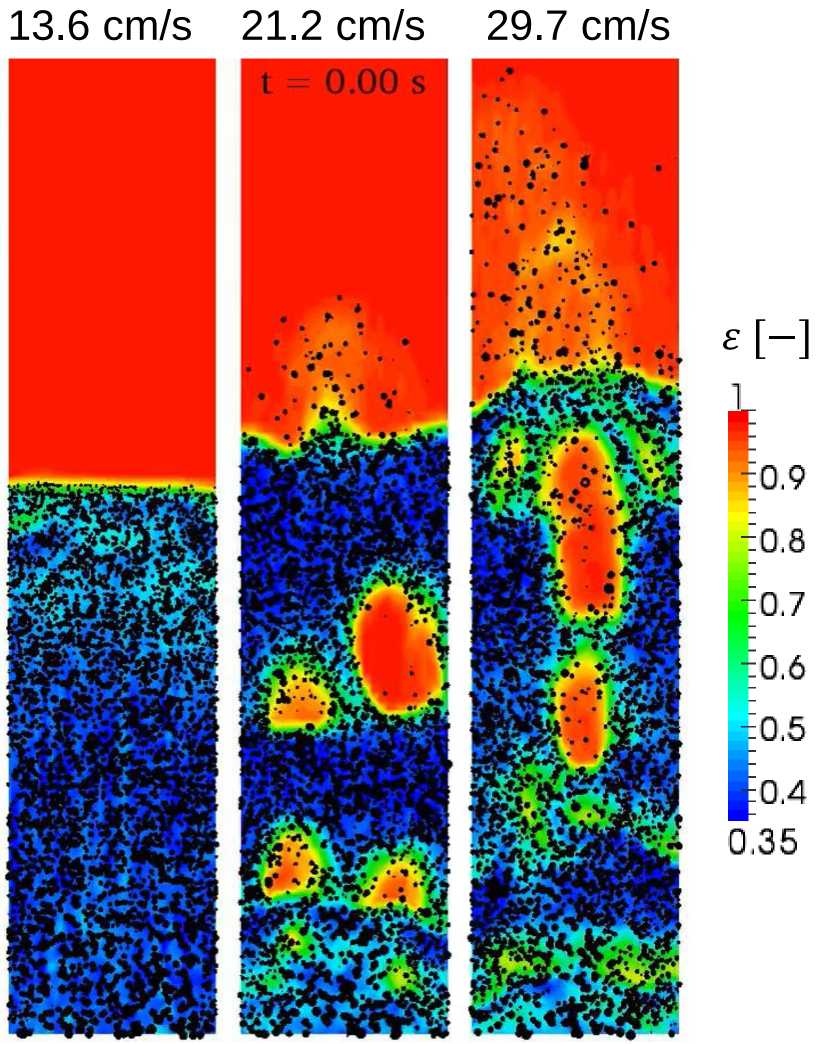
Fluidization behavior

Bed inventory m_S ↑



$u_g = 21\ cm/s$

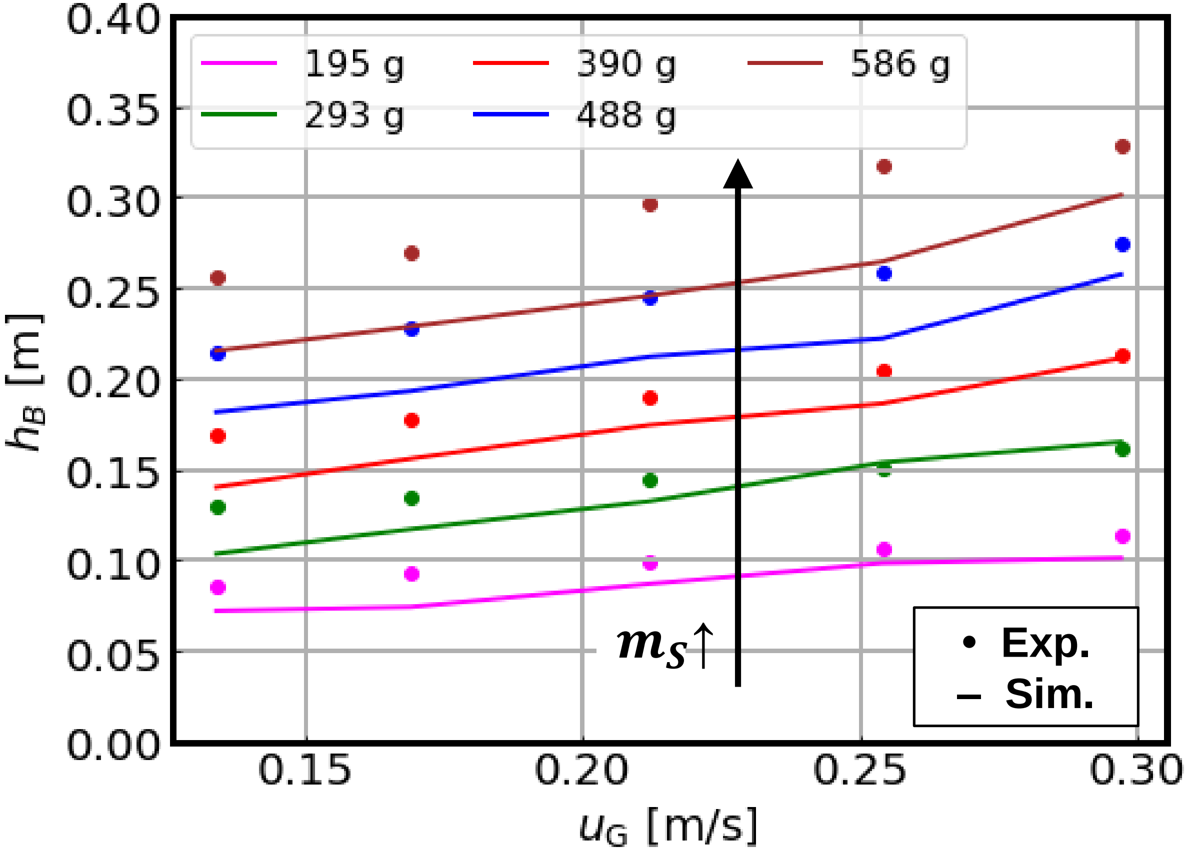
Superficial velocity u_g ↑



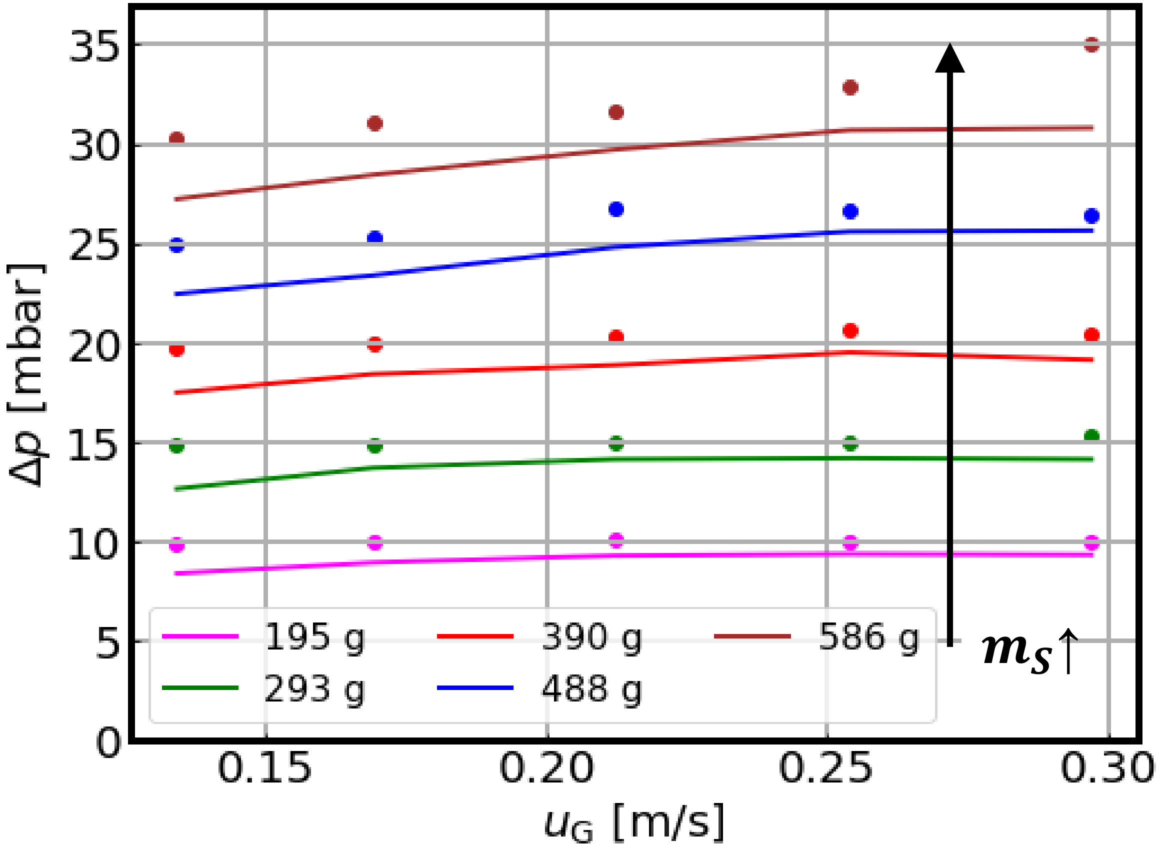
$m_S = 390\ g$

Comparison with experiments

- ☐ Bed height h_B increases with m_S and u_G
- ☐ Pressure drop Δp increases with m_S and remains almost constant with u_G

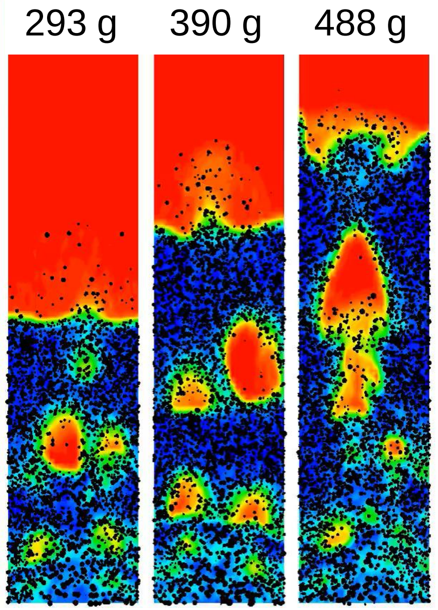


Bed height h_B



Pressure drop Δp

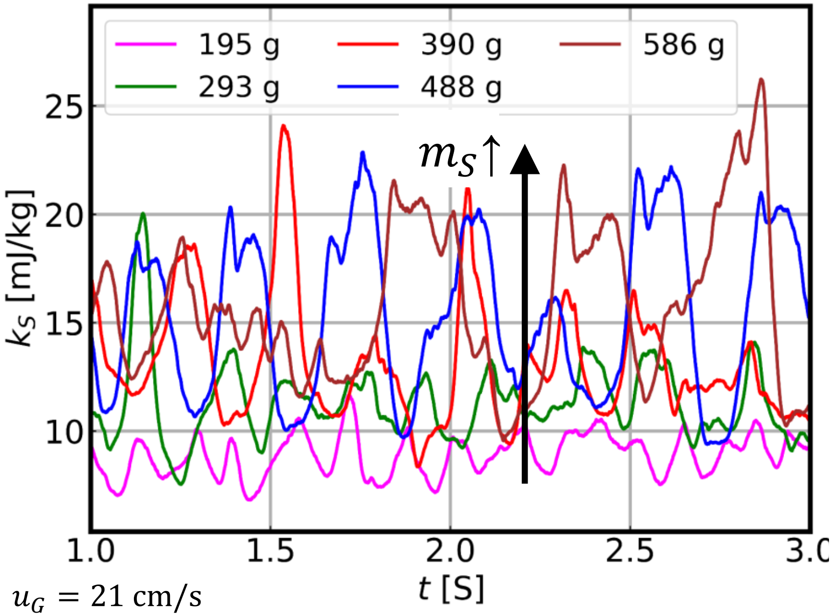
Dynamic properties of fluidized bed



Specific kinetic energy of sand k_S and bubble frequency f_B

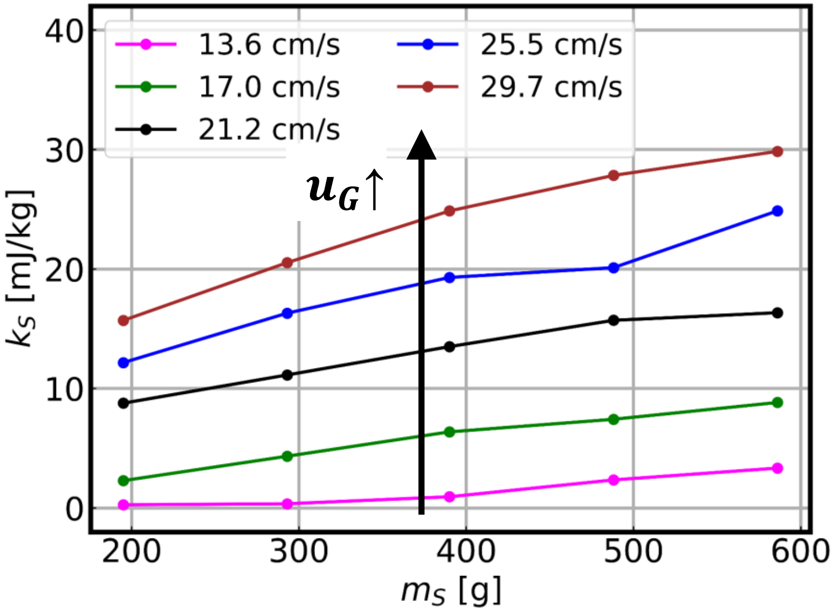
- ☐ Increase of k_S with m_S and u_G
- ☐ f_B decreases inversely proportionally with m_S

$$K_S = \frac{1}{2}\sum_{i=1}^{N_p} m_{p,i}u_{p,i}^2\,, \qquad k_S = K_S/m_S$$

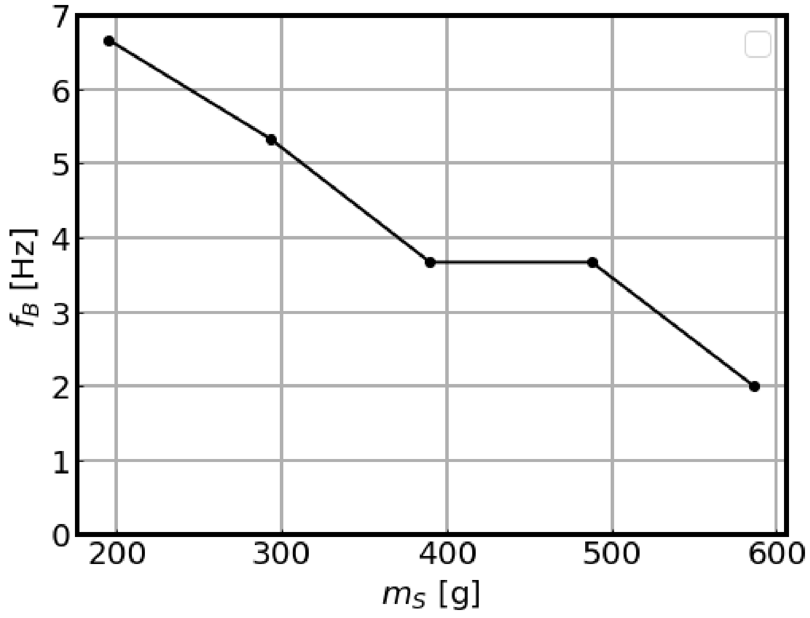


$u_G = 21$ cm/s

Kinetic energy of sand k_S [mJ/kg]



Bubble frequency f_B [Hz]

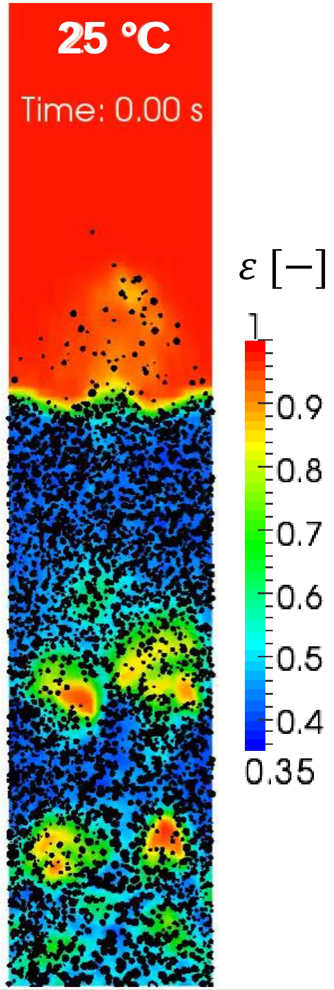


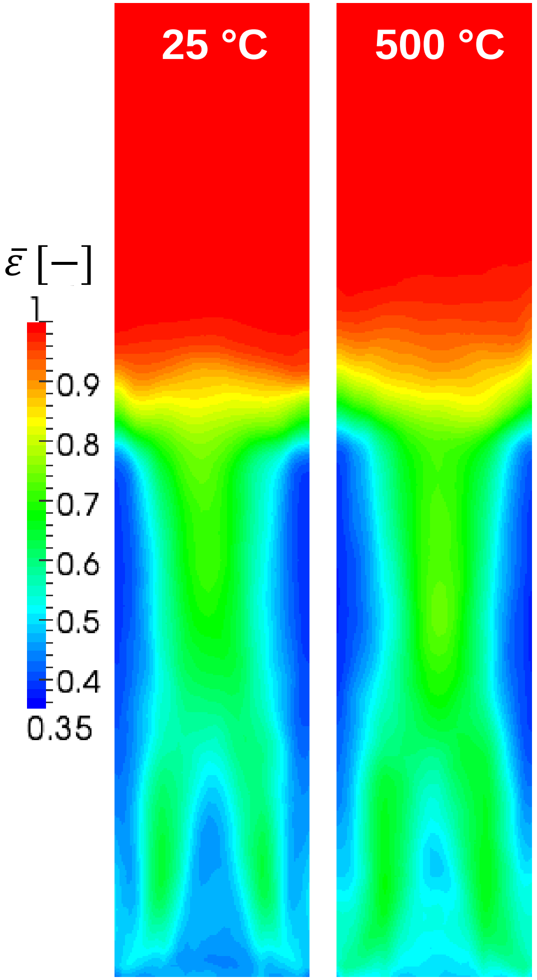
Impact of gas temperature

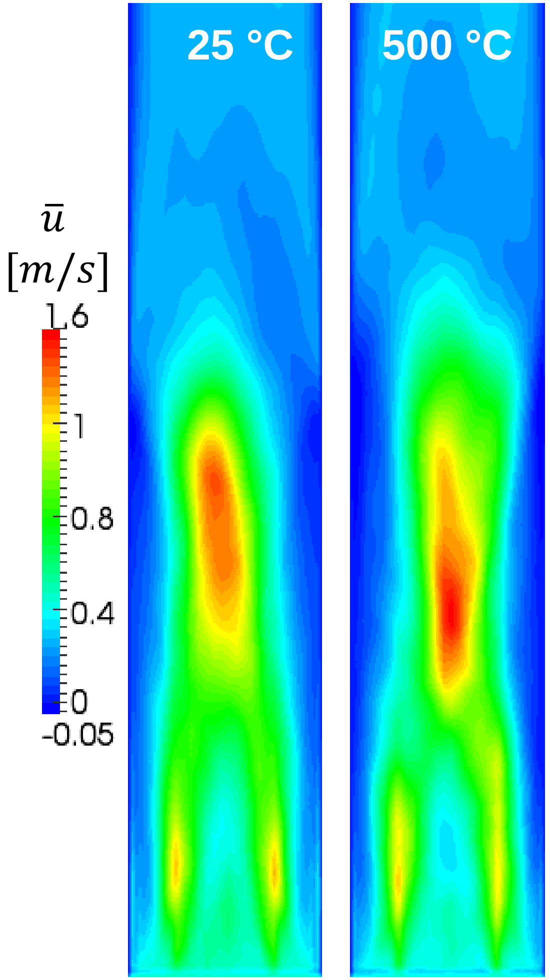
- ☐ Increase of gas density and viscosity with T_G
- ☐ Same fluidization behavior at increased T_G
- ☐ Slight increase of h_B and Δp

T_G [℃]	25	500
ρ_G [kg/m³]	1.14	0.44
υ_G [m²/s]	1.6e-5	8e-5
h_B [cm]	17.5	19.0
Δp [mbar]	18.9	19.8

m_S = 390 g, u_G = 21 cm/s


Gas volume fraction

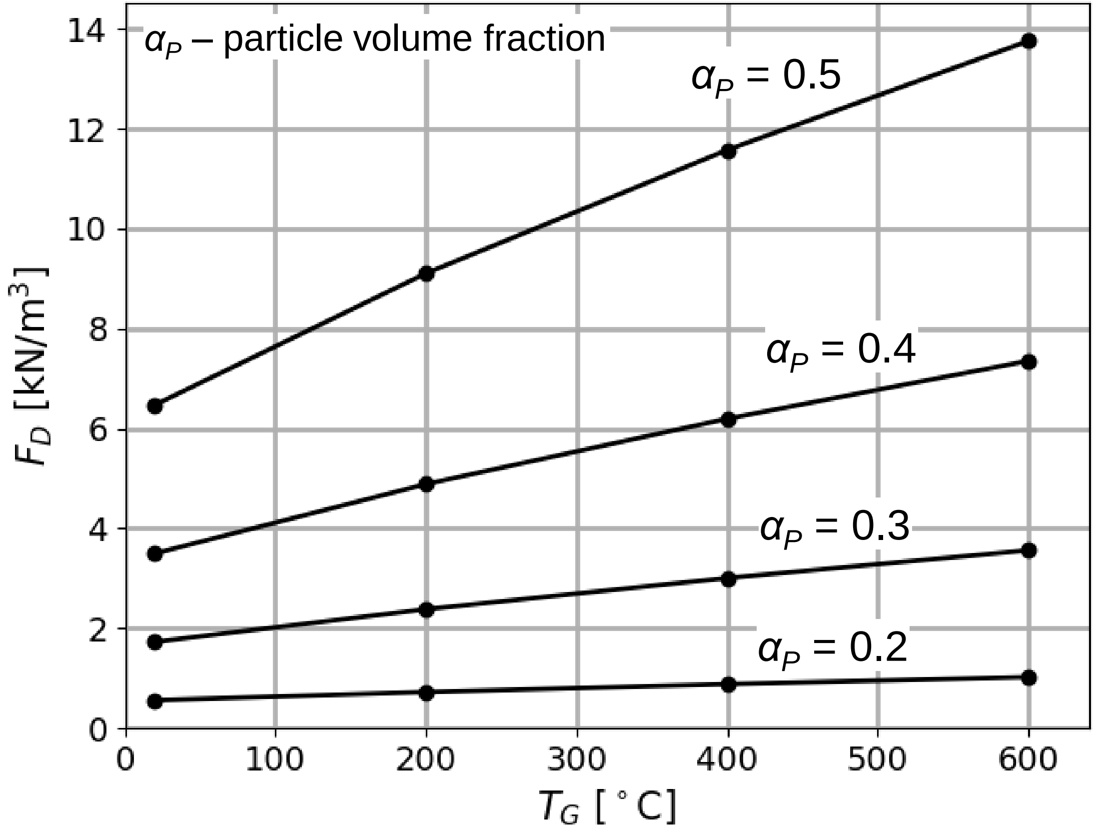

Gas volume fraction

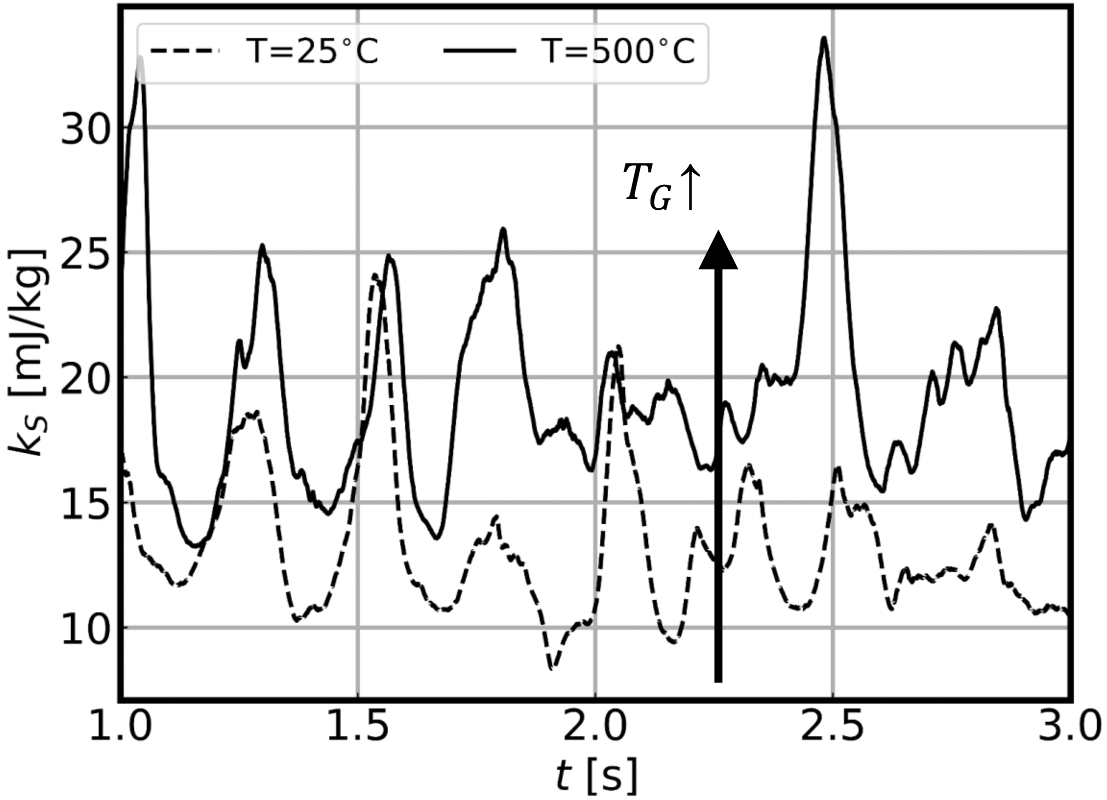

Gas velocity

Impact of gas temperature

- Increase of drag force with T_G
  - Increase of k_S by ca. 50%
  - f_B remains almost constant

T_G [°C]	25	500
k_S [mJ/kg]	13.6	19.2
f_B [Hz]	3.7	4.0



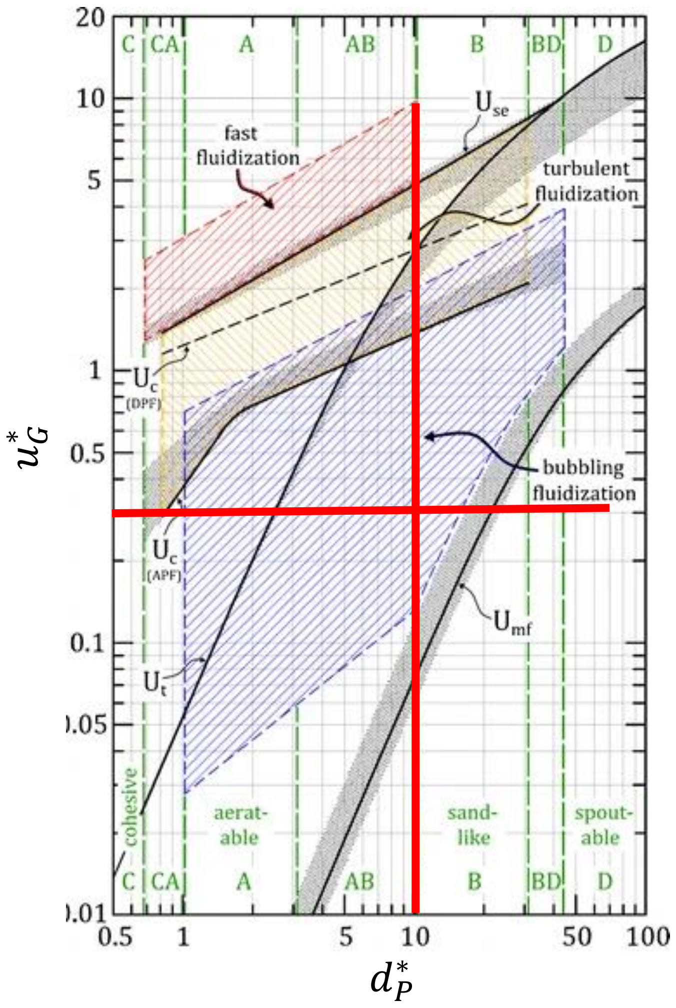


Impact of scale-up: setups

- Up-scaling at
  - Constant Δp and h_B
  - Bubbling fluidization regime
- Increase of m_S with d_R: $m_S \propto {d_R}^2$
- Simulation setups
  - Same resolution for gas phase (1 mm)
  - Proportionally increased No. of Lagrange parcels with m_S

d_R	3 cm	5 cm	10 cm
m_S	140 g	390 g	1600 g
u_G	21 cm/s	21 cm/s	21 cm/s
N_P	2.9 mil.	8.0 mil.	32.0 mil.

Regime diagram for gas-solid fluidized bed according to Grace



Grace JR, Contacting modes and behaviour classification of gas–solid and other two-phase suspensions.1986

$$u_G^* = 0.30$$

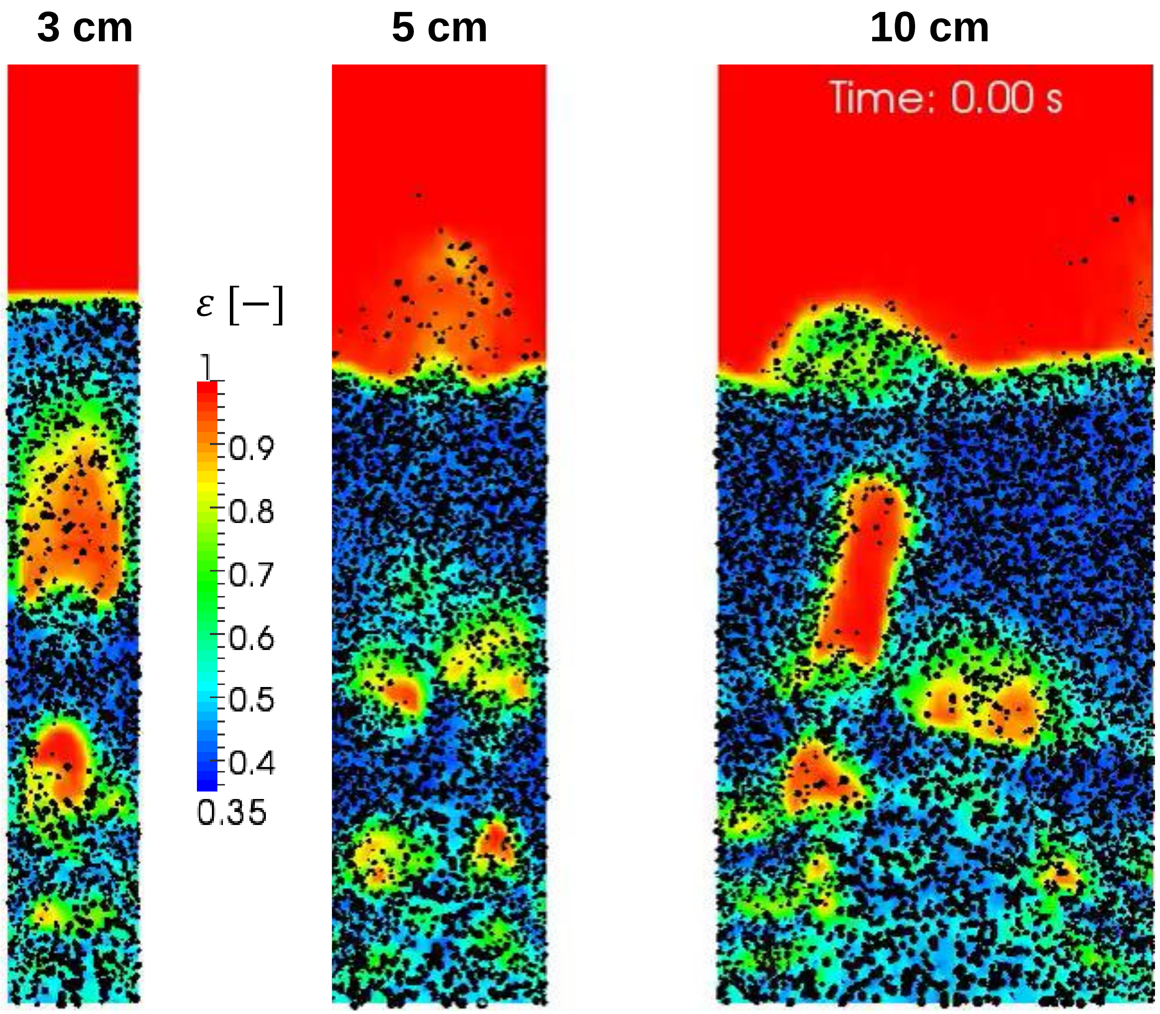
$$d_p^* = 10.24$$

$$u_G^* = u_G \sqrt[3]{\frac{\rho_g^2}{\mu_g(\rho_s - \rho_g)g}}$$

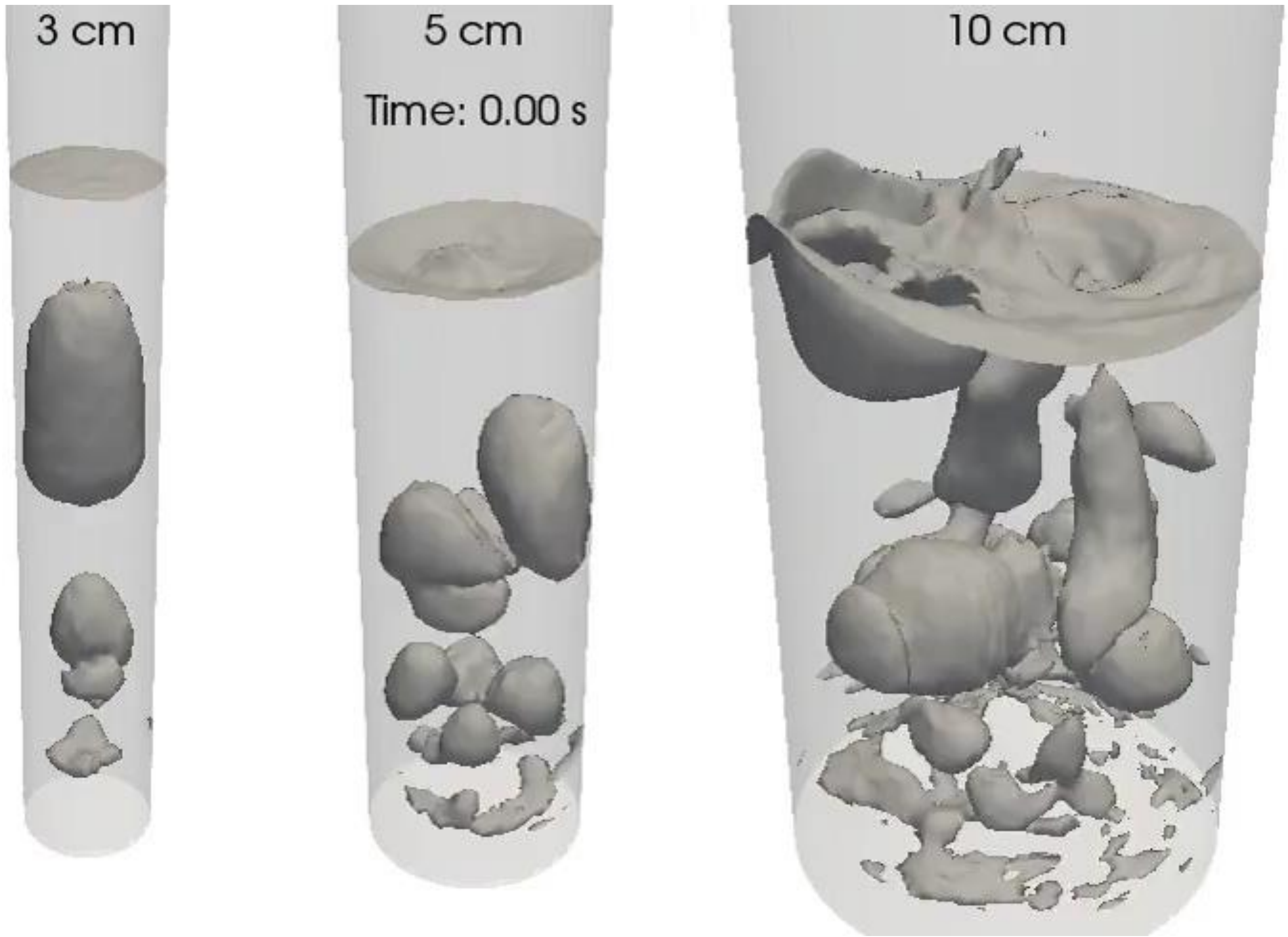
$$d_P^* = d_P \sqrt[3]{\frac{\rho_g(\rho_s - \rho_g)g}{\mu_g^2}}$$

Impact of scale-up: bubble formation

Gas volume fraction



Iso-surface α_g = 0.65



Impact of scale-up: dynamic properties

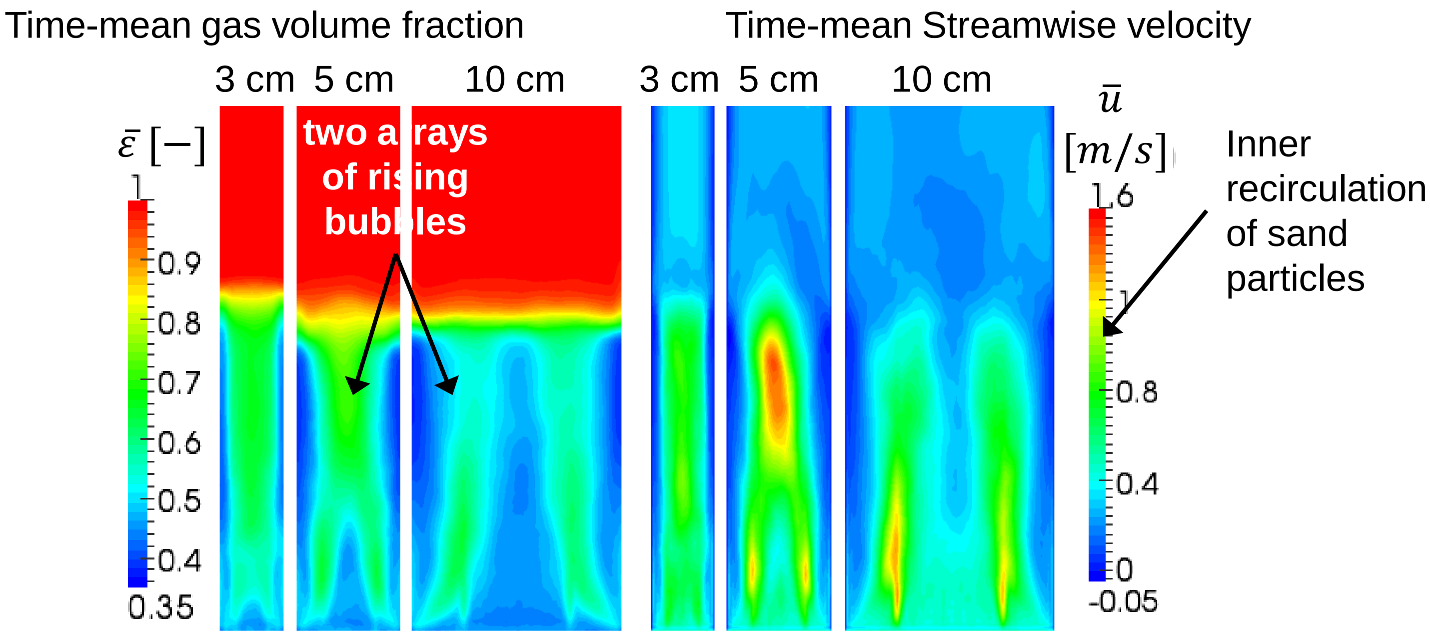
- Increased bubble-to-wall distance
- Enhanced bubble formation
- Multiple arrays of rising bubbles at d_R = 10 cm
- Specific kinetic energy remains constant
- Bubble frequency increases

h_B, Δp $\approx$ const.

$k_S \approx$ const.

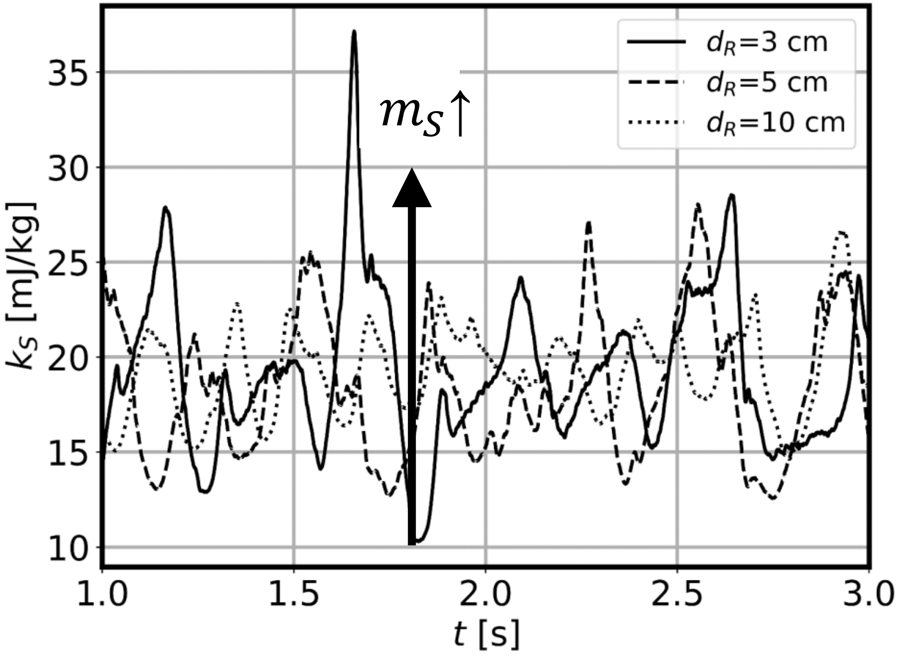
$f_B\uparrow$

d_R [cm]	3	5	10
h_B [cm]	18.0	17.5	17.4
Δp [mbar]	21.0	20.2	20.0
$\bar{k}_S$ [mJ/kg]	18.8	19.6	19.3
f_B [Hz]	2	3.2	3.8


Time-mean gas volume fraction

Time-mean Streamwise velocity

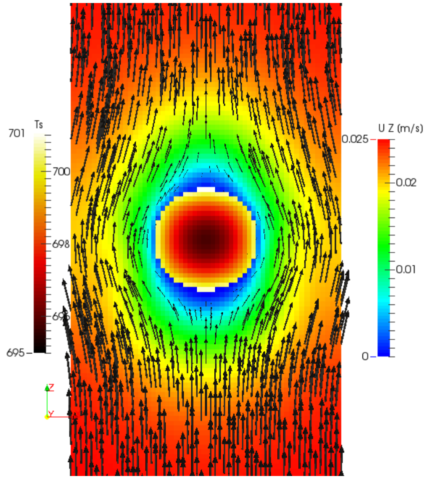
Inner recirculation of sand particles



Summary

- Simulation of cold-mode fluidized bed
- k_S increases with m_S and u_G
- f_B decreases with m_S and remains constant with u_G
- k_S increases at elevated gas temperature, while $f_B \approx \mathrm{const.}$
- Up-scaling leads to enhanced bubble formation and an increase of f_B while $k_S \approx \mathrm{const.}$
- Importance of k_S and f_B for characterizing hydrodynamic behaviors of fluidized bed

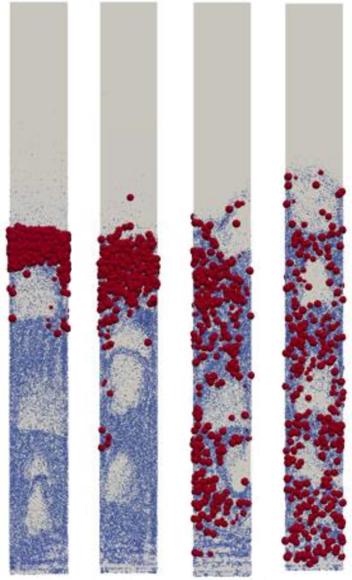
Particle-resolved simulation



Outlook

- Mixing of plastic particles, contact heat transfer, pyrolysis reactions
- Correlation of k_S and f_B with heating rate and pyrolysis reaction

Plastic pyrolysis in fluidized bed



Thank you for your attention!