MULTI-SCALE SIMULATION APPROACH FOR THE FLUIDISED BED SPRAY GRANULATION PROCESS

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FLUIDIZED BED SPRAY GRANULATION
motivation


free flowing


dust-free


redispersible


compact

product formulation

tailor-made properties


instant milk


culinary powders


soluble coffee

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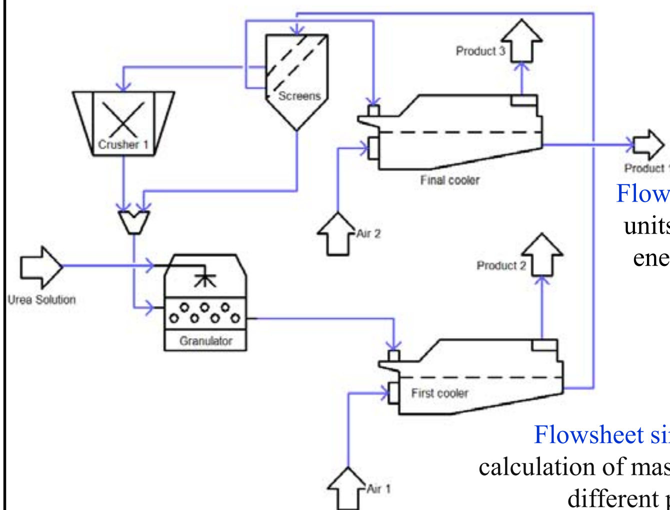
MULTISCALE SIMULATION APPROACH
industrial production process

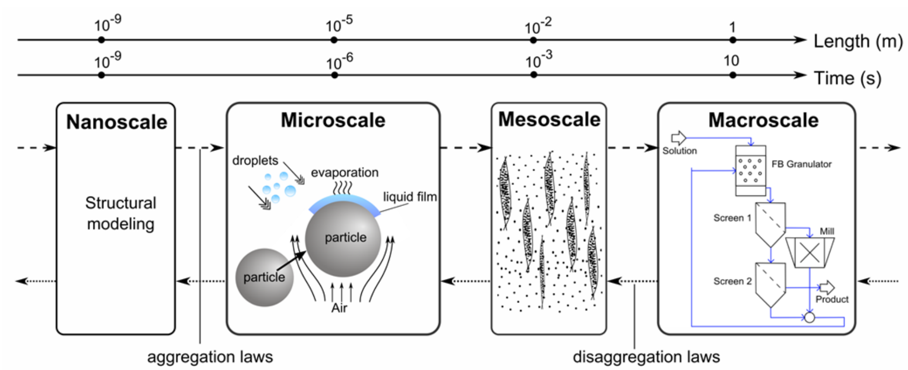
Most industrial processes consists of complex interconnection of different apparatuses and production steps



Flowsheet: Network of process units, which are connected by energy and material streams

Flowsheet simulation: Numerical calculation of mass and energy balances for different process structures

MULTISCALE SIMULATION APPROACH
process treatment on different scales



On the macroscale **empirical** or **semi-empirical** models are used, material properties are **poorly** considered

Description of the process on lower scales leads to exponential **increase** of computational volume

J. Werther, S. Heinrich, M. Dosta, E.-U. Hartge, Particuology, Vol. 9, 320-329, 2011

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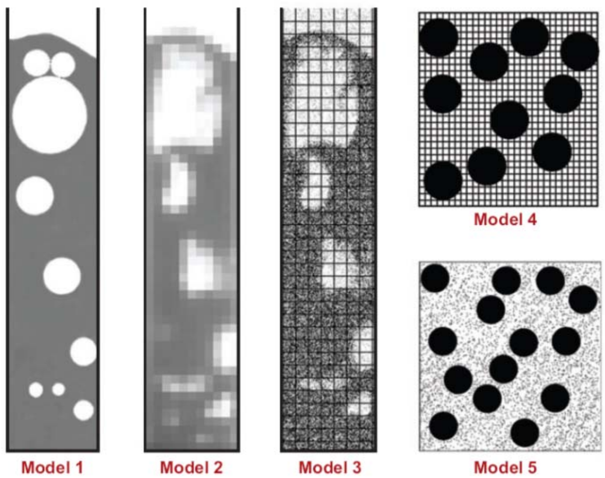
MULTI-SCALE MODELLING



Van der Hoef et al., Annu. Rev. Fluid M., 2008

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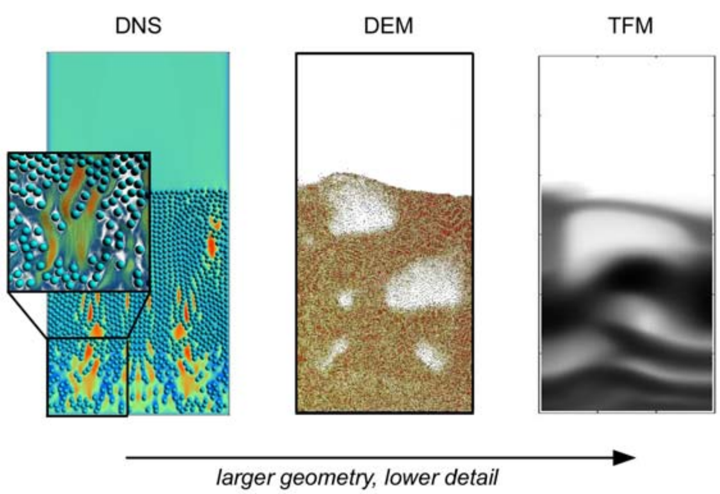
MULTI-SCALE MODELLING



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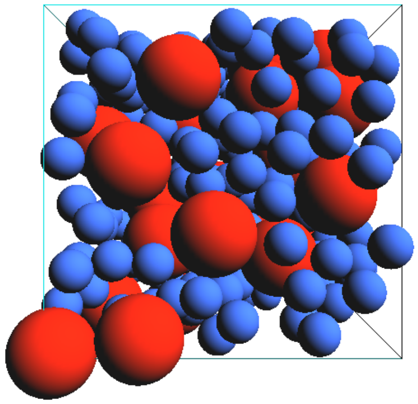
RESULTS OF LATTICE BOLTZMANN MODEL

static array of bi-disperse particles at low Re_p



example of initial particle configuration for a bi-disperse system generated with a Monte Carlo procedure

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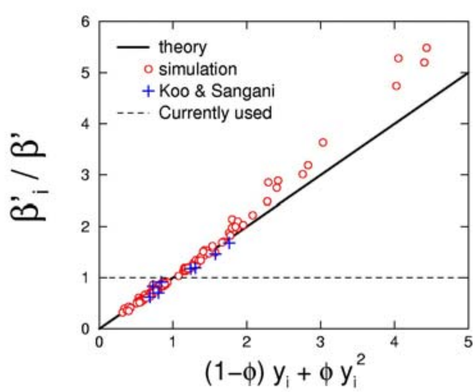
RESULTS OF LATTICE BOLTZMANN MODEL

static array of bi-disperse particles at low Re_p



$$\beta_i' = \left[(1-\phi)\,y_i + \phi\,y_i^2\right]\beta' \qquad y_i = \frac{d_i}{\langle d \rangle}$$

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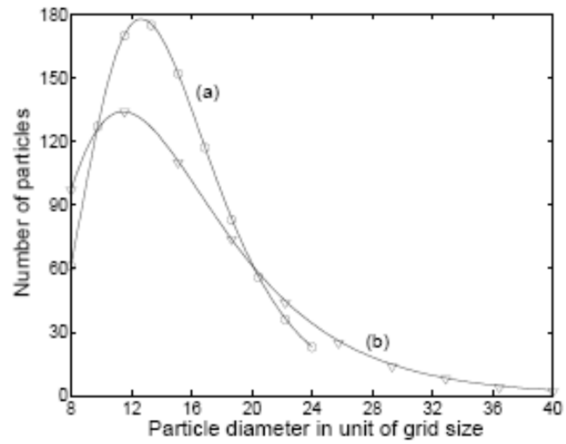
RESULTS OF LATTICE BOLTZMANN MODEL

static array of particles with log-normal PSD



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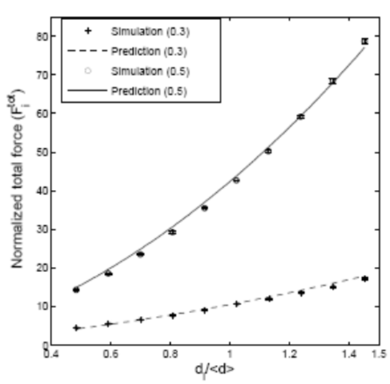
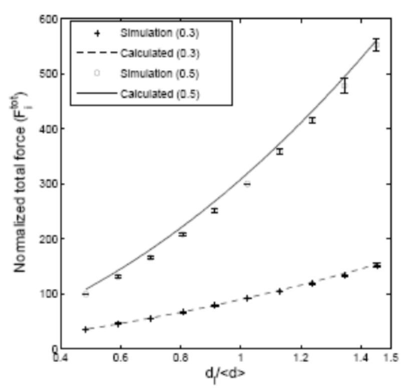
RESULTS OF LATTICE BOLTZMANN MODEL

static array of particles with log-normal PSD

Re=0.1



Re=500



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RESULTS OF LATTICE BOLTZMANN MODEL

final drag closure for mono-disperse and poly-disperse particles

$$\frac{\bar{\mathbf{F}}_{g\to i}}{3\pi\mu d_i\varepsilon_g(\mathbf{u}_g-\mathbf{v}_i)} = \left[\varepsilon_g\frac{d_i}{\langle d\rangle} + \varepsilon_s\frac{d_i^2}{\langle d\rangle^2} + 0.064\varepsilon_g\frac{d_i^3}{\langle d\rangle^3}\right] \times \left[\frac{10\,\varepsilon_s}{\varepsilon_g^3} + \varepsilon_g + 1.5\,\varepsilon_g\varepsilon_s^{1/2} + \frac{0.413\,\mathrm{Re}}{24\varepsilon_g^3}\left(\frac{\varepsilon_g^{-1}+3\varepsilon_s\varepsilon_g+8.4\,\mathrm{Re}^{-0.343}}{1+10^{3\varepsilon_s}\,\mathrm{Re}^{-(1+4\varepsilon_s)/2}}\right)\right]$$

good fit (deviation less then 8%) of basic LB simulation data generated over wide range of ε_g and Re

strictly valid for homogeneous arrays of particles

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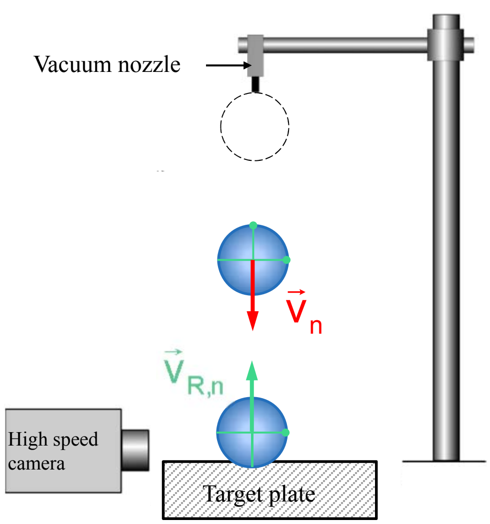
MECHANICAL PARTICLE PROPERTIES

measurement of restitution coefficient



$$e_n = \left|\frac{\vec{v}_{R,n}}{\vec{v}_n}\right|$$

e_n normal restitution coefficient

v_n normal impact velocity

$v_{R,n}$ normal rebound velocity

van Buijtenen, M.S., Deen, N.G., Heinrich, S., Antonyuk, S. and J.A.M. Kuipers: A discrete element study of wet particle-particle interaction during granulation in a spout fluidized bed, *Canadian Journal of Chemical Engineering* (2009), Vol. 9999, 1-10.

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MECHANICAL PARTICLE PROPERTIES

measurement of restitution coefficient

Restitution coefficient:

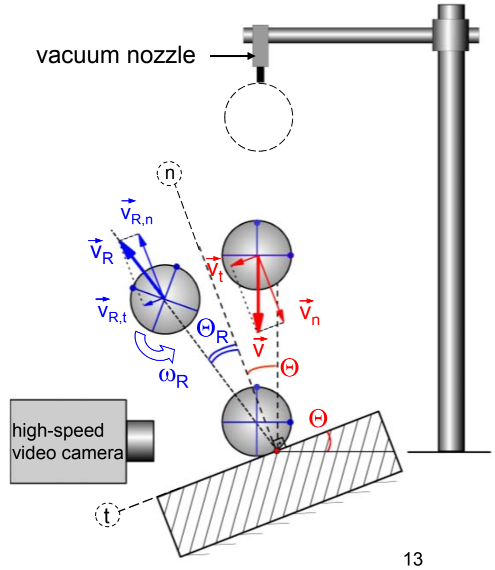
$$e = \sqrt{\frac{E_{kin,R}}{E_{kin}}} = \sqrt{1-\frac{E_{diss}}{E_{kin}}} = \frac{|\vec{v}_R|}{|\vec{v}|}$$

v_R/v relative rebound/impact velocity

n/t normal and tangential component

$$e_n = \left|\frac{\vec{v}_{R,n}}{\vec{v}_n}\right|$$ normal

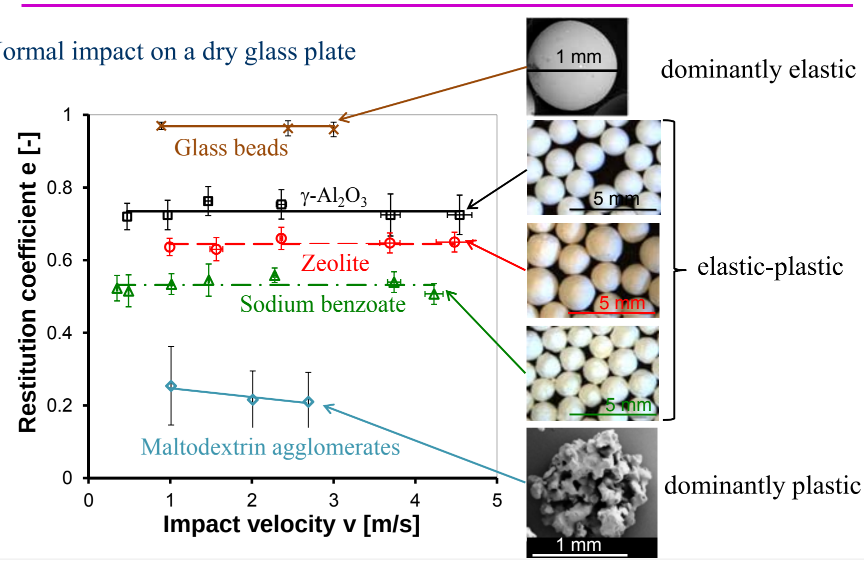
$$e_t = \left|\frac{\vec{v}_{R,t}}{\vec{v}_t}\right|$$ tangential



MECHANICAL PARTICLE PROPERTIES

measurement of “dry” restitution coefficient

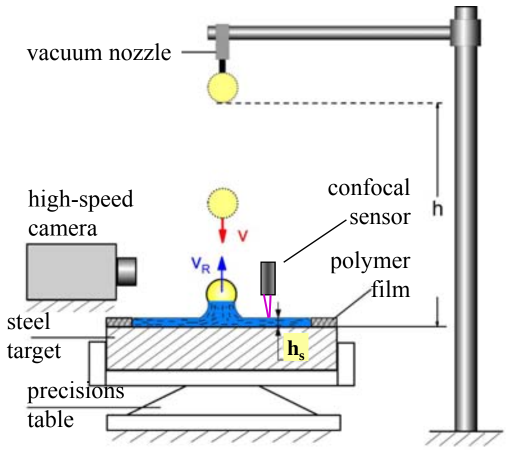
Normal impact on a dry glass plate



Antonyuk, S., Heinrich, S., Tomas, J., Deen, N.G., van Buijtenen, M.S. and J.A.M. Kuipers: Energy absorption during compression and impact of dry elastic-plastic spherical granules, Granular Matter (2010) 1, 12.

MECHANICAL PARTICLE PROPERTIES

measurement of “wet” restitution coefficient



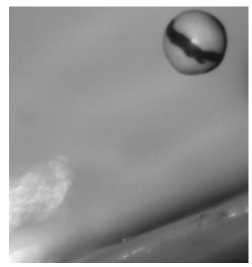
$$e = \sqrt{\frac{E_{kin,R}}{E_{kin}}} = \frac{v_R}{v}$$

v_R/v relative rebound/impact velocity

$E_{kin,R}$ elastic rebound energy

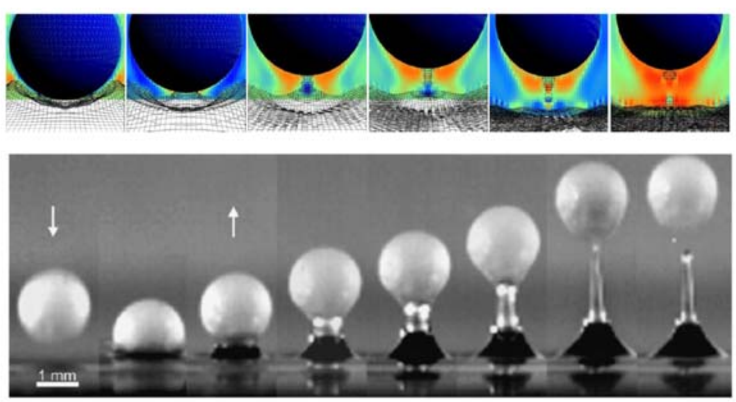
E_{kin} impact energy

E_{diss} irreversible absorbed energy



Objectives of the study: e = *f* (impact velocity, liquid film thickness and viscosity)

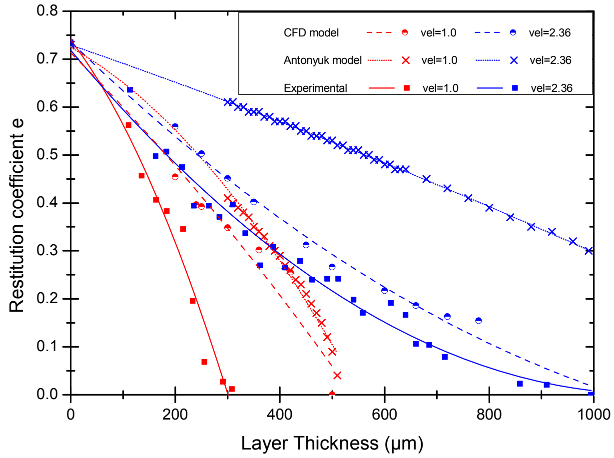
PARTICLE COLLISION IN WET SYSTEMS



(above) Formation, thinning & eventual breakup of the liquid bridge (simulation results)

(below) Images from high-speed recording of α-Al_2O_3 granule impacting with velocity of 2.36 m/s on wall with a water layer (thickness 0.4 mm) (Antonyuk et al. (2009)).

PARTICLE COLLISION IN WET SYSTEMS



Influence of impact velocity on restitution coefficient of the Al_2O_3 granules impacting on water layers with varying thickness.

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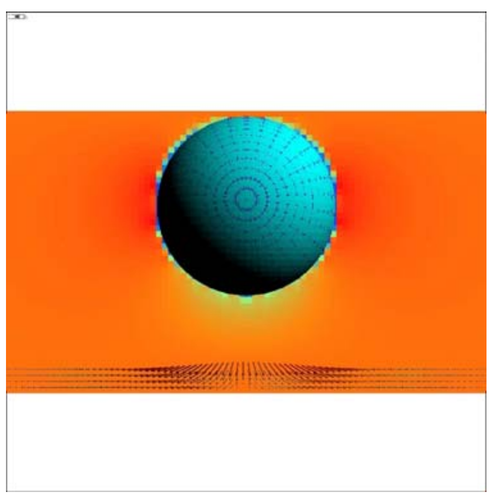
PARTICLE COLLISION IN WET SYSTEMS



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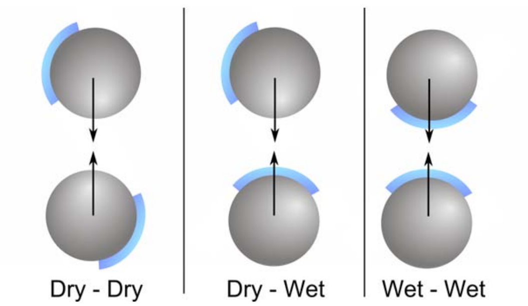
PARTICLE COLLISION IN WET SYSTEMS
collision types for different moisture contents

- During fluidized bed granulation the particles are covered by a liquid film
- Different types of collisions can occur:

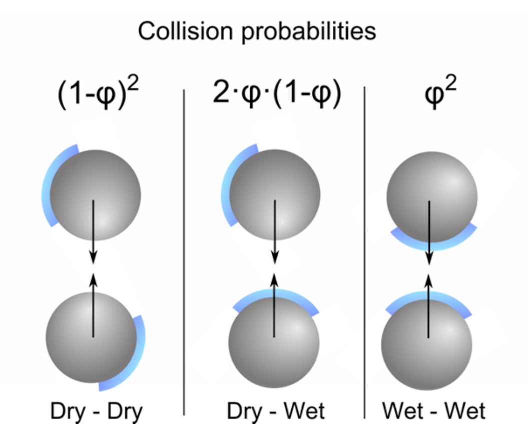


$$e = \sqrt{\frac{E_{kin,R}}{E_{kin}}} = \frac{v_R}{v}$$

How can the influence of the liquid film be predicted?

PARTICLE COLLISION IN WET SYSTEMS
collision types for different moisture contents

- For the description of the liquid film, the wetted surface fraction φ is used
- φ obtained from the calculations of the model on the macroscale



$$\varphi = \frac{A_{wet}}{A_{tot}}$$

A_{wet} wetted surface
A_{tot} total particle surface

$$e = \sqrt{\frac{E_{kin,R}}{E_{kin}}} = \frac{v_R}{v}$$

$$e = e_1 \cdot (1-\varphi)^2 + e_2 \cdot 2 \cdot \varphi \cdot (1-\varphi) + e_3 \cdot \varphi^2$$

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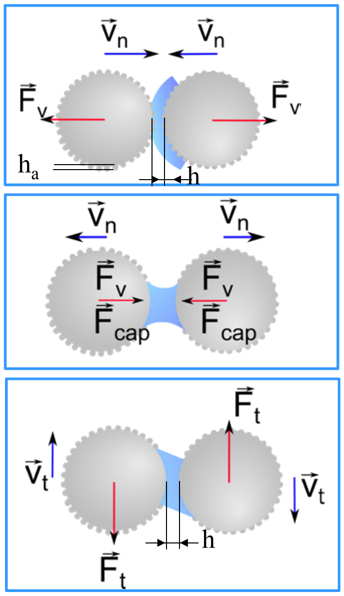
PARTICLE COLLISION IN WET SYSTEMS

contact model for wet collisions



Viscous forces

Normal impact[1]

$$F_{v,n} = \frac{6\,\pi\,\eta\,R^{*2} v_{n,rel}}{h}$$

Tangential impact[2]

$$F_{v,t} = 2\,\pi\,\eta\,R^{*}\,v_{t,rel}\,\ln\left(1+\frac{R^{*}}{2\,h}\right)$$

$$h \geq 2\,h_a$$

$v_{n,rel}$	normal relative velocity
$v_{t,rel}$	tangential relative velocity
h	minimum separation distance
h_a	roughness
η	viscosity
R^*	average curvature radius in contact
F_{cap}	capillary force

[1]Adams, M.J., Edmondson, B. (1987). Tribology in particulate technology.
[2]Popov, V. (2009) Kontaktmechanik und Reibung, Springer.

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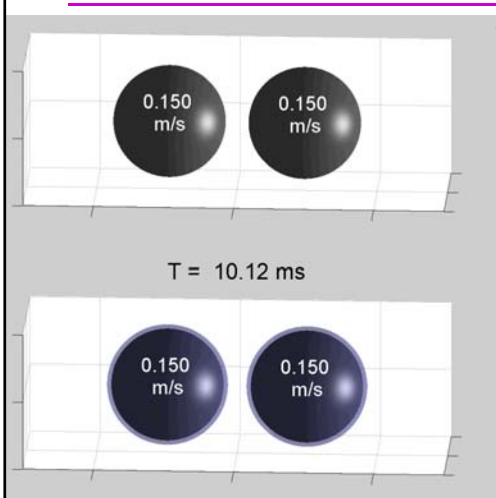
PARTICLE COLLISION IN WET SYSTEMS

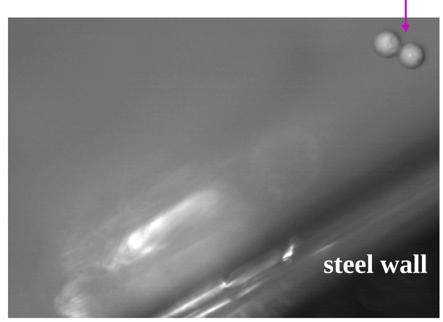
application of viscous contact model



← **model: $F_{Hertz\text{-}Tsuji}$**

e_{dry} = 0.6

Liquid bridge



← **model: $F_{Hertz\text{-}Tsuji}$ + F_v**

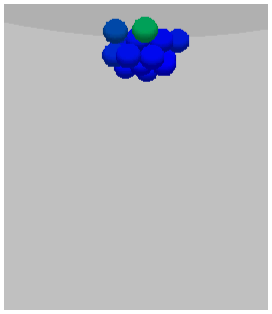
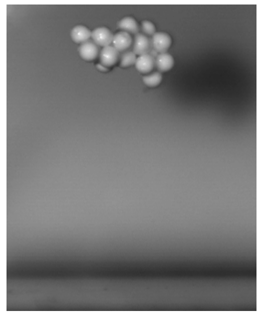
e_{wet} = 0.05

Particles: R = 0.4 mm, ρ = 190 kg/m³, e_{dry} = 0.6, G = 6.3 MPa

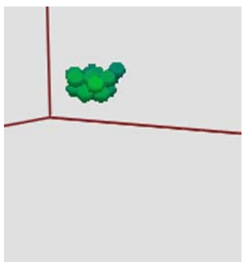
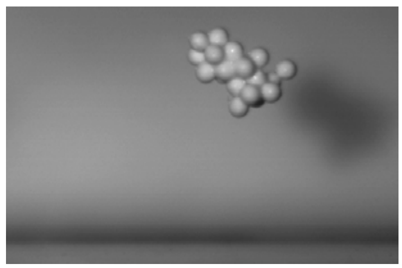
Liquid layer: η = 1 mPa·s, h = 60 µm, h_a = 2.5 µm

PARTICLE COLLISION IN WET SYSTEMS

application of viscous contact model

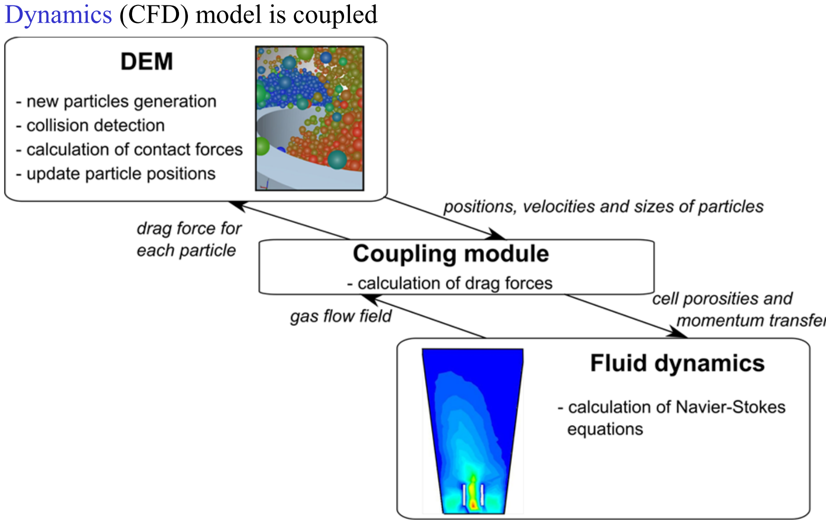
d_p = 0.8 mm
v_{imp} = 1.2 m/s
liquid layer:
η = 8 mPa·s, $h_m \approx$ 60 µm

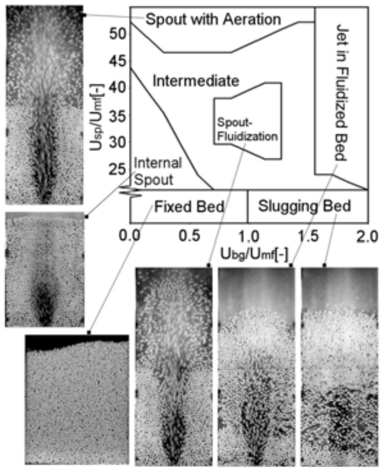
d_p = 0.8 mm
v_{imp} = 1.2 m/s
liquid layer:
η = 4 mPa·s, $h_m \approx$ 60 µm

COUPLING BETWEEN DEM AND CFD

- For the description of particle motion in the fluid field the Computational Fluid Dynamics (CFD) model is coupled



RESULTS DISCRETE PARTICLE MODEL
spouted bed



"CAPABILITIES" OF DPM
(COLLISION PARAMETERS!!!)
(Link et al., CES, 2005)

REGIME PREDICTION

GAS BUBBLES BEHAVIOUR

PRESSURE FLUCTUATIONS

SOLIDS MOTION

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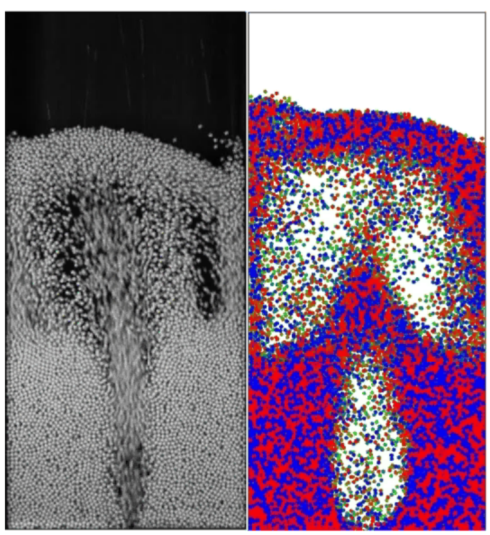
RESULTS DISCRETE PARTICLE MODEL
spouted bed (dry system)



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DISCRETE PARTICLE MODEL
nozzle region

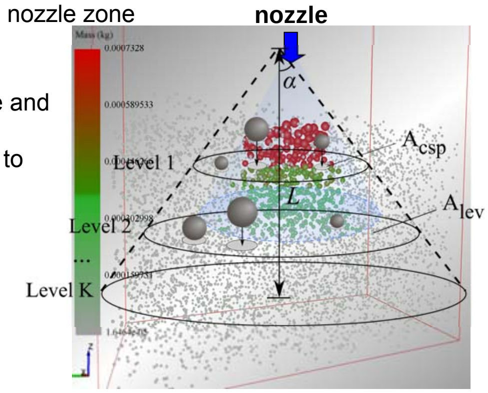
- For the description of particle wetting the nozzle zone model has been developed
- The nozzle zone is described by the suspension mass stream, spraying angle and the height of cone area
- The suspension mass flow which comes to the particle *j* in the level *i* is defined as:

$$\dot{M}_{susp,j} = \dot{M}^{i}_{susp} \cdot \frac{A_{csp,j}}{A_{lev,i}}$$

- Mass stream on the level *i+1*:

$$\dot{M}^{i+1}_{susp} = \dot{M}^{i}_{susp} \cdot \left(1 - \frac{\sum A_{csp,j}}{A_{lev,i}}\right)$$

- In apparatus the different nozzles can be defined simultaneously



$A_{csp,j}$	cross-cut surface of particle *j* [m²]
$A_{lev,i}$	cross-cut surface of level *i* [m²]

L. Fries, M. Dosta, S. Antonyuk, S. Heinrich, S. Palzer, Chemical Engineering Technology, 34, 2011

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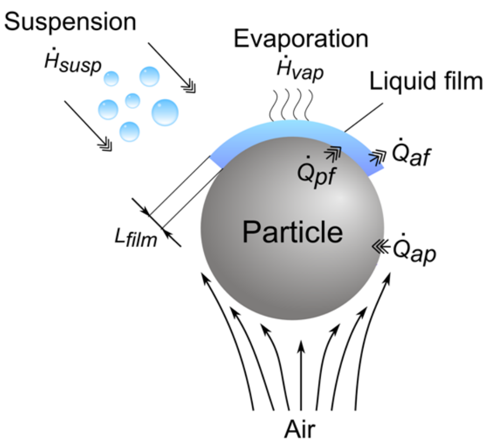
DISCRETE PARTICLE MODEL
heat and mass transfer

- For the calculation of liquid film drying the equations of energy and mass balance are used
- The heat and mass transfer coefficients α and β are calculated for each particle



$$\dot{Q}_{af} = \alpha_{af} \cdot A_{film} \cdot (\vartheta_{air} - \vartheta_{film})$$

$$\dot{Q}_{ap} = \alpha_{ap} \cdot (A_p - A_{film}) \cdot (\vartheta_{air} - \vartheta_p)$$

$$\dot{Q}_{pf} = \alpha_{pf} \cdot A_{film} \cdot (\vartheta_p - \vartheta_{film})$$

$$\frac{dH_{film}}{dt} = \dot{H}_{susp} + \dot{Q}_{pf} - \dot{H}_{vap} + \dot{Q}_{af}$$

A_{film}	Surface of liquid film [m²]
A_p	Particle surface [m²]
ϑ_p	Particle temperature [°C]
ϑ_{film}	Temperature of liquid film [°C]

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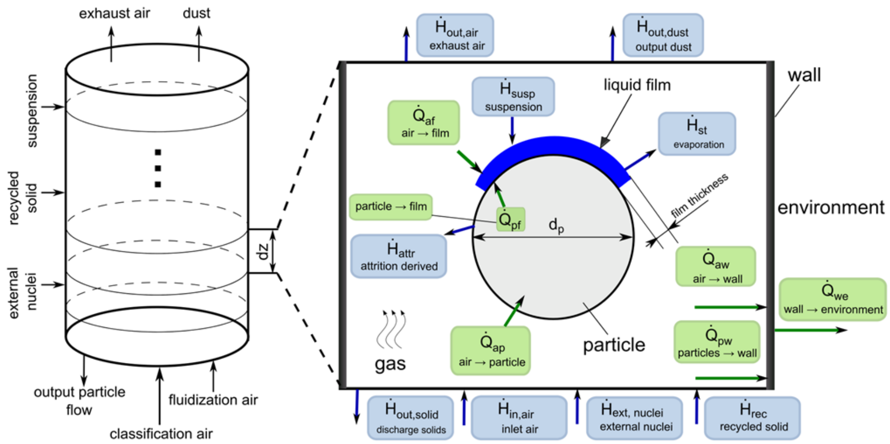
DISCRETE PARTICLE MODEL
heat and mass transfer and particle growth



- growth rate for each particle:

$$\frac{dR_p}{dt} = \frac{\dot{M}_{vap} \cdot (1 - x_w)}{4 \cdot \pi \cdot R_p^2 \cdot x_w \cdot \rho_s}$$

R_p	Particle radius [m]
$\dot{M}_{vap}$	Vapor mass stream [kg/s]
ρ_s	Solid density [kg/m³]

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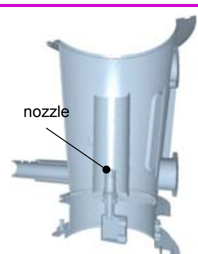
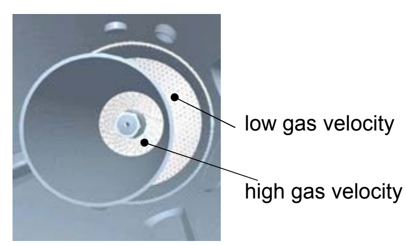
RESULTS DISCRETE PARTICLE MODEL / CFD
real granulators – Wurster coater

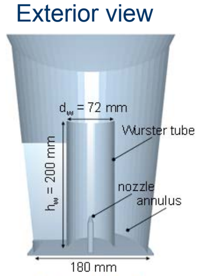

Exterior view



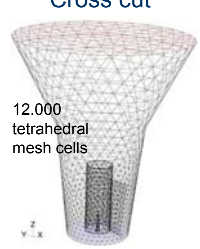
Cross cut



Segmented distributor plate



Simplified geometry for DPM



Mesh for CFD-simulation

Design and process parameters
- Gap distance below Wurster
- Height and diameter of Wurster
- Injection velocity
- Fluidization gas velocity
- Air split ratio Wurster/annulus

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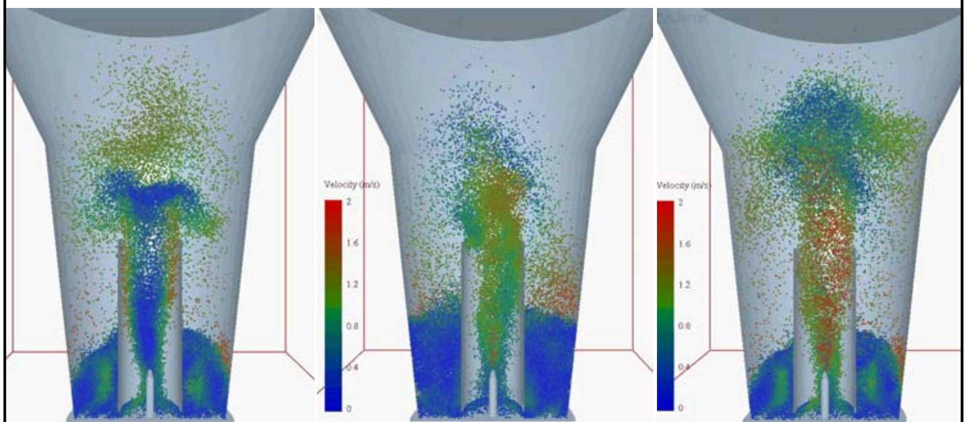
RESULTS DISCRETE PARTICLE MODEL / CFD
real granulators – Wurster coater

150.000 particles, d_p = 2 mm, ρ_p = 1500 kg/m³, total mass = 0.94 kg, e = 0.8, simulation time t = 2.5 s, fluidization velocity: Wurster: u_W = 8 m/s = 10.1·u_{mf}, annulus: u_{ann} = 3 m/s = 3.8·u_{mf}



v_{nozzle} = 20 m/s **v_{nozzle} = 100 m/s** **v_{nozzle} = 160 m/s**

- High spout velocity provides stable circulation regime
- Backmixing is prevented

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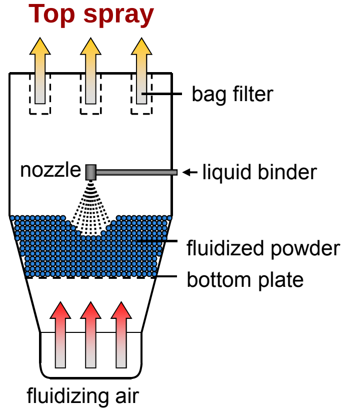
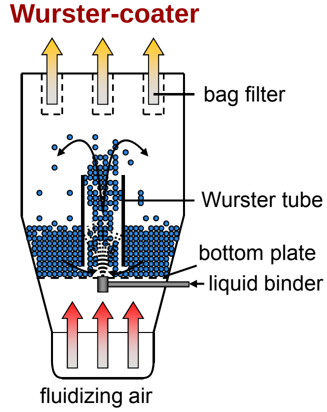
RESULTS DISCRETE PARTICLE MODEL / CFD
comparison of granulator configurations

Top spray



Application:
Granulation and agglomeration of food and fertilizers.

Wurster-coater



Application:
tablet coating, encapsulation of flavors.

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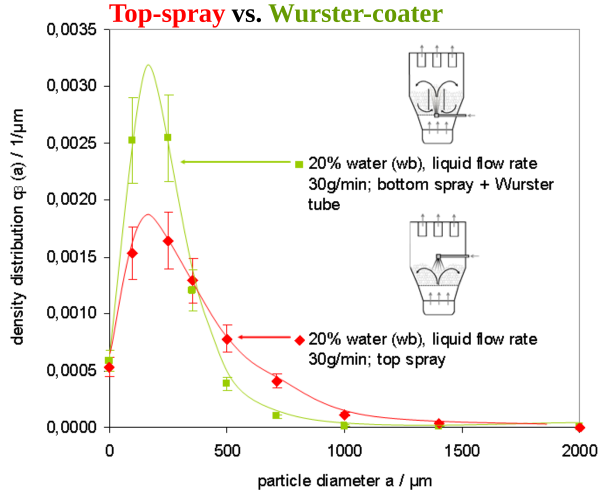
RESULTS DISCRETE PARTICLE MODEL / CFD

comparison of granulator configurations

Top-spray vs. **Wurster-coater**



Nestlé Research™

Process conditions

Glatt GCPG 3.1
Dextrose syrup (DE21)
Fluidization air: 250 m³/h

Injection: water,
20% of bed mass
at constant spray rate

- Top-spray-configuration produces wide size distribution of the product
- Circulating regime allows more homogeneous wetting at equal process conditions

L. Fries, S. Antonyuk, S. Heinrich, S. Palzer, Chemical Engineering Science, 2011

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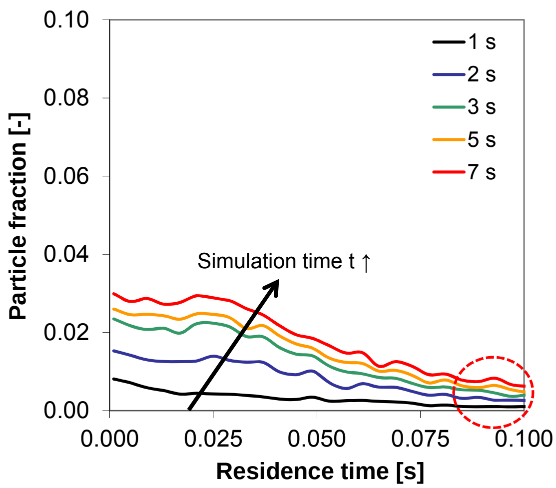
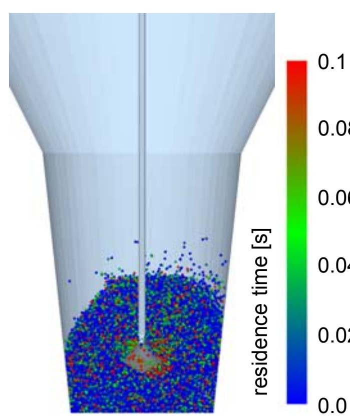
RESULTS DISCRETE PARTICLE MODEL / CFD

comparison of granulator configurations

Top spray granulator

Broad residence time distribution





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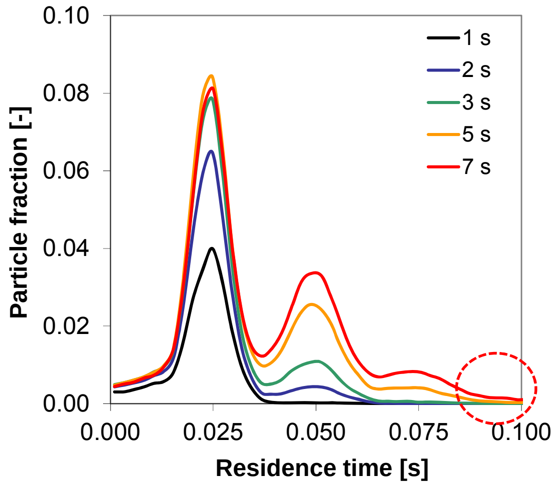
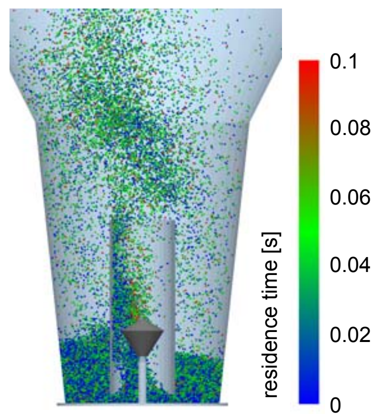
RESULTS DISCRETE PARTICLE MODEL / CFD
comparison of granulator configurations

Wurster-coater
Cyclic wetting
Defined residence time per cycle





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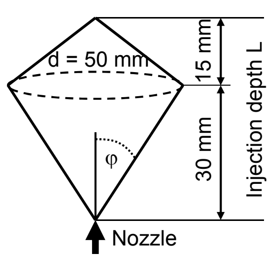
RESULTS DISCRETE PARTICLE MODEL / CFD
particle collision dynamics

Collisions between surface-wet particles

Parameter	Wurster-coater	Top Spray
Particle fraction inside spray zone	0.53 %	0.36 %
Average angular velocity inside spray zone	43 rad/s	54rad/s
Average collision frequency (inside spray zone)	88 s^{-1}	864 s^{-1}
Average relative collision velocity inside spray zone	0.39 m/s	0.15 m/s



Wurster-coater:
- Lower collision frequency
- Higher kinetic energy

→ Reduced agglomeration probability

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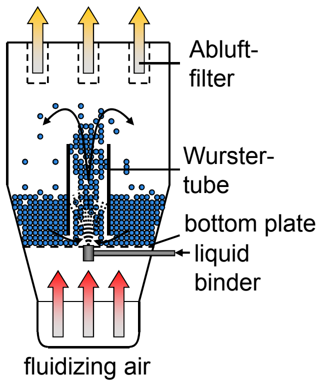
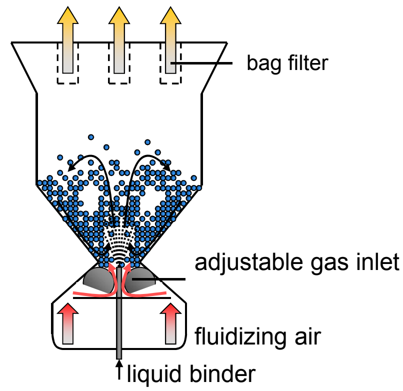
RESULTS DISCRETE PARTICLE MODEL / CFD
comparison of granulator configurations

Wurster-Coater



Application:
tablet coating,
encapsulation of flavors.

Spouted bed



Application:
very fine, cohesive and non-spherical particles

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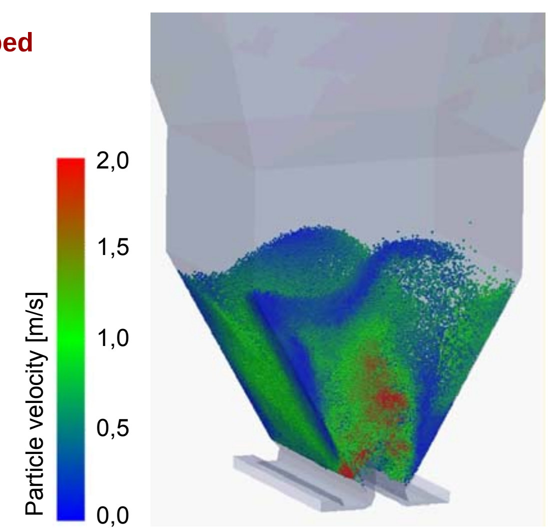
RESULTS DISCRETE PARTICLE MODEL / CFD
comparison of granulator configurations

Spouted bed

Joint STW/DFG project



150.000 Particle, d_p = 2 mm, Density ρ_p = 1500 kg/m³, Bed mass = 0.94 kg, e = 0.8, Simulation time = 5 s

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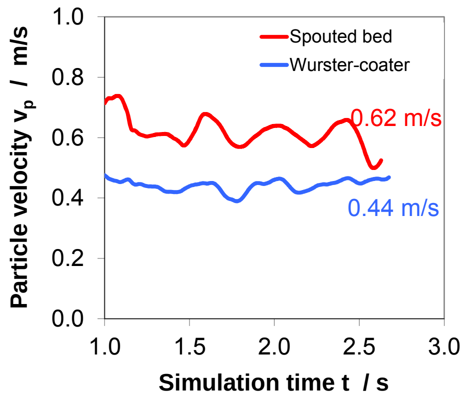
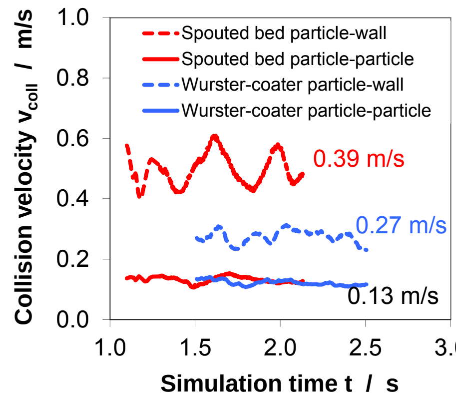
RESULTS DISCRETE PARTICLE MODEL / CFD
comparison of granulator configurations

Translation: mean particle velocity



Collision dynamics



Spouted bed: Higher impact energy for particle-wall collisions
→ Increased agglomerate strength

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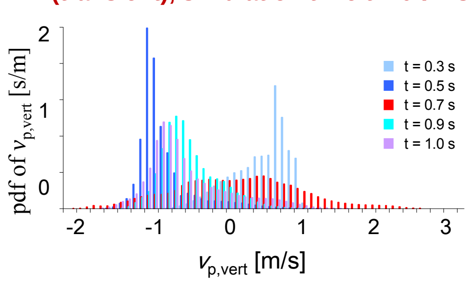
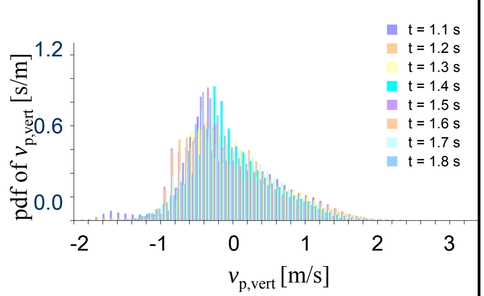
RESULTS DISCRETE PARTICLE MODEL / CFD
spouted bed behaviour

start-up process from fixed bed (transient), simulation time t = 0→1 s



steady-state spouting, t > 1 s



- Typical distribution of vertical particle velocities for spouted bed was found
- This kind of parameters can't be measured up-to-day by available methods. They can be obtained only from a simulation.

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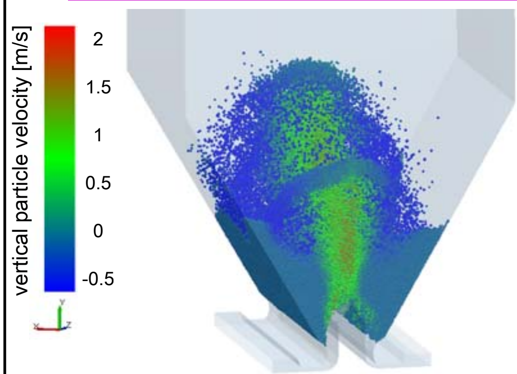
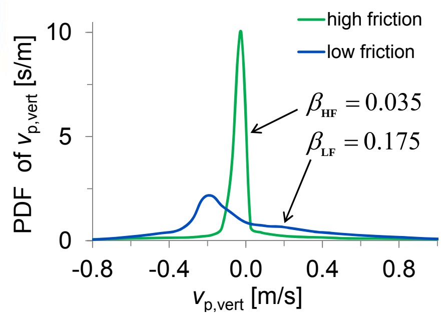
RESULTS DISCRETE PARTICLE MODEL / CFD
stable spouted bed behaviour





- High friction influences the particle mobility β
- The spread of the function strongly decreases
- The shape of velocity distribution changes from Gumbel Max to Gumbel Min (skewed to the left)

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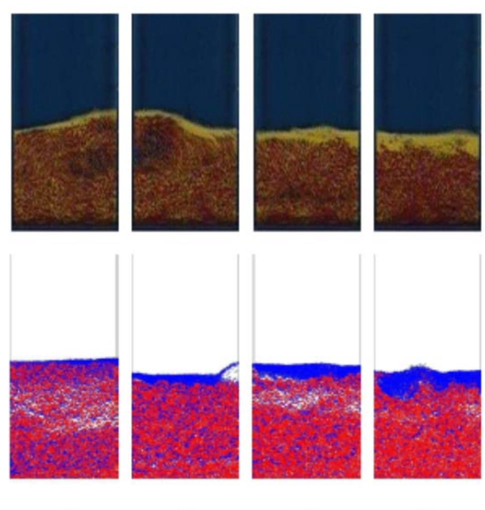
RESULTS DPM MODEL
segregation in bidisperse systems



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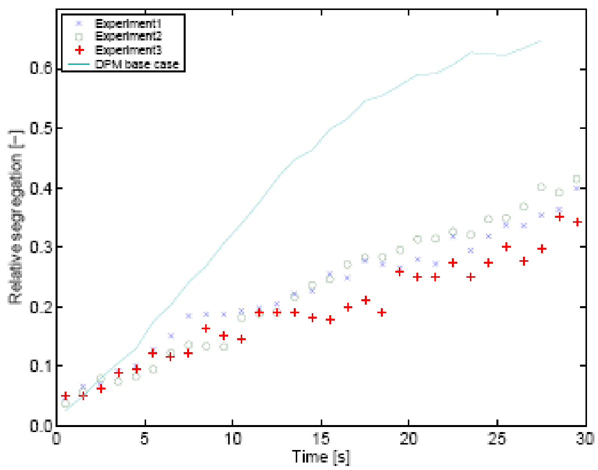
RESULTS DPM MODEL
segregation in bidisperse systems



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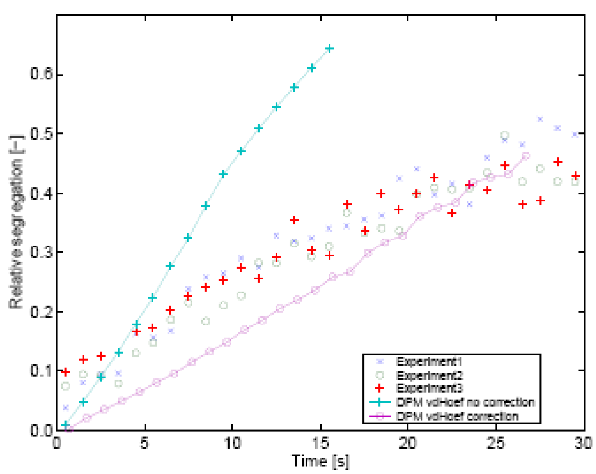
RESULTS DPM MODEL
segregation in bidisperse systems



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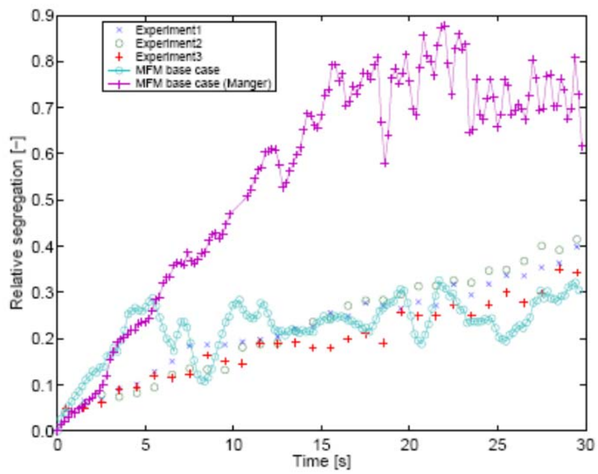
RESULTS MFM MODEL

segregation in bidisperse systems



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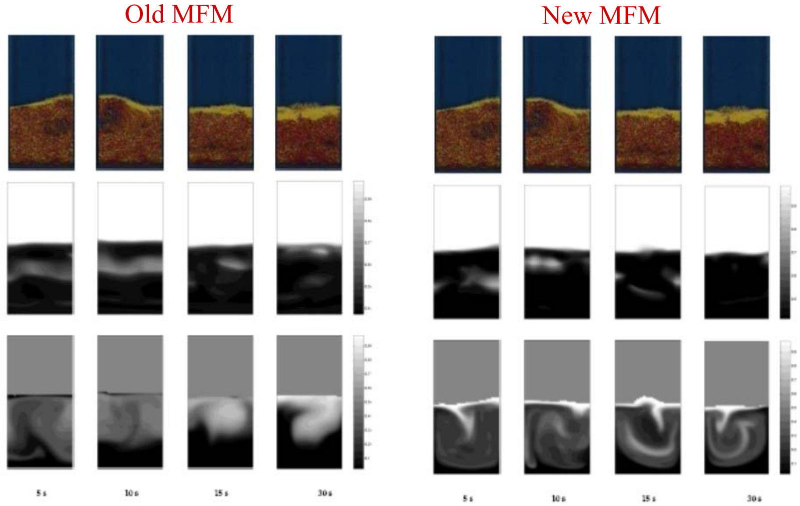
RESULTS MFM MODEL

segregation in bidisperse systems

Old MFM

New MFM



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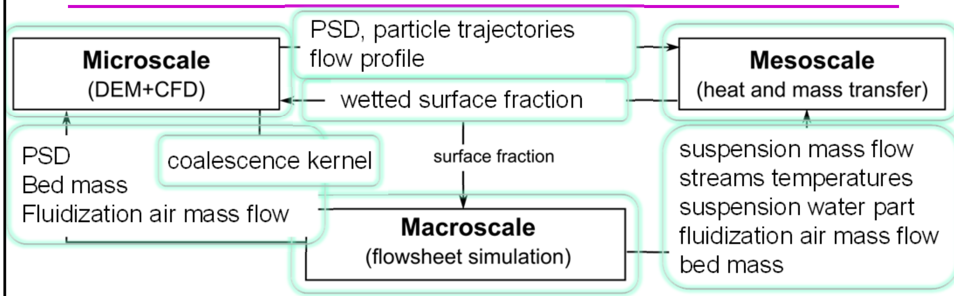
INTERSCALE COUPLING
granulation agglomeration in fluidized beds



1. Calculation of the process on the macroscale up to steady-state
2. Generation of initial conditions for DEM+CFD simulation
3. Microscale calculation for short time interval (in order of seconds)
4. Transmission of particle trajectories and fluid profile to the mesoscale
5. Mesoscale calculation of wetting, drying, growth, …
6. Recreation of microscale simulation according to new parameters
7. Microscale simulation -> calculation of coalescence kernel
8. Repeating of the calculation on the macroscale with new kernel

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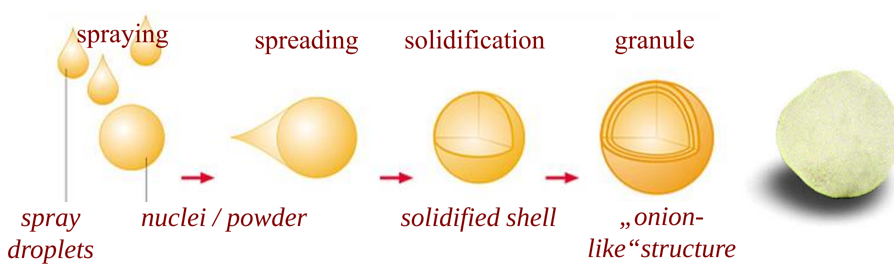
MACROSCALE
granulation

Granulation (granum (lat.) = grain)

Transfer of solids from **liquids** (suspensions, solutions, melts) or **dusty solids** to a well defined **granule structure**



e.g. detergents, food technology, preservatives

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MACROSCALE
population balance model for granulation

For the description of the change of particle size distribution, a one-dimensional Population Balance Model (PBM) has been used

$$\frac{\partial n_{tot} q_{0,b}}{\partial t} = -\underbrace{\frac{\partial G_e n_{tot} q_{0,b}}{\partial d_p}}_{\text{Growth rate}} + \underbrace{\dot{n}_{in} q_{0,in} - \dot{n}_{out} q_{0,out}}_{\text{Input and output streams}}$$

Growth rate

Input and output streams

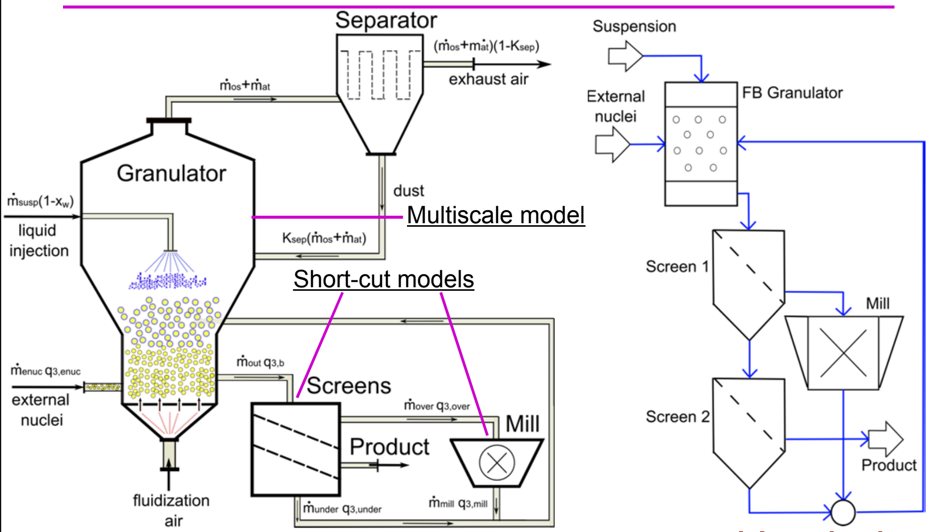
Empirical model:

$$G_e = \frac{2 \cdot \dot{M}_e}{\rho \cdot A_{tot}}$$

$$\dot{M}_e = \dot{M}_{susp} \cdot (1 - x_w)$$

G_e	Growth rate [m/s]
A_{tot}	Total particle surface [m^2]
$\dot{M}_e$	Effective mass stream [kg/s]
ρ	Particle density [kg/m^3]
$\dot{M}_{susp}$	Suspension mass stream [kg/s]
x_w	Water part in suspension [%]

MACROSCALE
flowsheet of granulation process



Production process *SolidSim Flowsheet*

M. Dosta, S. Heinrich, J. Werther, Powder Technology, 204, 71-82, 2010

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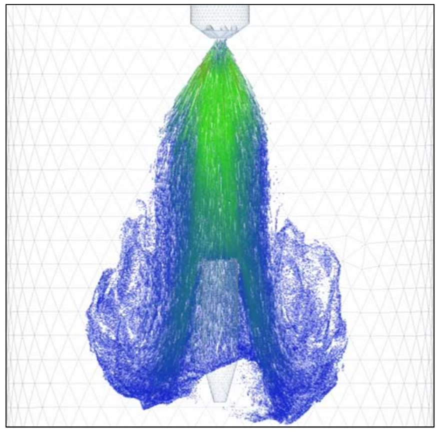
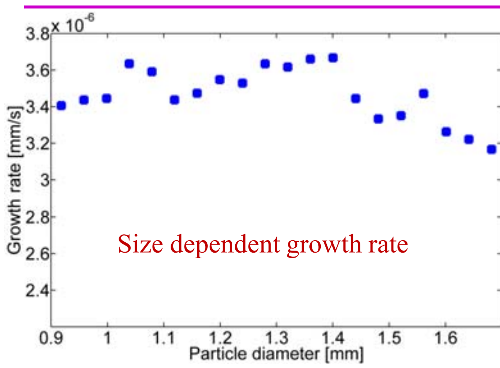
MICROSCALE
DEM simulation of the nozzle zone

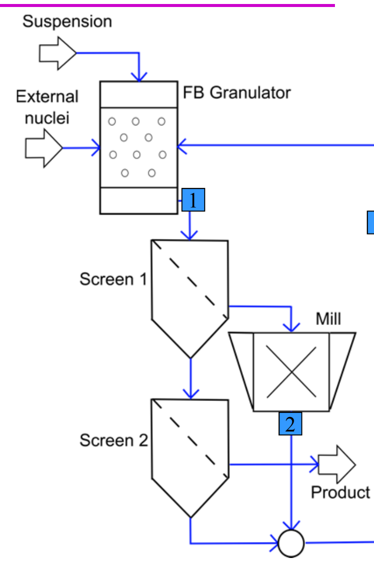


MACROSCALE
simulation results



Empirical model / Growth rate from multiscale model

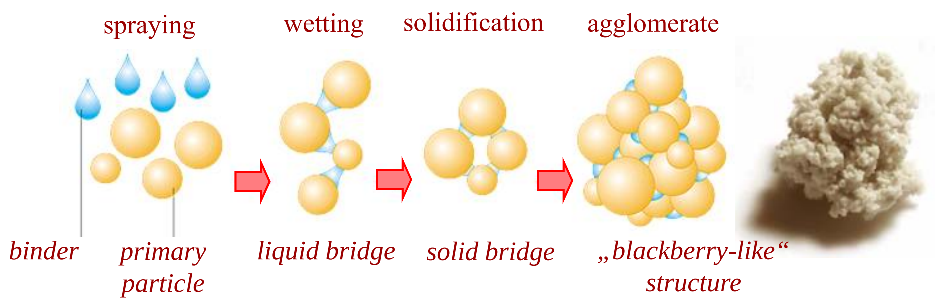
Stream	Median [mm]	Mass stream [g/s]
1	1.03 / 0.954	2.25 / 2.32
2	0.9 / 0.9	0.305 / 0.219
3	0.941 / 0.868	1.6 / 2.45



Process flowsheet

MACROSCALE
agglomeration

Agglomeration (agglomerare (lat.) = to agglomerate)
of primary particles (powder)



e.g. pharmaceutical technology, combination of active agents and excipients, instant coffee

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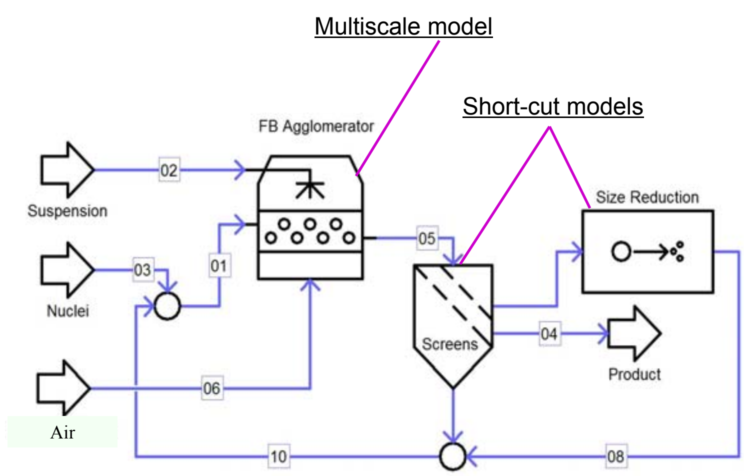
MACROSCALE
flowsheet of agglomeration process

- As an simulation example the continuous agglomeration process has been used



MACROSCALE

population balance model for agglomeration

- The agglomeration process on the macroscale has been described by population balance model
- PBM of pure agglomeration (no growth, breakage or attrition)

$$\frac{\partial n(t,v)}{\partial v} = B_{agg}(t,v) - D_{agg}(t,v) + \dot{n}_{in}(t,v) - \dot{n}_{out}(t,v)$$

where

$$B_{aggl}(t,v) = \frac{1}{2N_{tot}(t)} \int_0^v \beta(t, v-u, u) \cdot n(t,u) \cdot n(t, v-u) du$$ **birth rate**

$$D_{aggl}(t,v) = \frac{1}{N_{tot}(t)} \int_0^\infty \beta(t, v, u) \cdot n(t,u) \cdot n(t,v) du$$ **death rate**

- One of the main process parameters – coalescence kernel $\beta(t,v,u)$

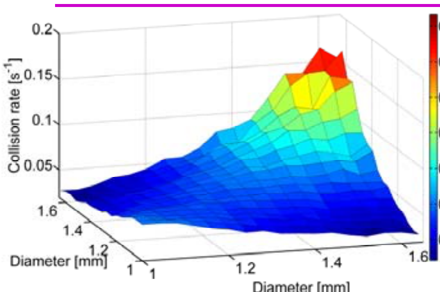
$$\beta(t,v,u) = \beta_0(t) \cdot \beta^*(v,u)$$

where $\beta_0(t)$ - time dependent part, $\beta^*(v,u)$ - size dependent part

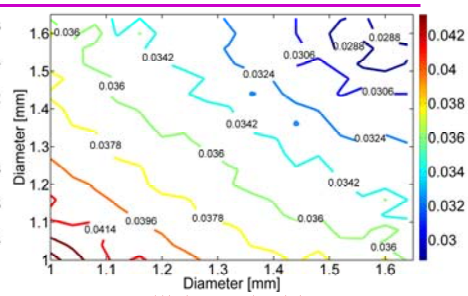
obtaining of physical based coalescence kernel

MICROSCALE

simulation results for agglomeration

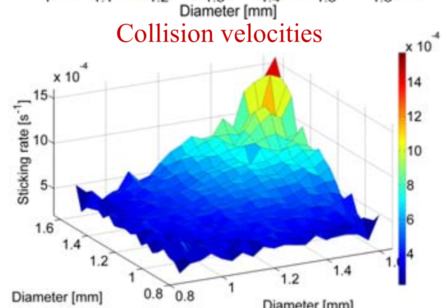


Collision rate



Collision velocities

Based on the calculation of viscous force, the sticking rate of particles can be obtained.

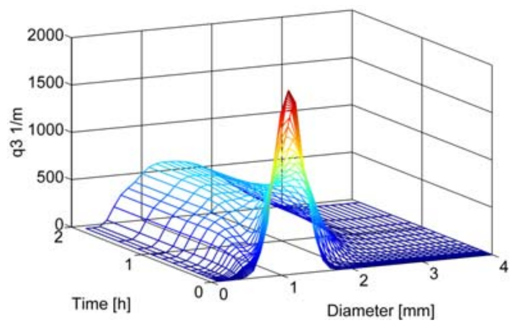


Sticking rate

MACROSCALE

simulation results for agglomeration

- The contact forces which arise from subsequent collisions with neighbour particles can cause the rupture of the formed liquid bridge
- A force balance including viscous adhesion forces in the liquid bridge and separating forces due to collisions is solved on the microscale
- The received results are used to calculate the probability for the destruction of a liquid bridges connecting two particles due to further collisions with other particles



Time progression of PSD of macro process

CONCLUSIONS

- The multiscale simulation leads to more detailed process description, where material microproperties can be considered
- Accurate closures are required for fluid-particle and particle-particle interactions
- Complex solids processes with multiple process units can be described by flowsheet simulation
- In this contribution the general view of simulation framework has been proposed and applied for granulation/agglomeration processes

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