Strategy in modelling irregular shaped particle behaviour in confined turbulent flows

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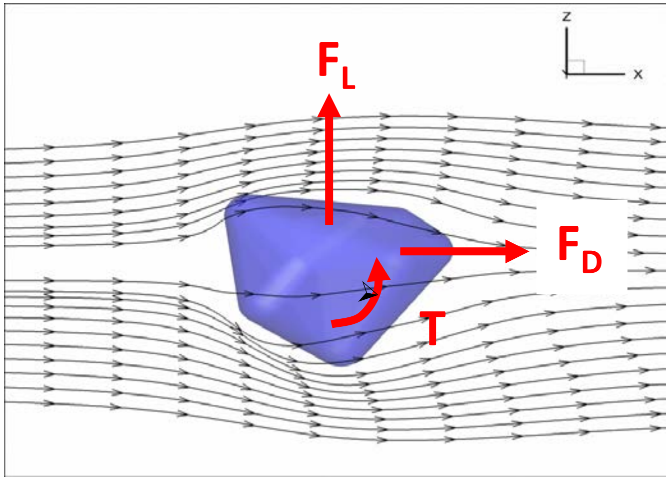
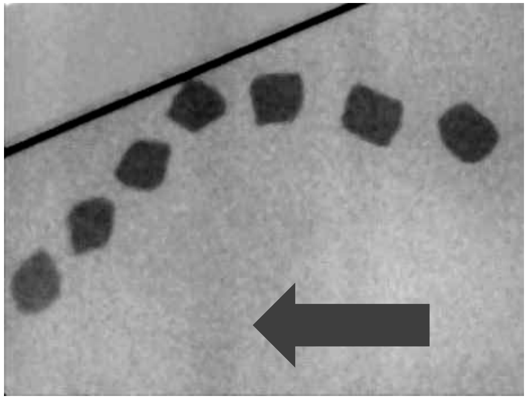




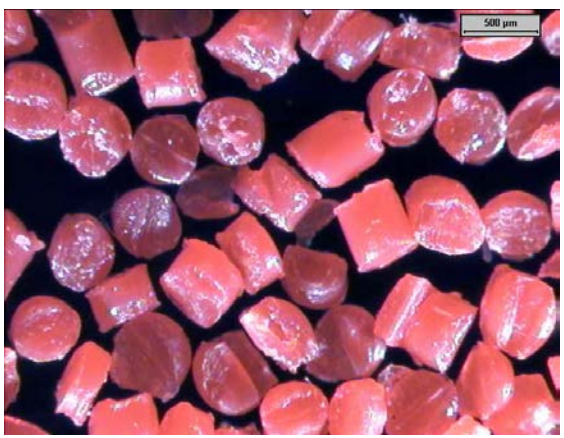
Content of the Lecture

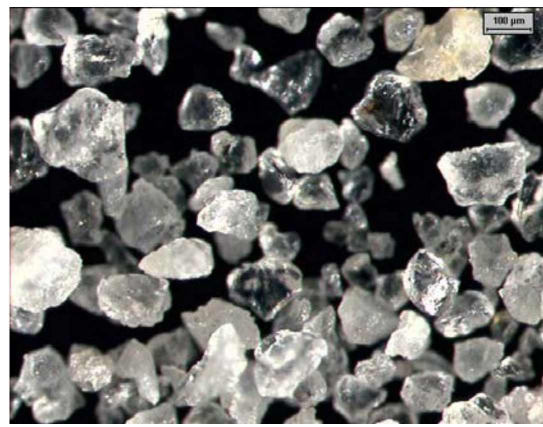
- **Introduction to non-spherical-particles treatment in a Lagrangian approach**
  - Statistical modelling of irregular shaped particles
- **Evaluation of flow resistance coefficients for irregular-shaped particles by the Lattice-Boltzmann method**
- **Derivation of PDF`s for the resistance coefficients**
- **Experimental analysis of irregular particle wall collisions using high-speed cameras**
- **Derivation of PDF`s for the restitution ratios**
- **Validation of model calculations for a horizontal channel flow**
- **Conclusions and outlook**

Introduction 1

- Numerical predictions of dispersed two-phase flows by the Euler/Euler- or Euler/Lagrange approach quite often rely on the **assumption of spherical particles** (fluid-dynamic forces and wall collision process).
- However, in most practical situations and industrial processes the particles are irregular in shape or have certain geometrical shapes, (e.g. fibres, cylinders, discs, ...) or are even agglomerates.

granulates





irregular particles

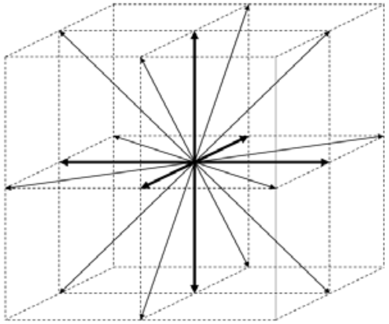
Introduction 2

Lagrangian treatment of non-spherical particles	
Regularly shaped non-spherical particles	**Irregular non-spherical particles**
Deterministic (forces) tracking of particles, new location, linear and translational velocities	Stochastic tracking of particles, new location, linear and translational velocities
Requires additionally tracking of the particle orientation using Euler angles/parameters or quaternions	Determine the instantaneous values of the resistance coefficients from a-priory determined distribution functions (random process), e.g. by Lattice-Boltzmann simulations
Particle orientation-dependent resistance coefficients are required (Hölzer and Sommerfeld 2009)	Apply these random resistance coefficients in the equation of motion each time step
Wall collisions: Solving the impulse equations for non-spherical particles considering particle orientation (Sommerfeld 2002)	Calculate the particle velocity change during a wall collision process from measured distribution functions of the restitution ratios

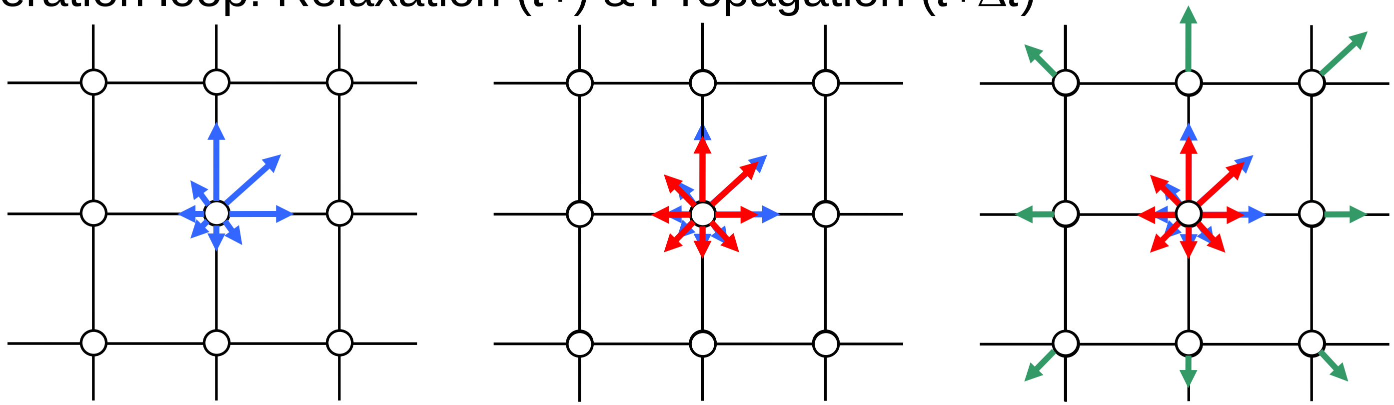
Lattice-Boltzmann equation: Behaviour of fluids on mesoscopic level

$$f_{\sigma i}(\mathbf{x}+\boldsymbol{\xi}_{\sigma i}\Delta t, t+\Delta t) - f_{\sigma i}(\mathbf{x},t) = -\frac{\Delta t}{\tau}\left(f_{\sigma i}(\mathbf{x},t) - f_{\sigma i}^{0}(\mathbf{x},t)\right) + \Delta t\, F_{\sigma i}$$

- Key variable: Discrete distribution function $f_{\sigma i}$
- Discretization of space by a regular grid
- Discretization of the velocity space: D3Q19
- Macroscopic parameters (density, momentum): Derived as moments of $f_{\sigma i}$



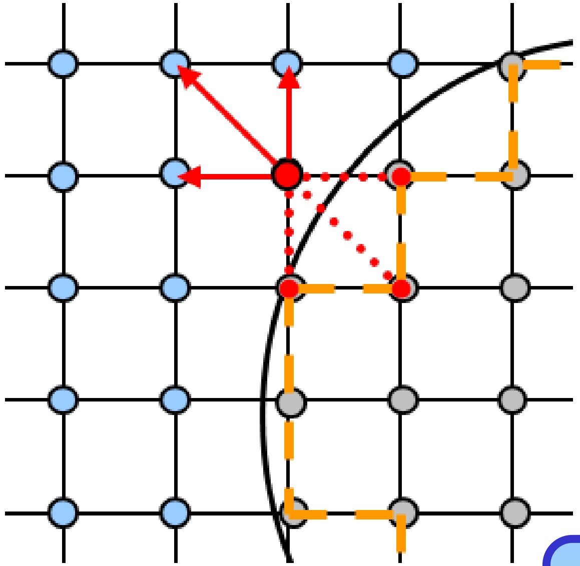
- Iteration loop: Relaxation (t+) & Propagation ($t+\Delta t$)



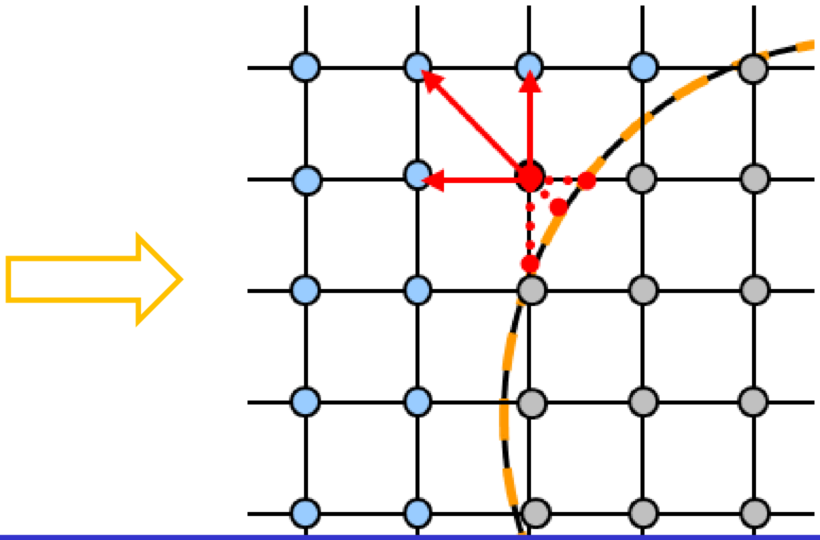
Point of time: t | Point of time: t+ | Point of time: $t+\Delta t$

Lattice-Boltzmann Method 2

Standard wall boundary condition:

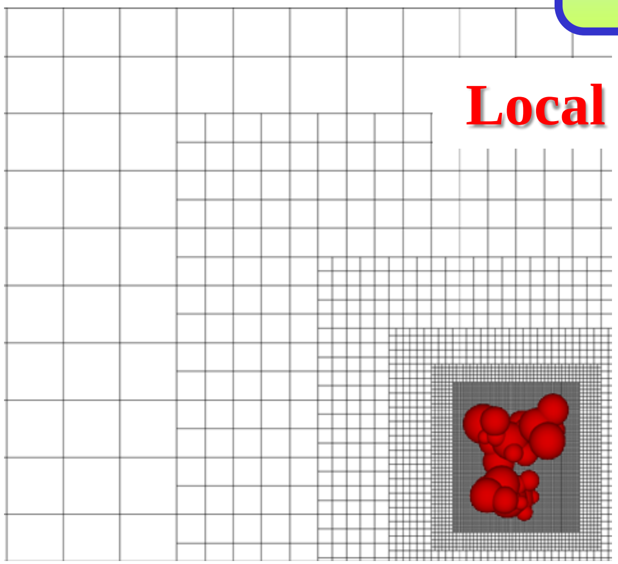


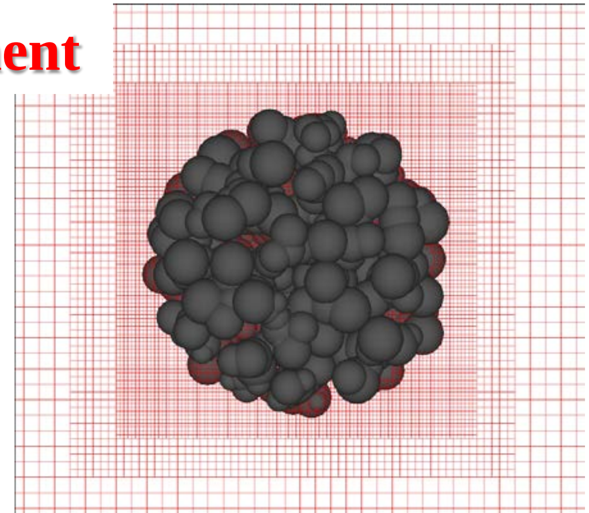
Curved wall boundary condition:



Forces over a particle are obtained from a momentum balance (reflection of the fluid elements)

Local grid refinement

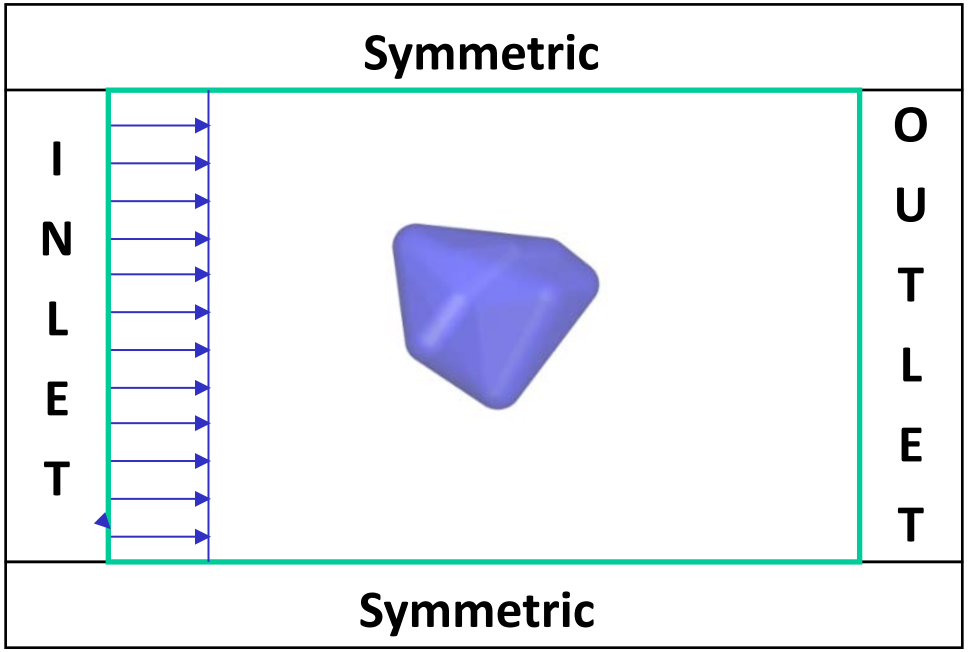




Simulations for Non-Spherical Particles 1

- Numerical calculation of a plug flow about an irregular shaped particle fixed in a cubic domain using the boundary conditions specified below.
- Determination of the resistance coefficients (drag, lift and torque) in dependence of particle Reynolds number.

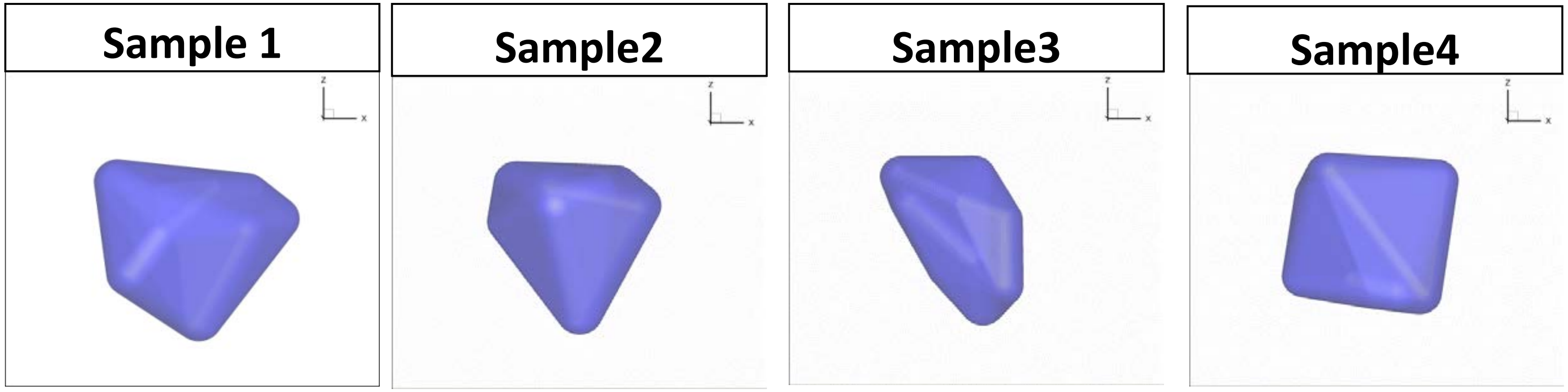
symmetry boundary condition $\left(\frac{dv}{dy} = 0\right)$



stress-free boundary condition $\left(\frac{dv}{dx} = 0\right)$

Simulations for Non-Spherical Particles 2

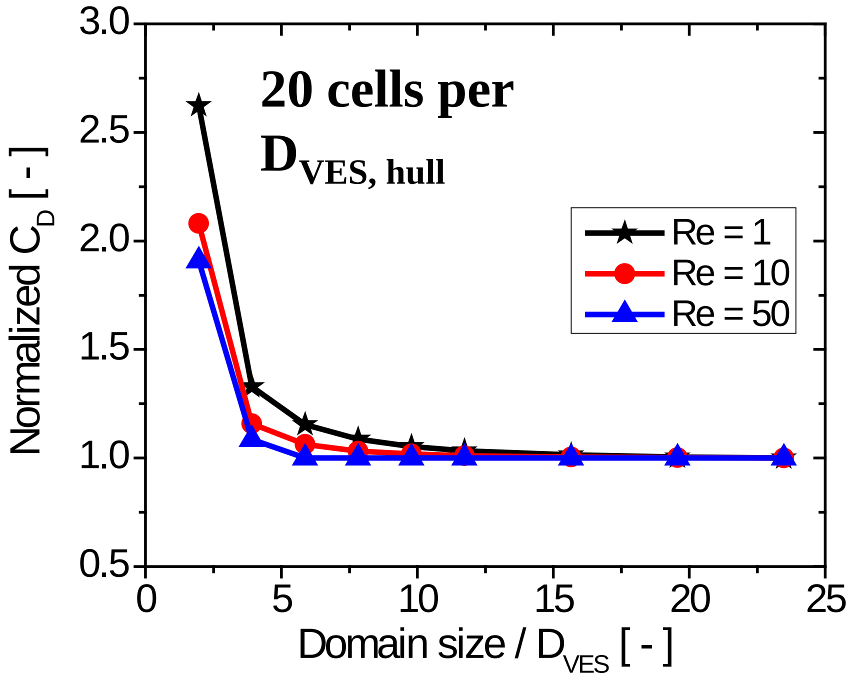
- The simulations were conducted for four different shaped particles with about the same sphericity ($D_{VES,hull} \approx 100\ \mu m$, $\psi \approx 0.87$)

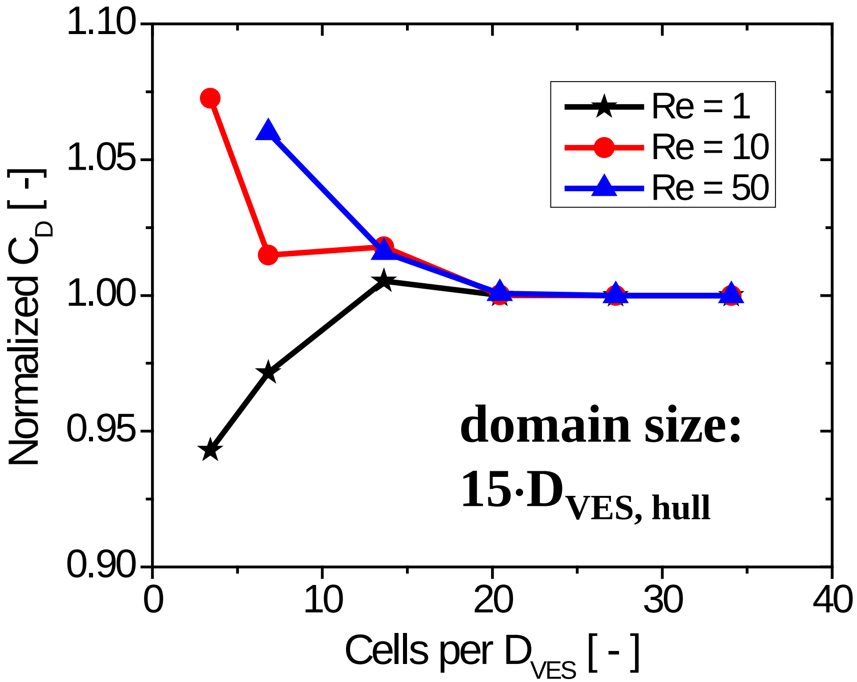


- For each Re-number the particle was randomly rotated to 71 positions with respect to the inflow in order to derive distributions of the resistance coefficients.
- Particle Reynolds number: $$Re = \frac{\rho\, U_0\, D_{VES}}{\mu}$$
- Drag coefficient: $$C_D = \frac{F_D}{\frac{\rho}{2} U_0^2\, A_{VES}}$$
- Lift coefficient: $$C_L = \frac{F_L}{\frac{\rho}{2} U_0^2\, A_{VES}}$$
- Torque coefficient: $$C_T = \frac{T}{\frac{\rho}{2} U_0^2\, D_{VES}\, A_{VES}}$$

Simulations for Non-Spherical Particles 3

- Study on the grid-independence of the results:

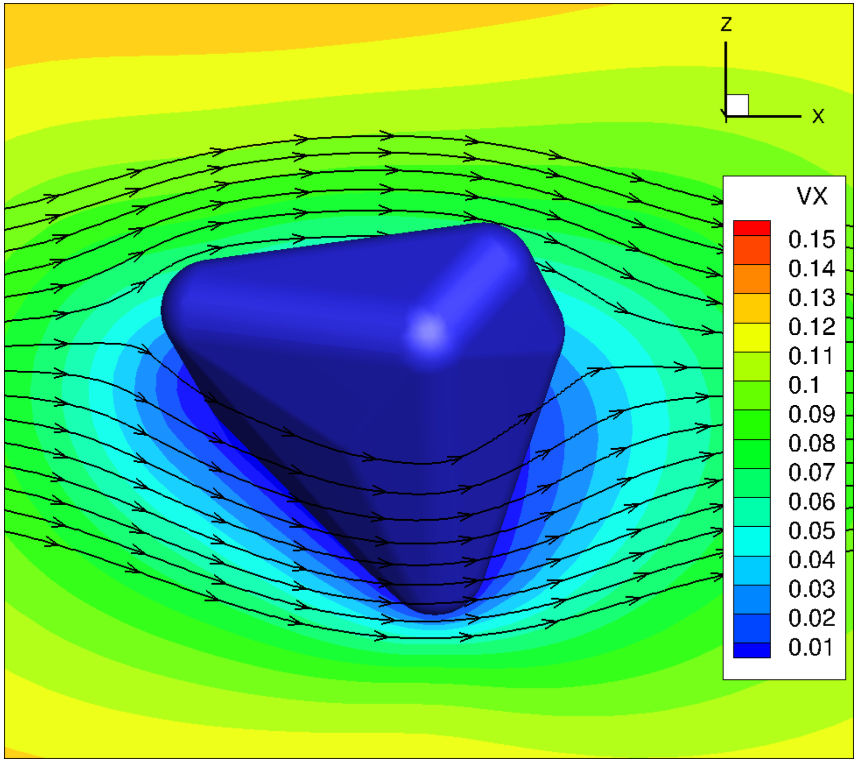




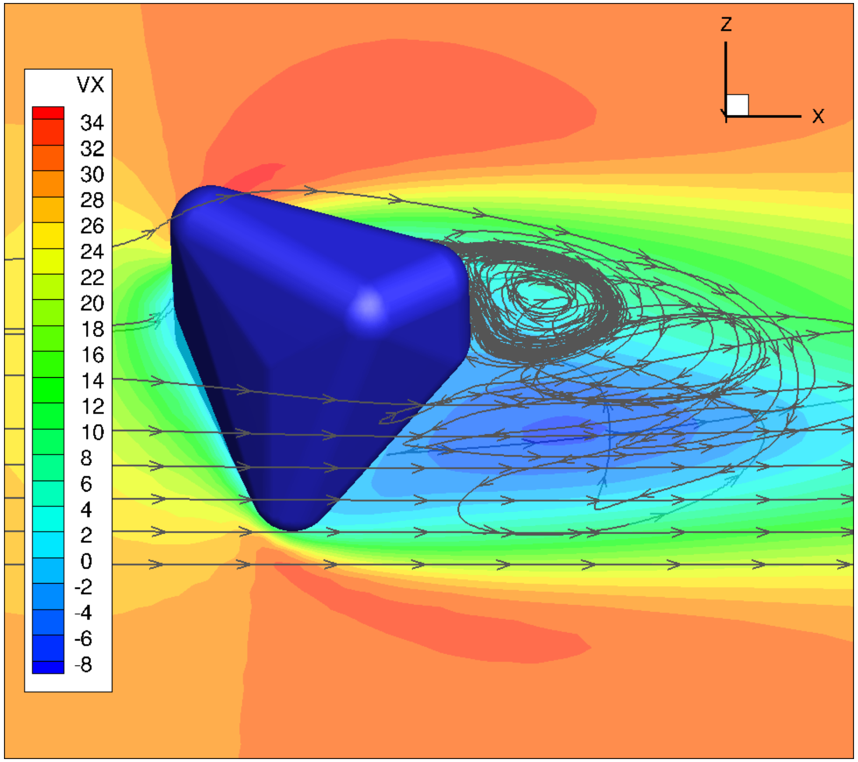
Reynolds number	Computational domain	Refinement regions	Cells per $D_{VES,\ hull}$
Re = 1, 10, 50	80 x 80 x 80	2	20
Re = 100	160 x 160 x 160	1	20
Re = 200	160 x 160 x 160	0	20

☞ **Velocity about an irregular particle at different Re:**

$Re_p = 1.0$

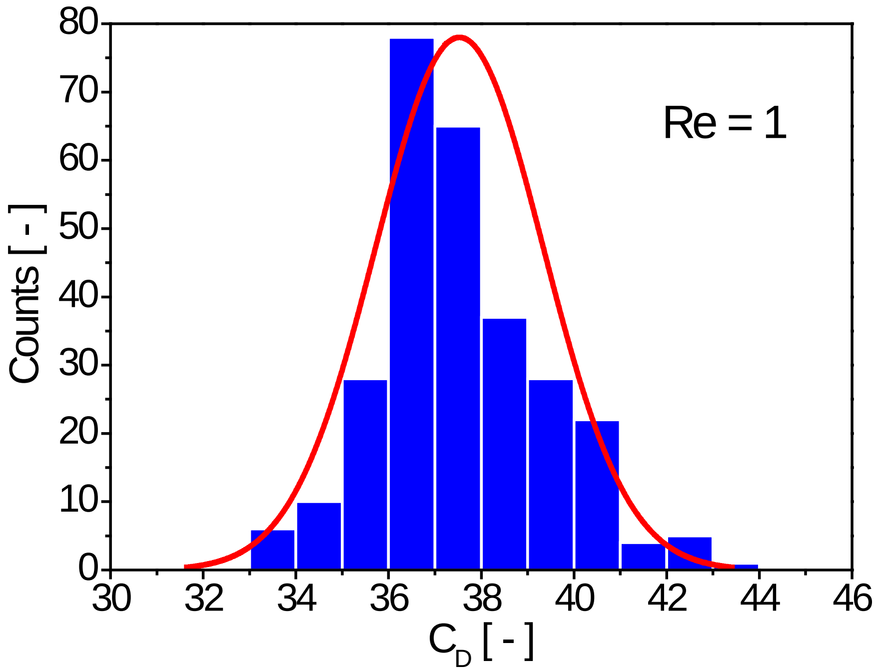


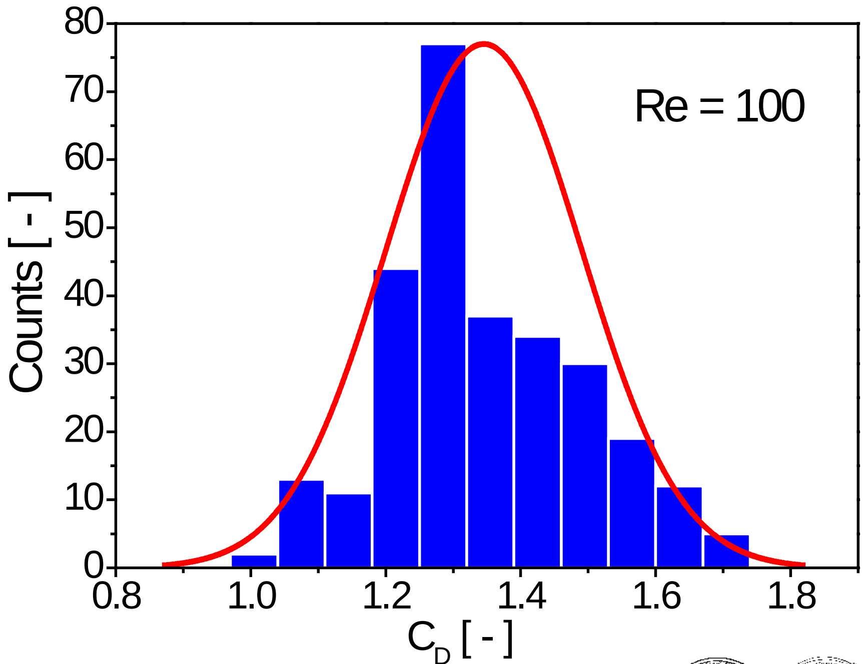
$Re_p = 200$



Resistance Coefficients 1

- **Typical PDF`s for the drag coefficient resulting from the different orientations and the 4 similar particles** ($D_{VES,hull}$ ≈ 100 μm, ψ ≈ 0.87)

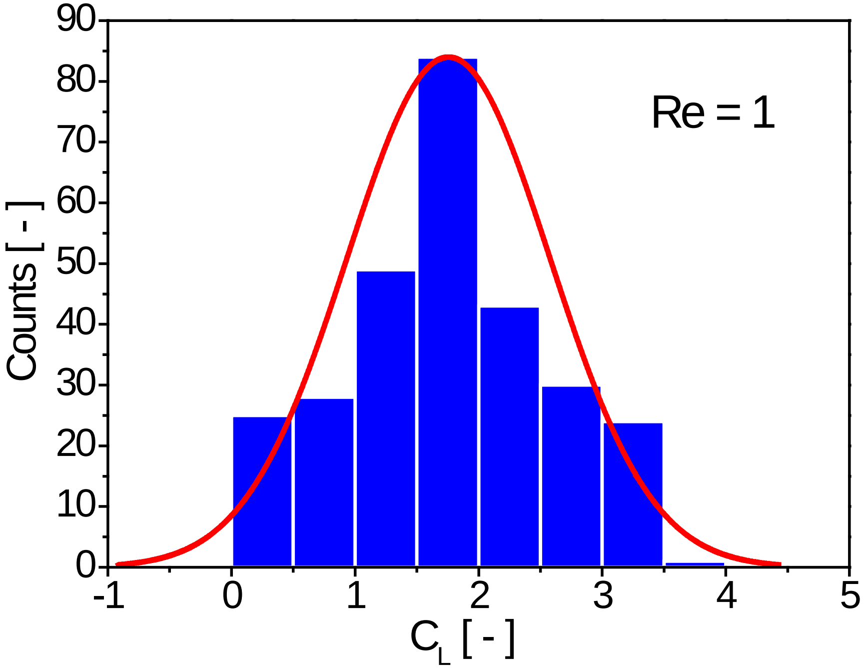


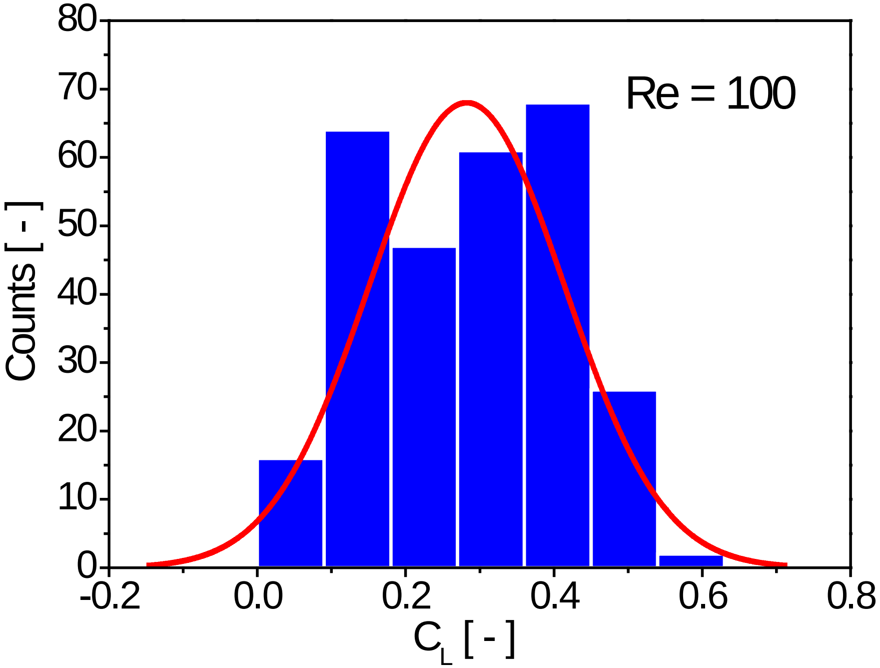


The PDF`s can be approximated by a normal distribution

Resistance Coefficients 2

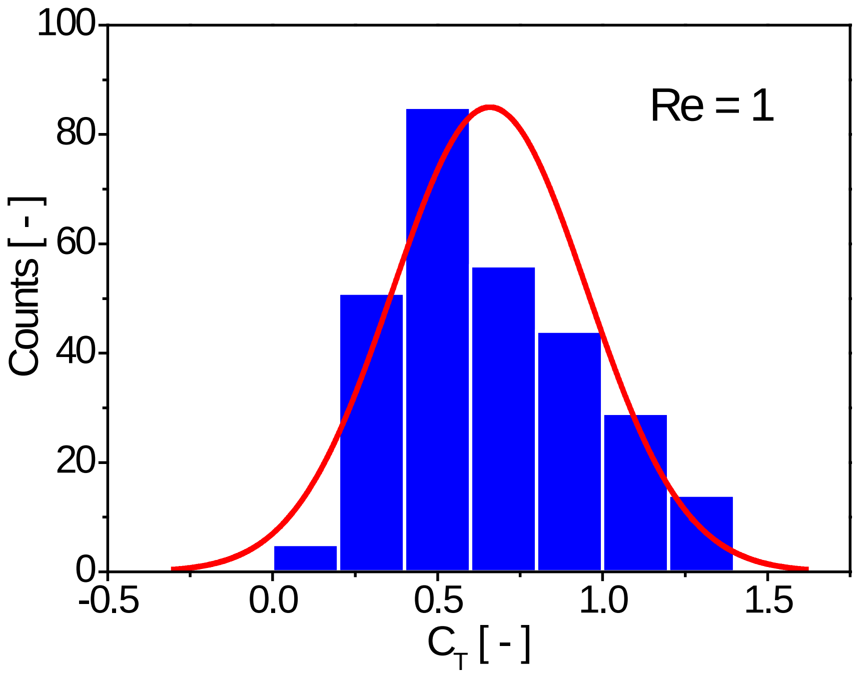
- **Typical PDF`s for the lift coefficient resulting from the different orientations and the 4 similar particles ($D_{VES,hull}$ ≈ 100 μm, ψ ≈ 0.87)**

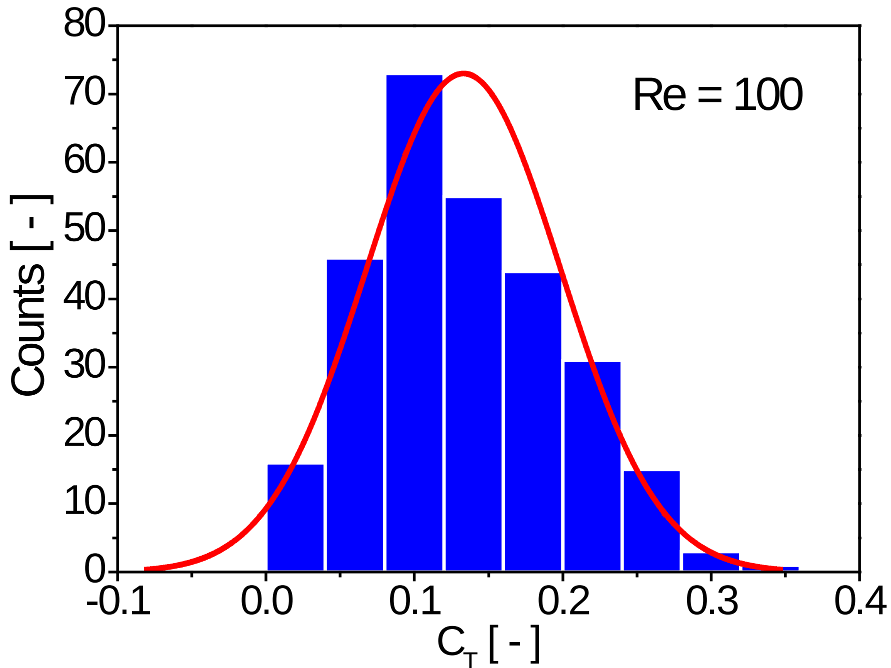




Resistance Coefficients 3

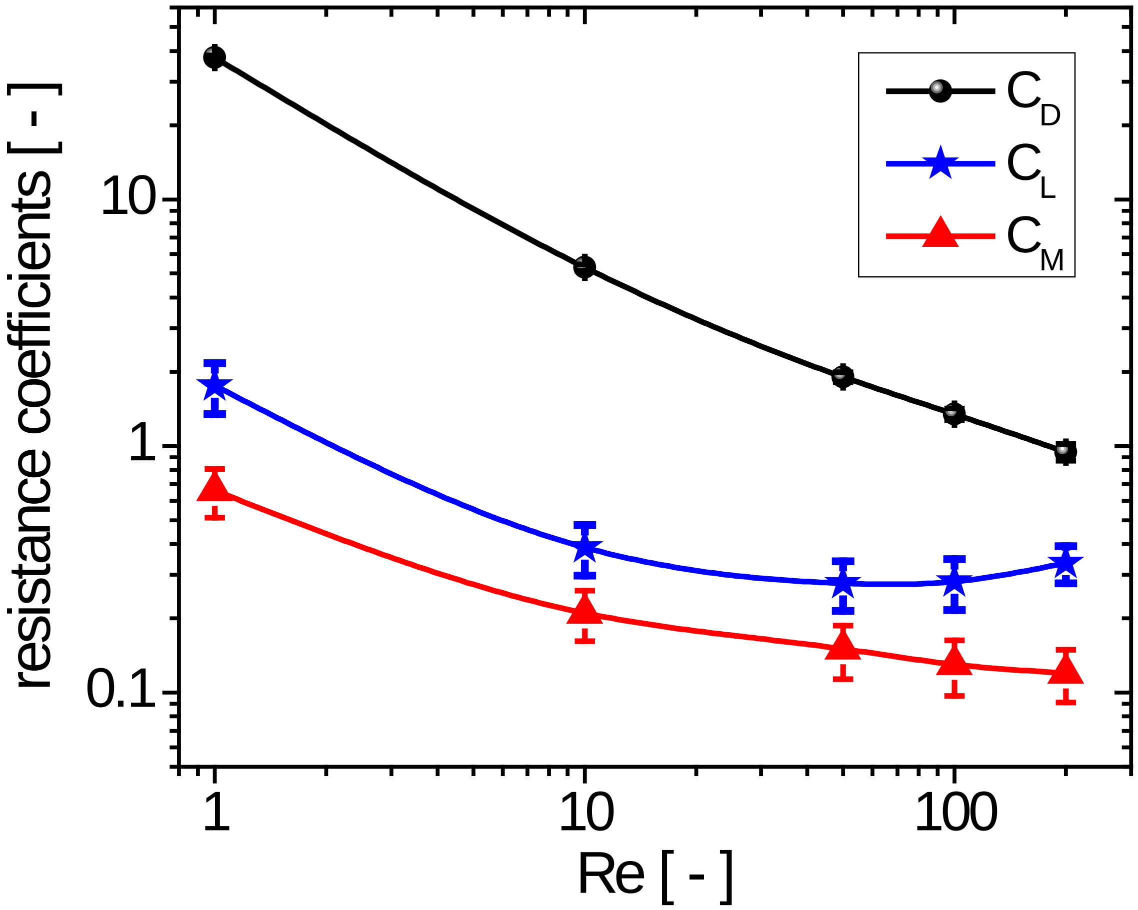
➢ **Typical PDF`s for the moment coefficient resulting from the different orientations and the 4 similar particles ($D_{VES,hull} \approx 100$ μm, $\psi \approx 0.87$)**





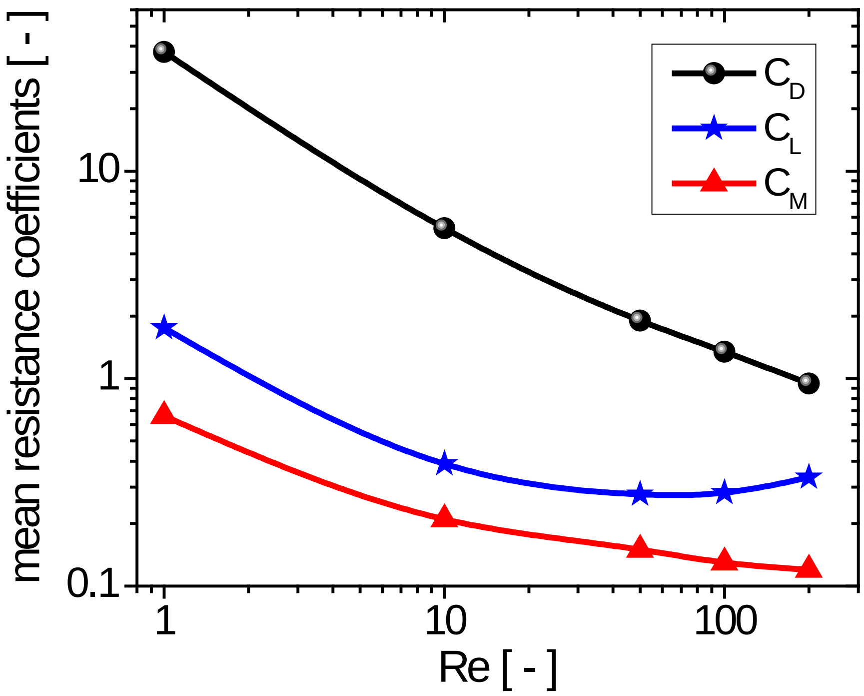
Resistance Coefficients 4

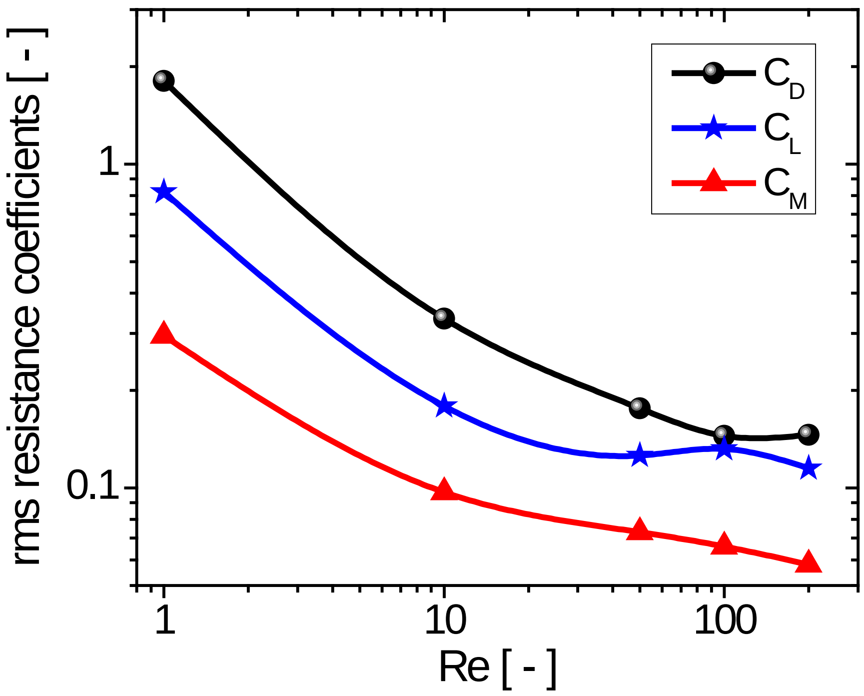
☞ **Resistance coefficients as a function of particle Reynolds number with standard deviation (vertical bars), $\psi \approx 0.87$**



Resistance Coefficients 5

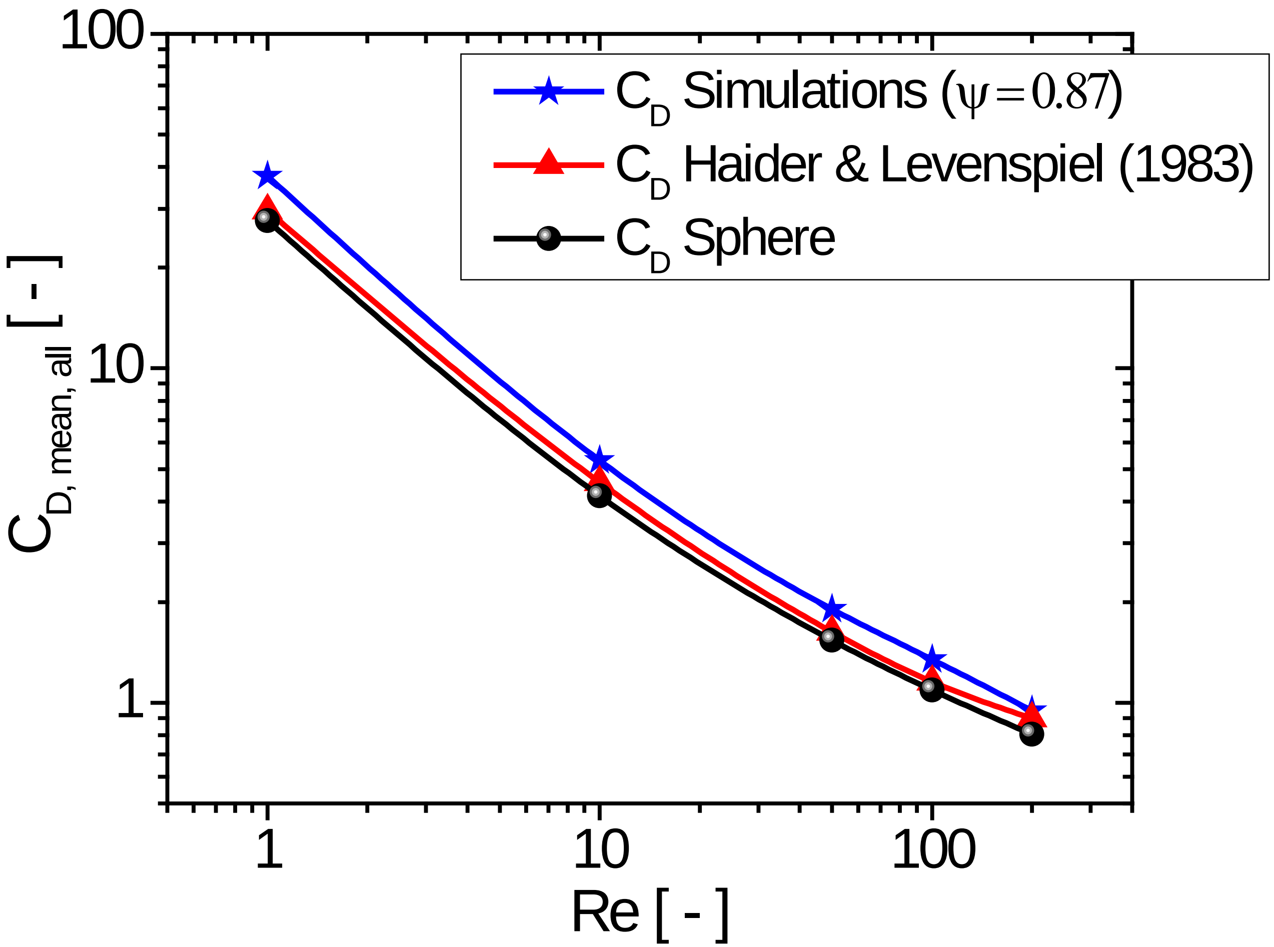
- **Resistance coefficients as a function of particle Reynolds number and standard deviation, $\psi \approx 0.87$**



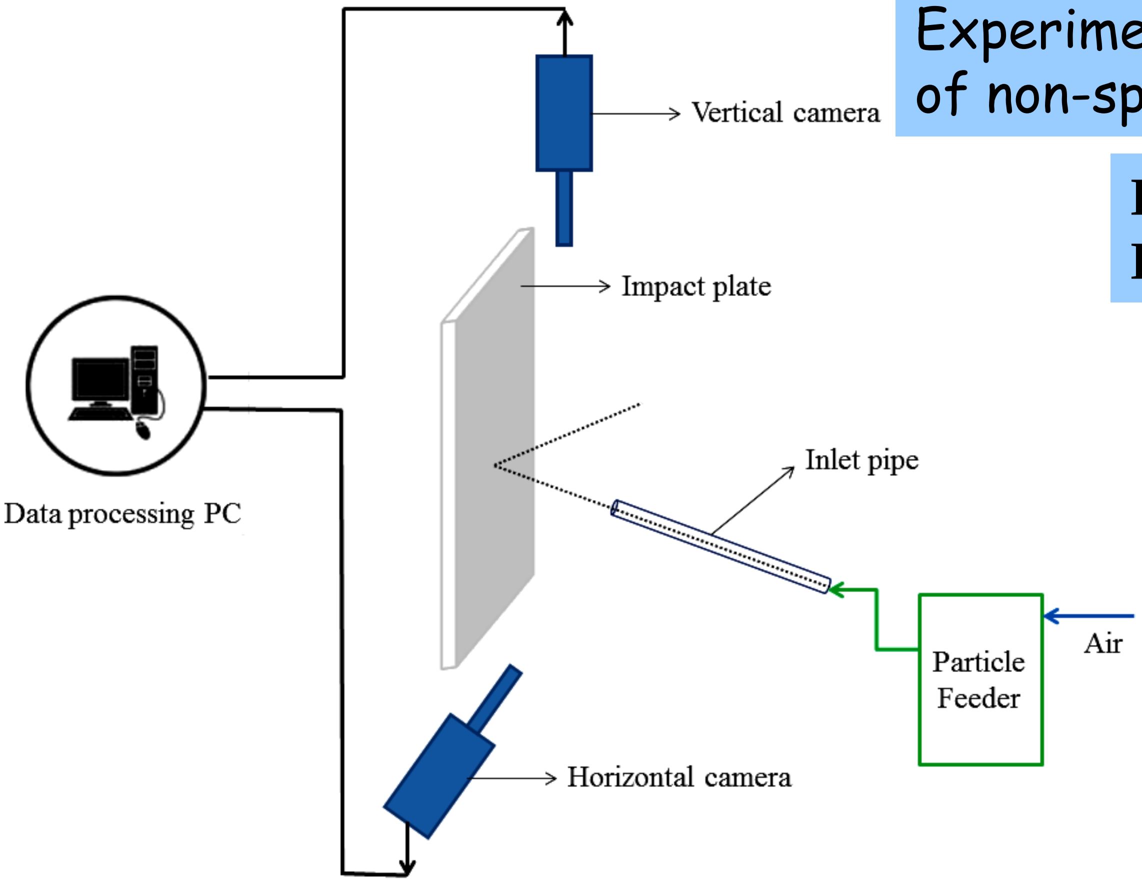


Resistance Coefficients 6

➢ **Drag coefficient as a function of particle Reynolds number, comparison with different correlations, $\psi \approx 0.87$**

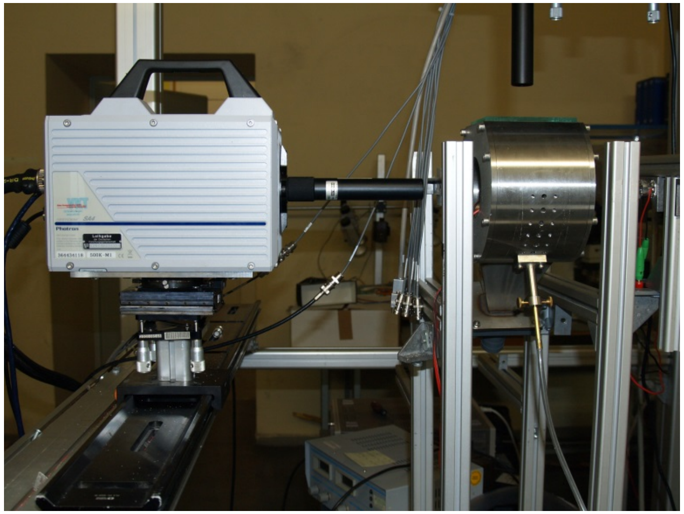


Wall-Collision Experiments 1



Experimental studies on wall collisions of non-spherical particles

Impact angles: 5° to 85°
Impact velocities: 8 and 21 m/s



- Photron High Speed Video Camera, FASTCAM SA4 RV operated at 60,000 fps
- LED illumination back-lightning
- Telecentric lens of T80 series
- Magnification ratio of 1:1

Wall-Collision Experiments 2

- **Properties of particles considered in the experiments**

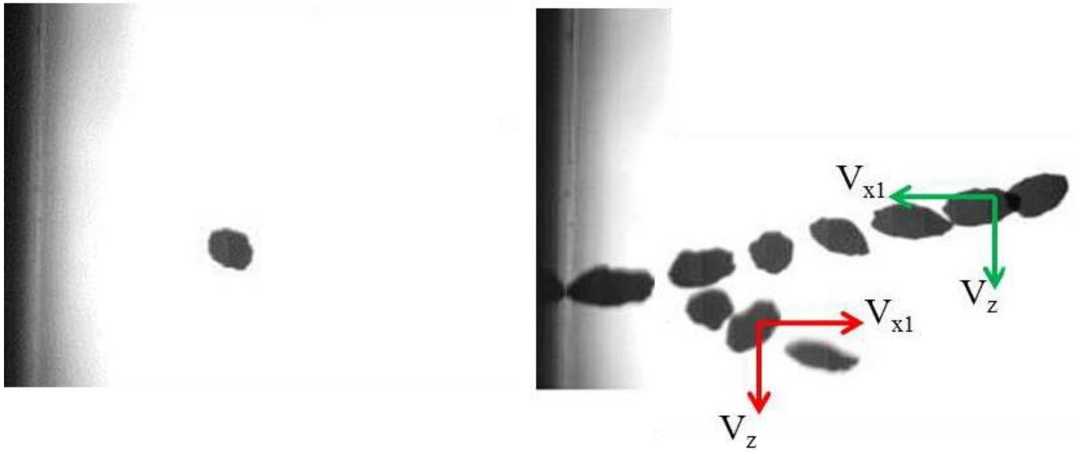
Material	Density (kg/m^3)	Size Distribution Diameters (µm)	Mean size (µm)	Sphericity
Granulates	1120	500 x 500	480	0.778
MC4 Duroplast	1480	250 - 350	300	0.773
Quartz Sand	2650	200 - 300	250	0.851
Cylinders	1100	500 x 1500	825	0.778

Wall-Collision Experiments 3

- **Wall collision of an irregular particle (Duroplast particles MC-4, projection diameter 300 µm, ψ = 0.773, velocity: 16.3 m/s)**

horizontal camera

before and after collision



vertical camera

Before and after collision

Wall-Collision Experiments 4

- Videos wall collision of Duroplast particles (MC-4)

horizontal camera view

vertical camera view

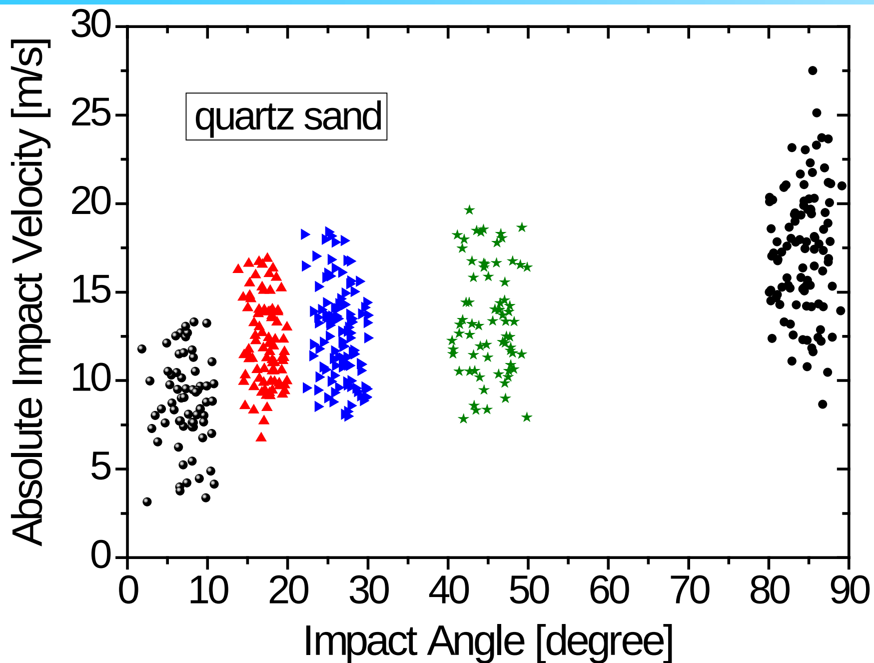
- **The restitution ratios are determined from the ratio of the velocities obtained by the particle tracking routine:**

$$e = \left|\frac{V_2}{V_1}\right| \qquad e_n = \left|\frac{V_{y2}}{V_{y1}}\right| \qquad e_t = \frac{V_{x2}}{V_{x1}}$$

- **From the impulse equations for spherical particles the friction coefficient is obtained in the following way:**

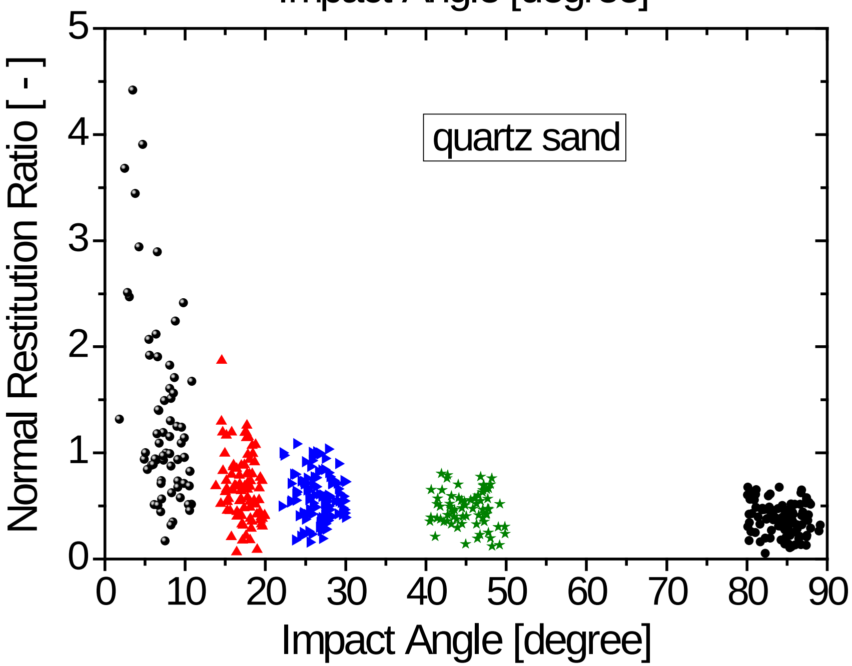
$$\mu = \frac{|V_{x1} - V_{x2}|}{(1+e)\,V_{y1}}$$

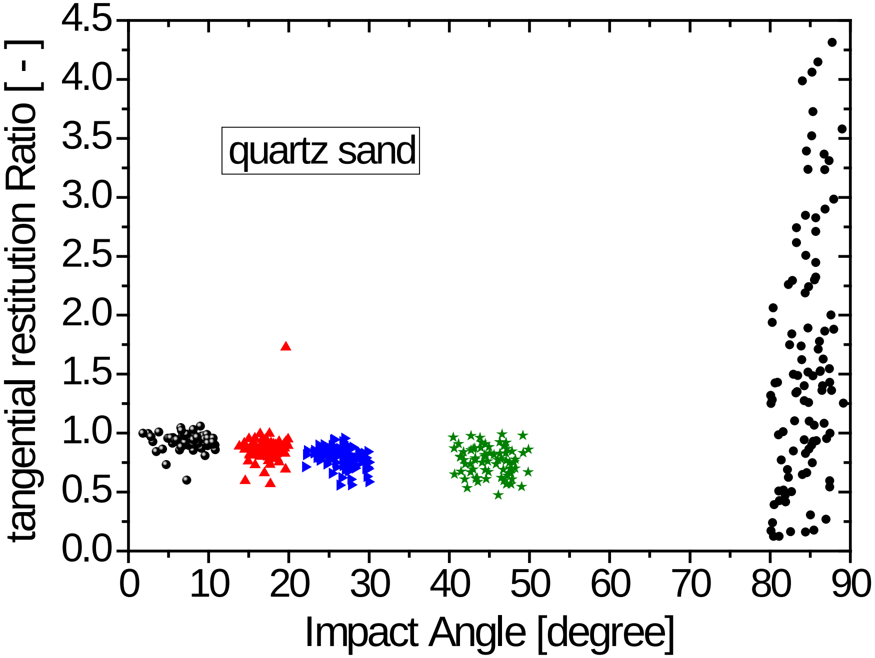
Wall-Collision Results 1



Correlations between wall collision properties and impact angle

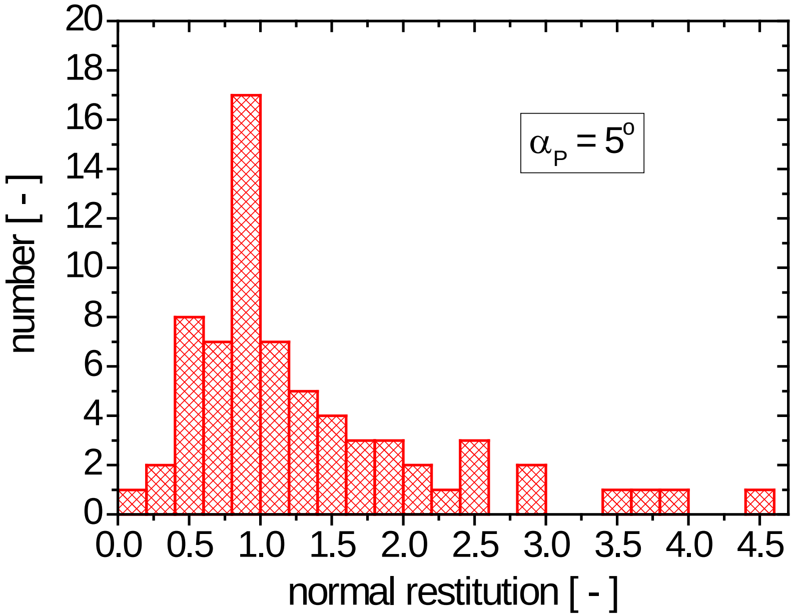
quartz sand

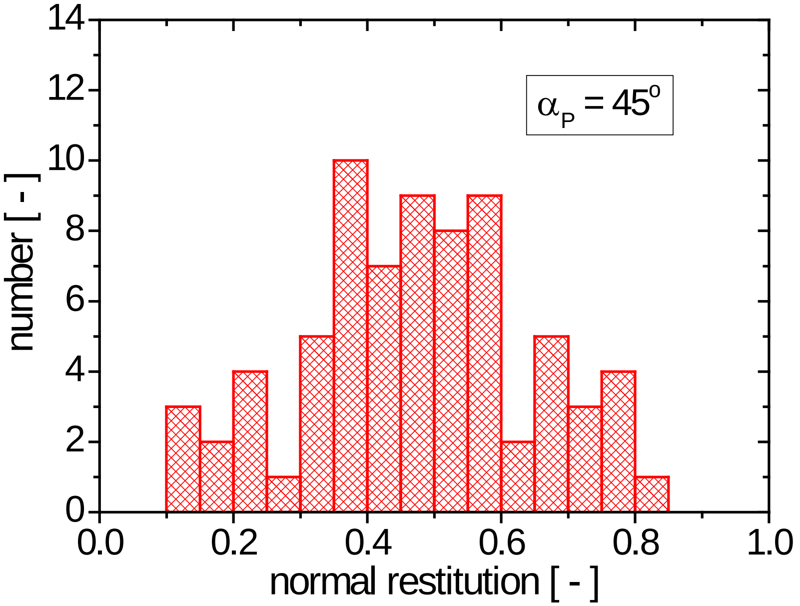


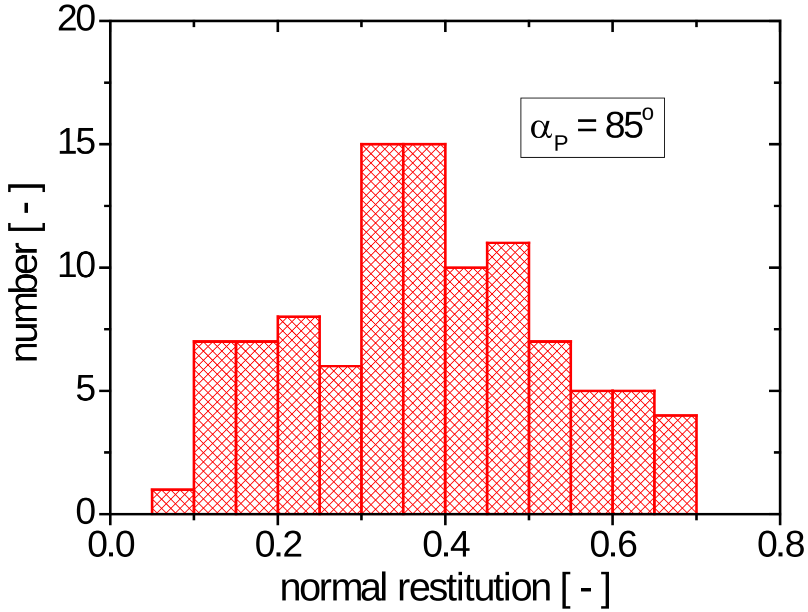


Wall-Collision Results 2

➢ **Normal restitution quartz sand**

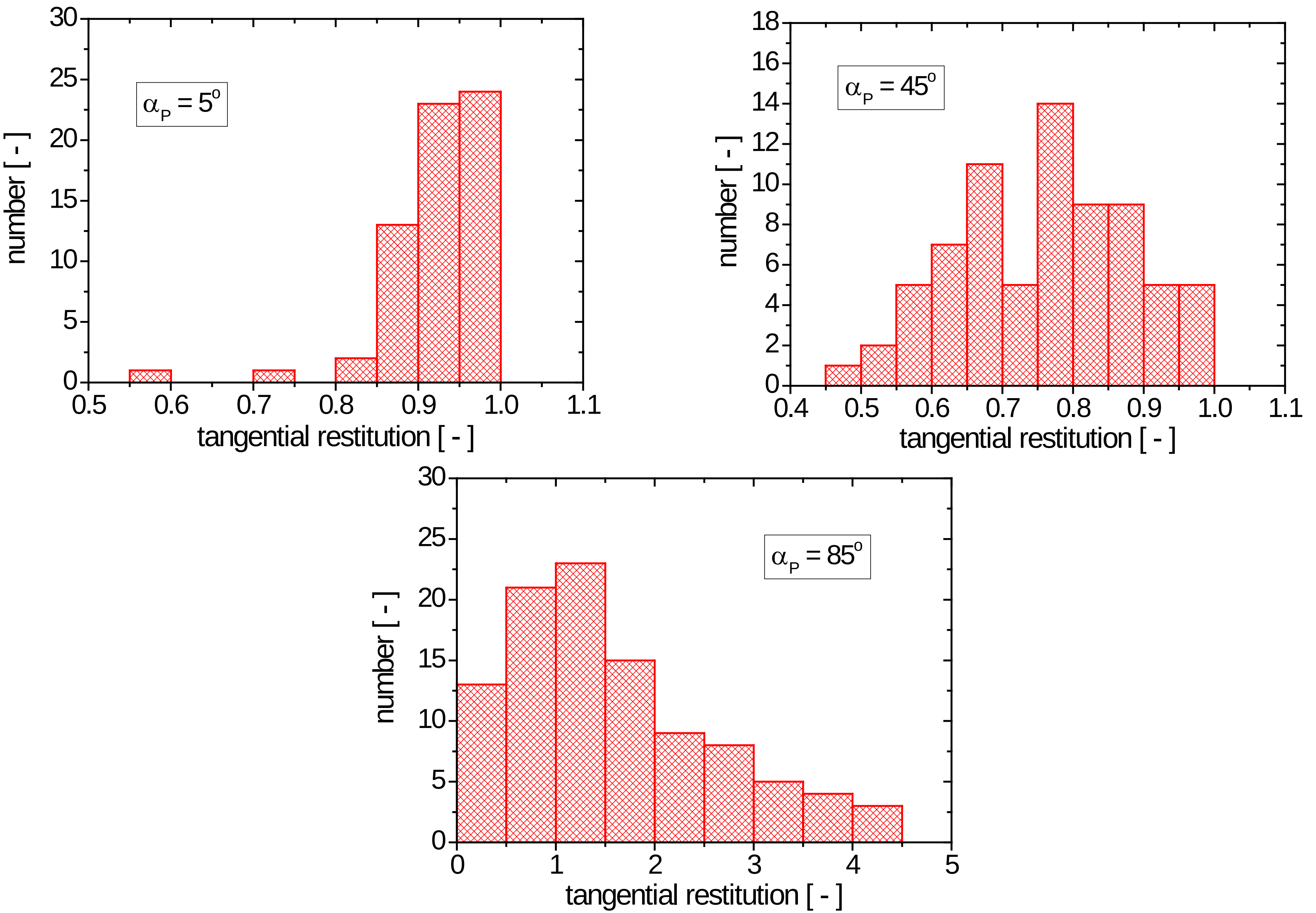






Wall-Collision Results 3

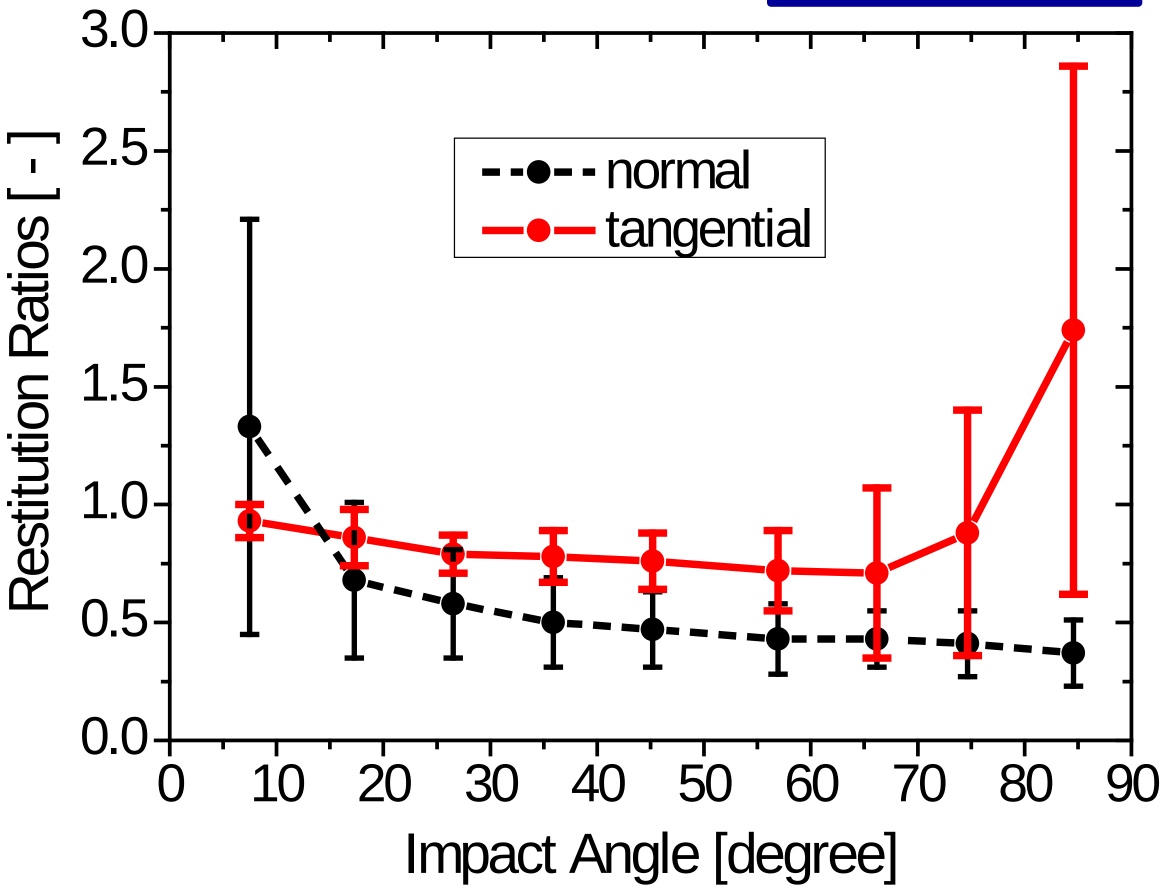
- **Tangential restitution quartz sand**



Wall-Collision Results 4

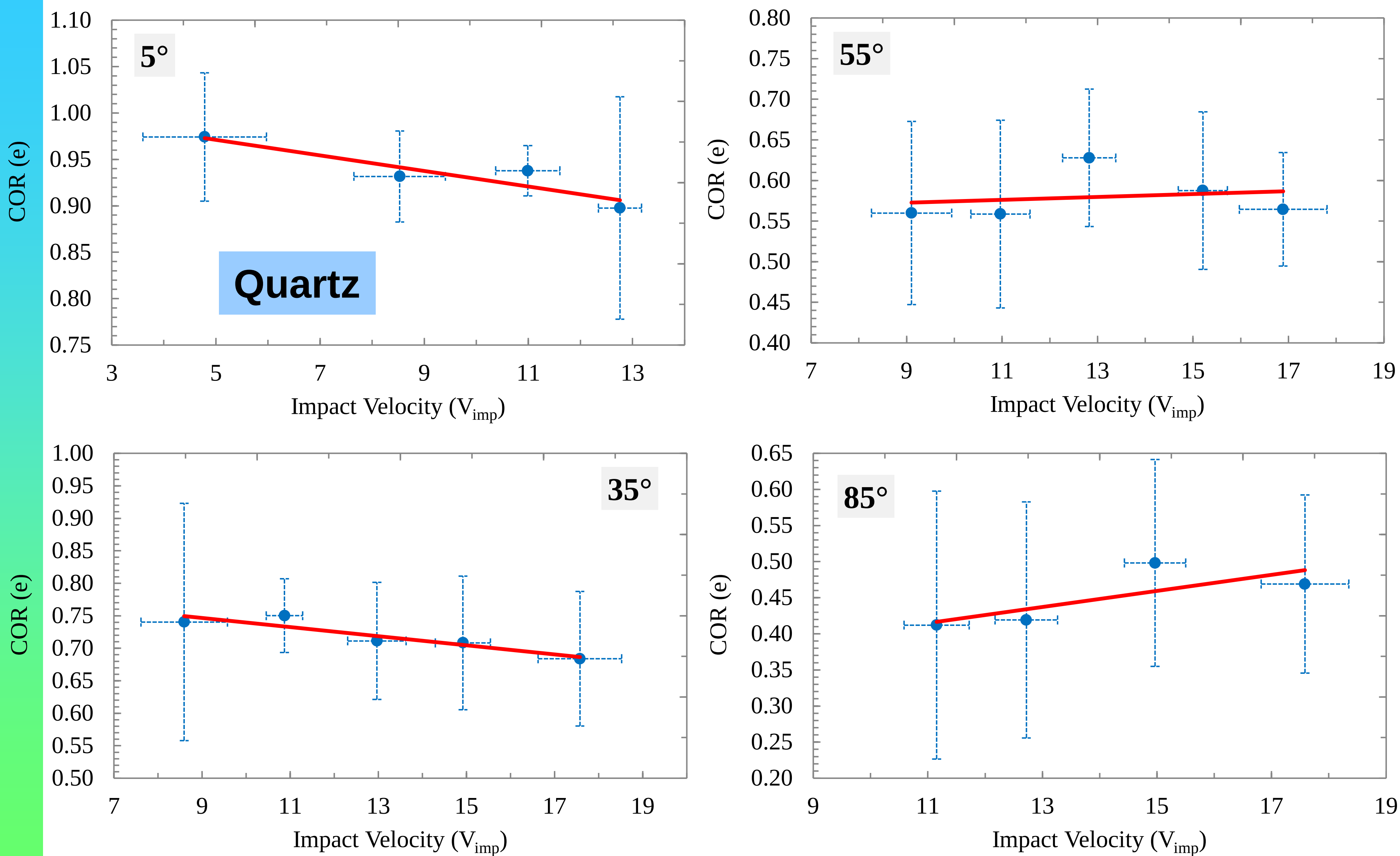
- **Dependence of normal and tangential restitution ratios on mean impact angle**

quartz sand



Wall-Collision Results 5

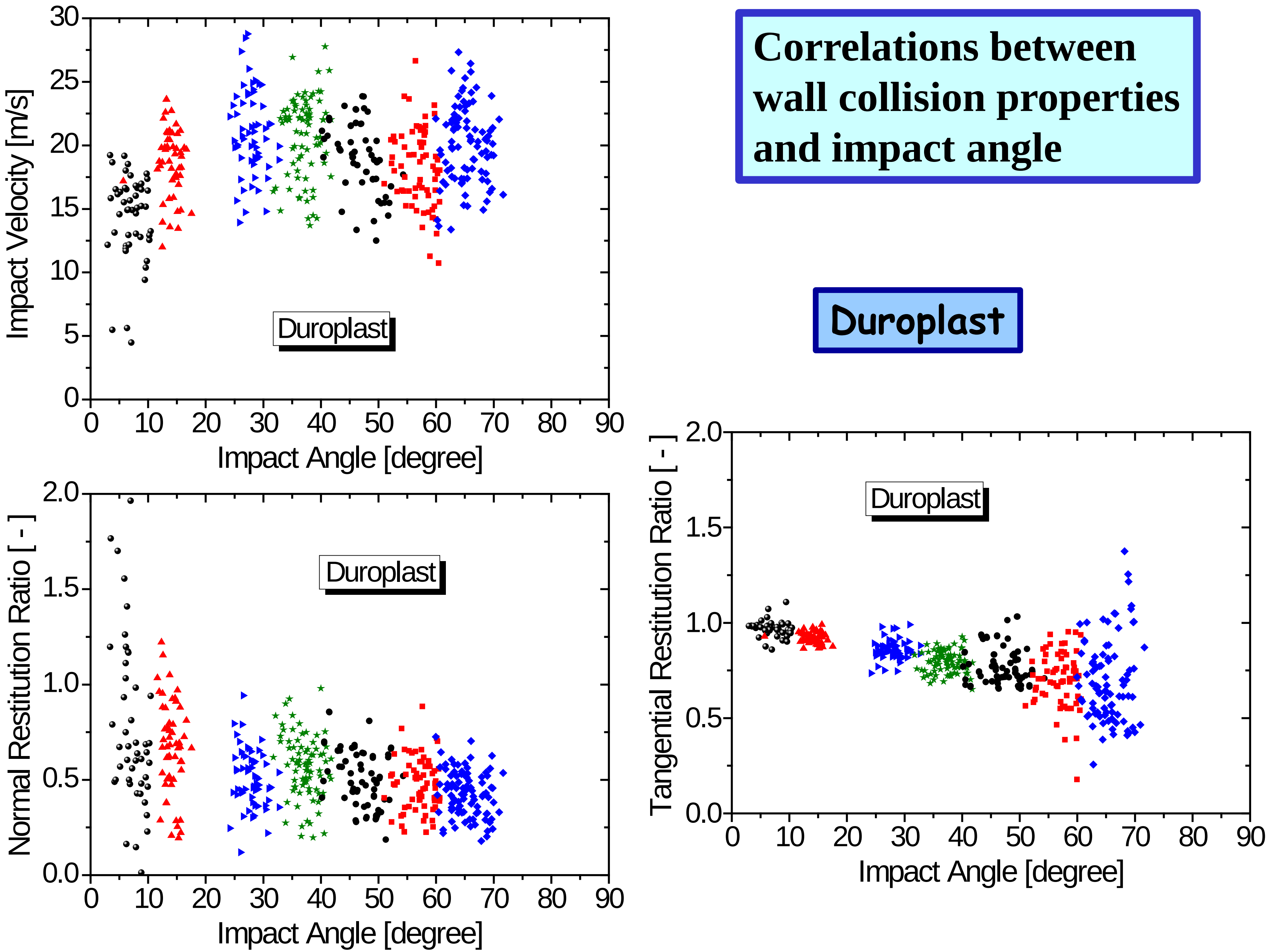
➢ **Dependence of total restitution coefficient on impact velocity:**



Wall-Collision Results 6

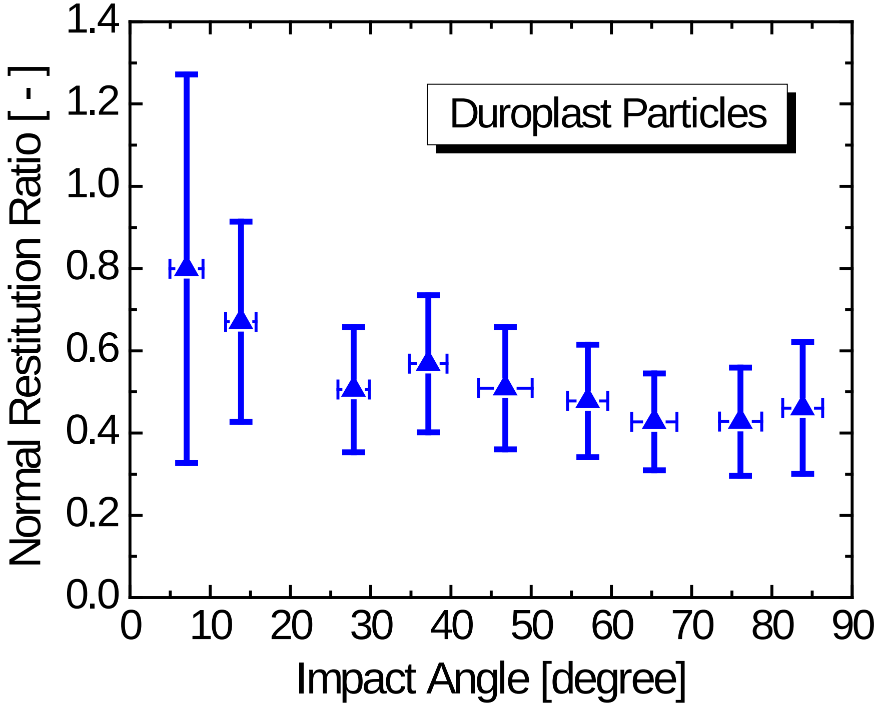
Correlations between wall collision properties and impact angle

Duroplast

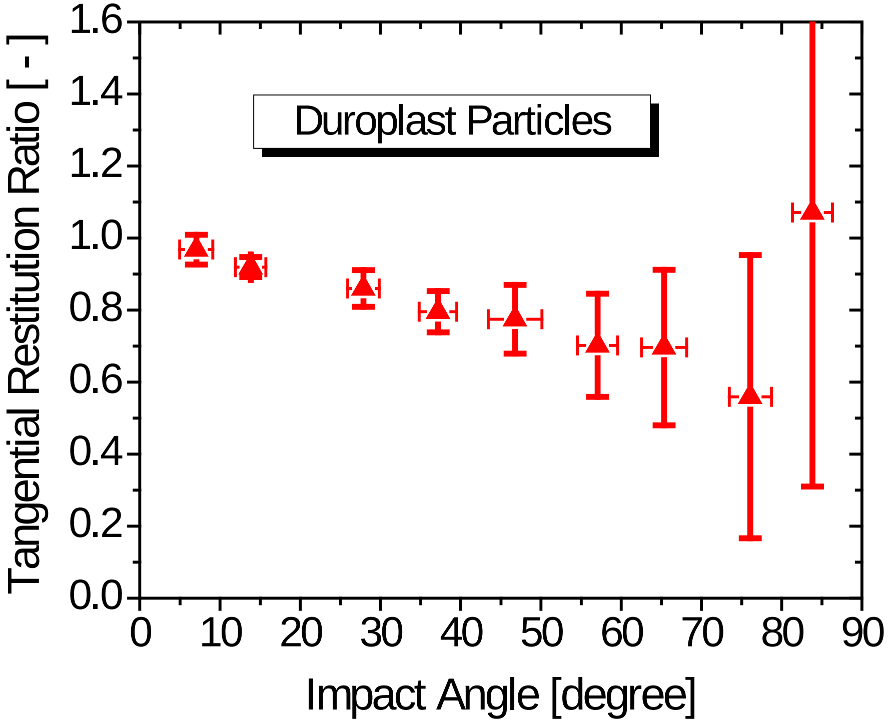


Wall-Collision Results 7

➢ **Dependence of normal and tangential restitution ratios on mean impact angle**

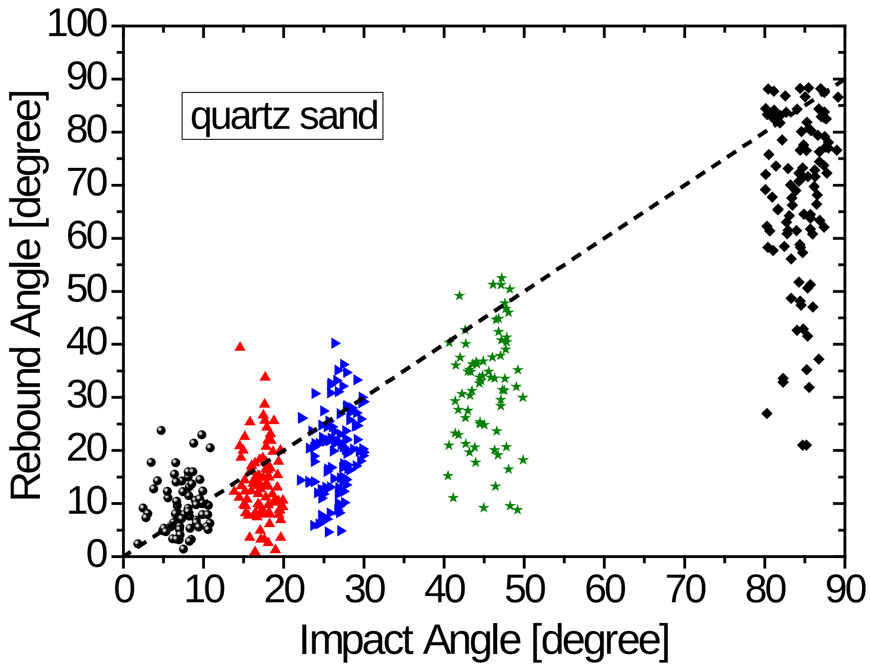


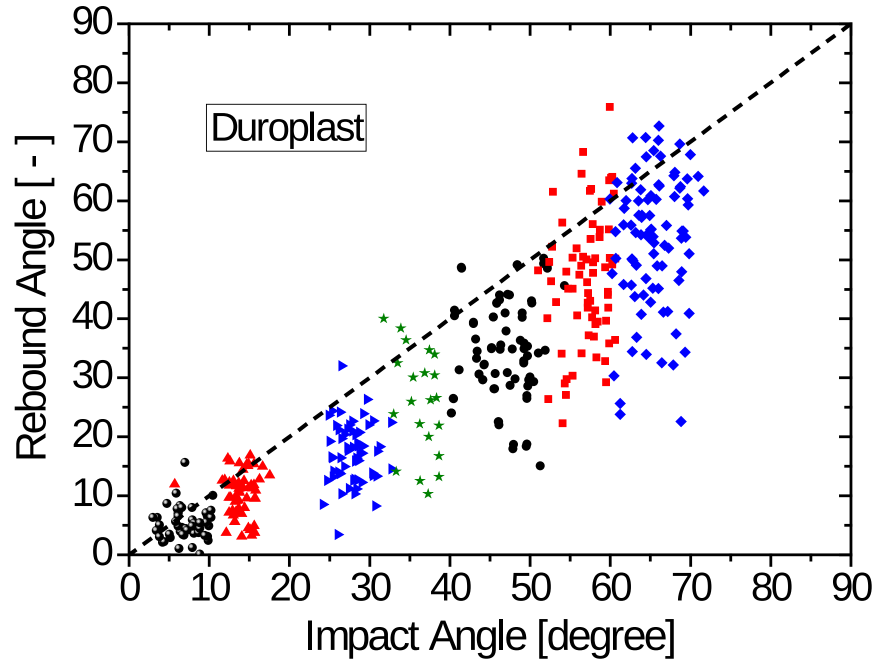
Duroplast



Comparison 1

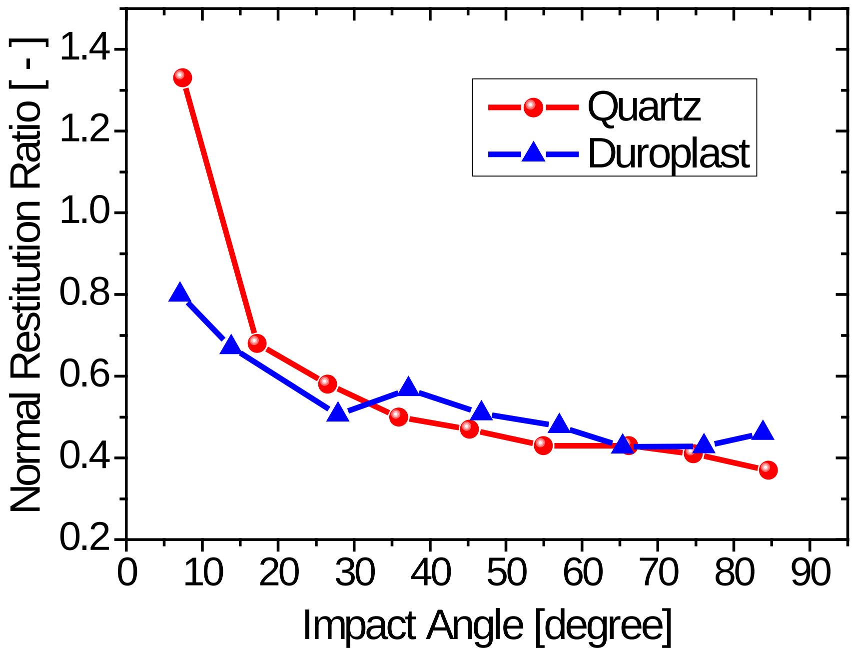
➢ **Rebound angle versus impact angle for quartz and Duroplast**

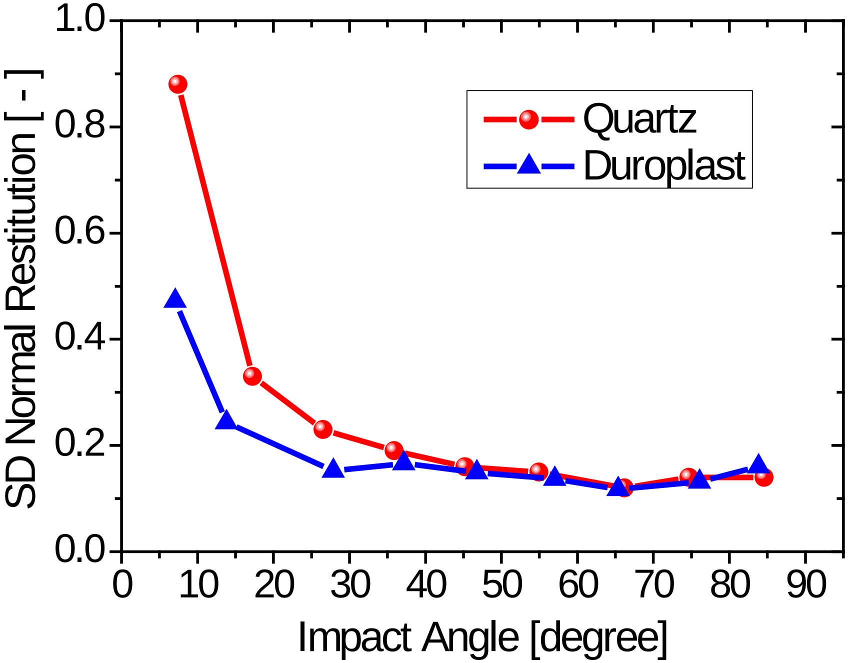




Comparison 2

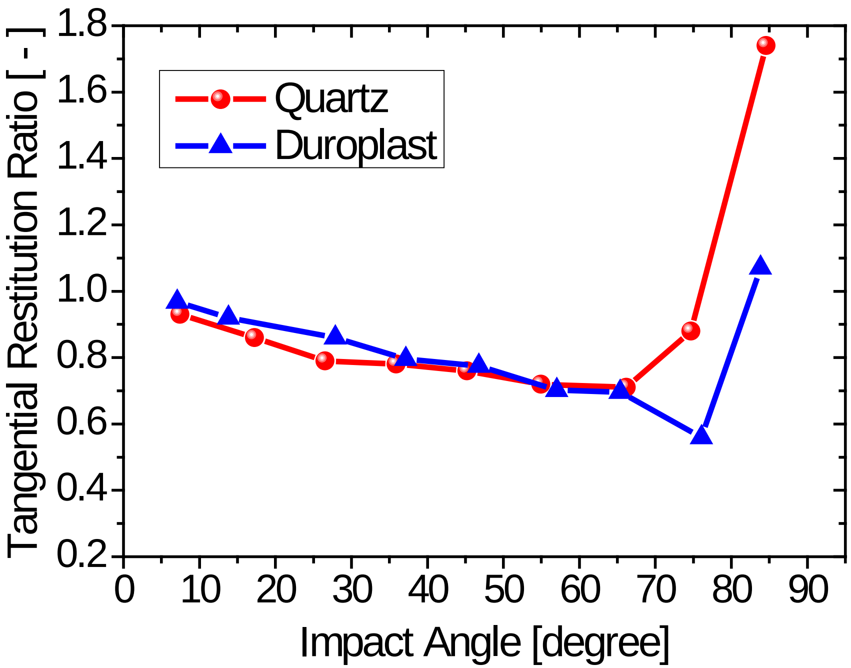
➲ **Comparison of the results for the irregular non-spherical particles**

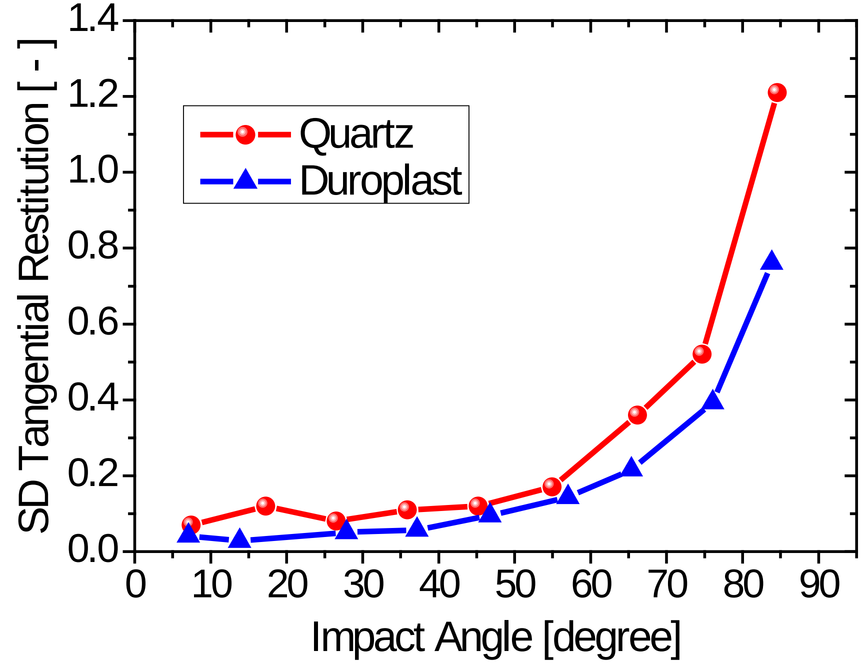




Comparison 3

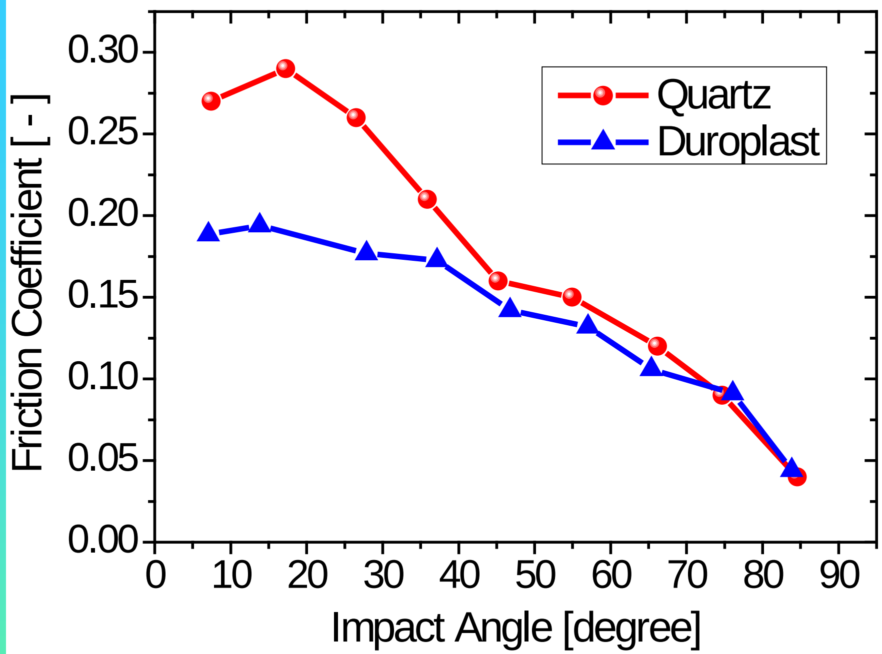
- Comparison of the results for the irregular non-spherical particles



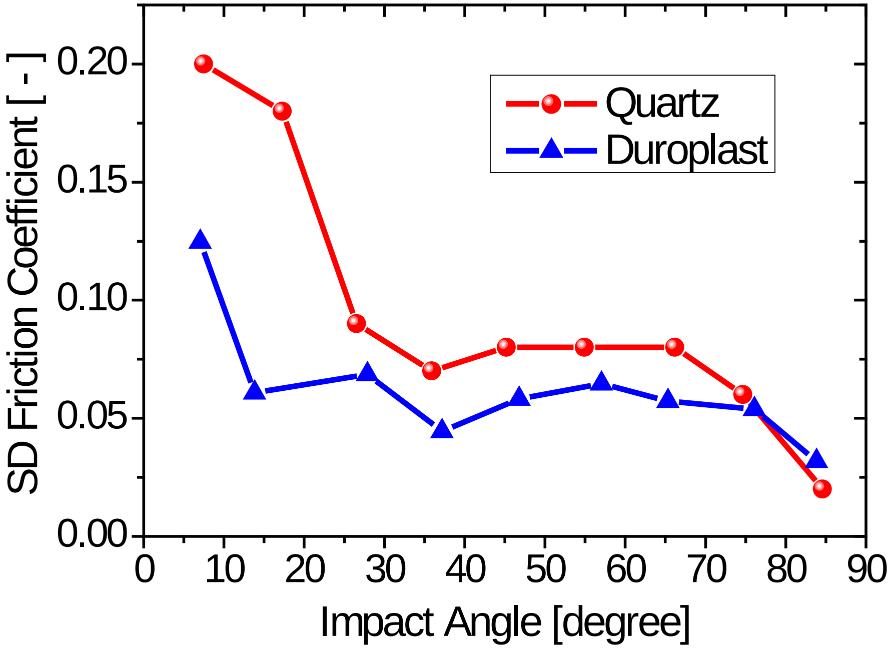


Comparison 4

➲ **Comparison of the results for the irregular non-spherical particles**



$$\mu = \frac{|V_{x1} - V_{x2}|}{(1+e)\,V_{y1}}$$



Measurements in the Horizontal Channel

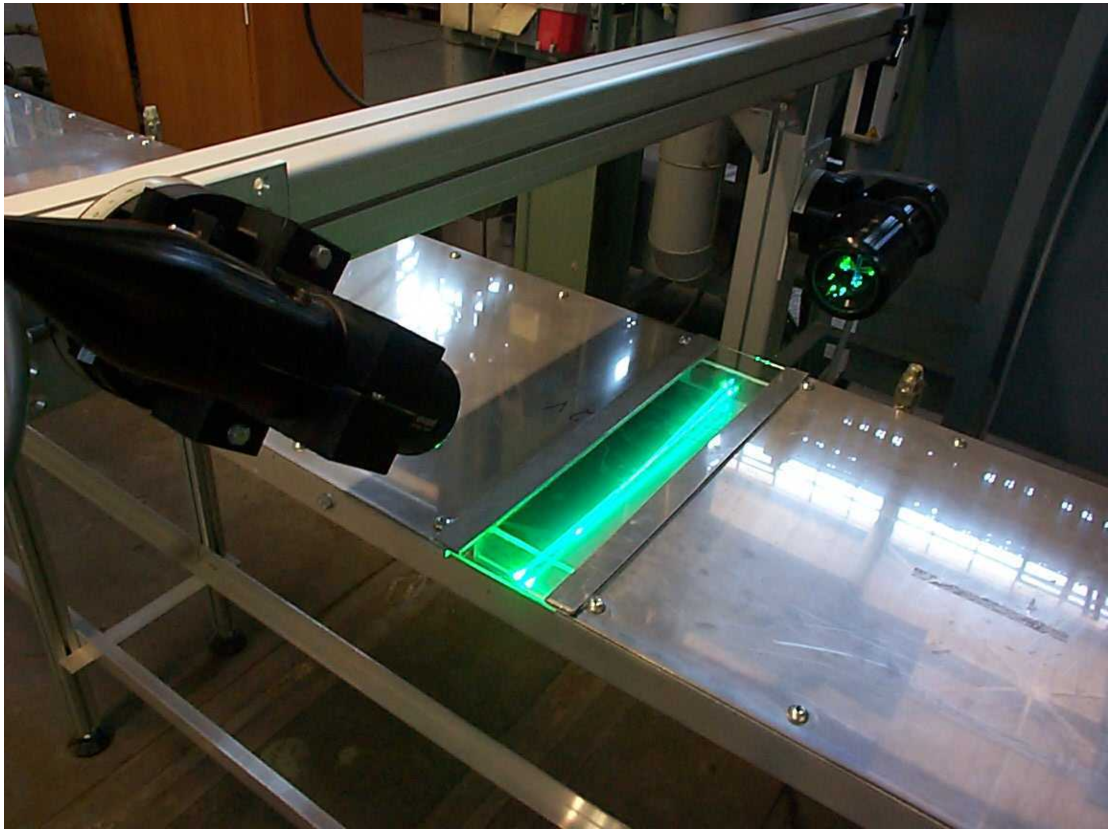
☞ For *providing experimental data for validation*, measurements in a horizontal channel (35 mm x 350 mm) or a pipe may be performed by using laser-Doppler anemometry and imaging techniques (Kussin 2004).

Tracer:
Glass beads 2 µm

Particle phase (without tracer):
Reflection: 120°

Tracer particles in two-phase flow:
Refraction: 33.5°

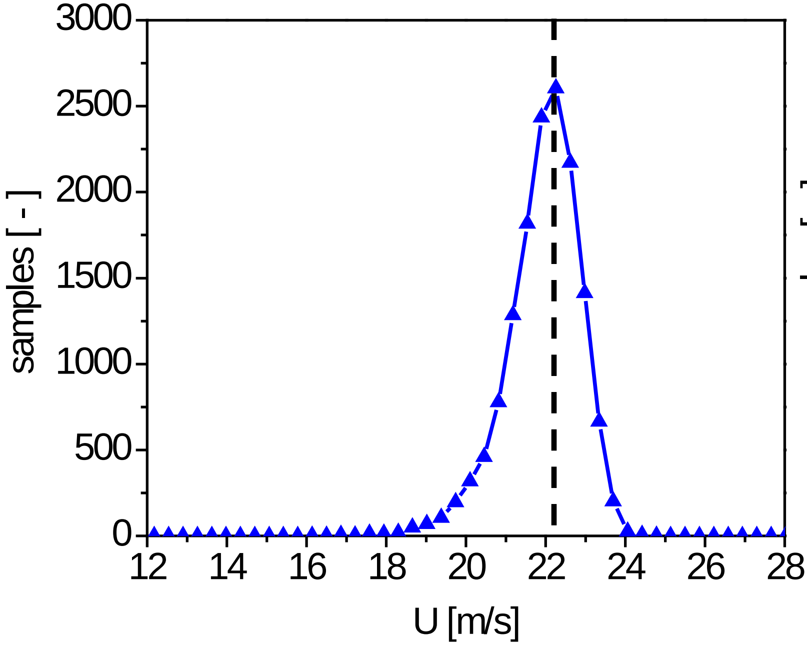
Conveying velocity:
19 – 20 m/s



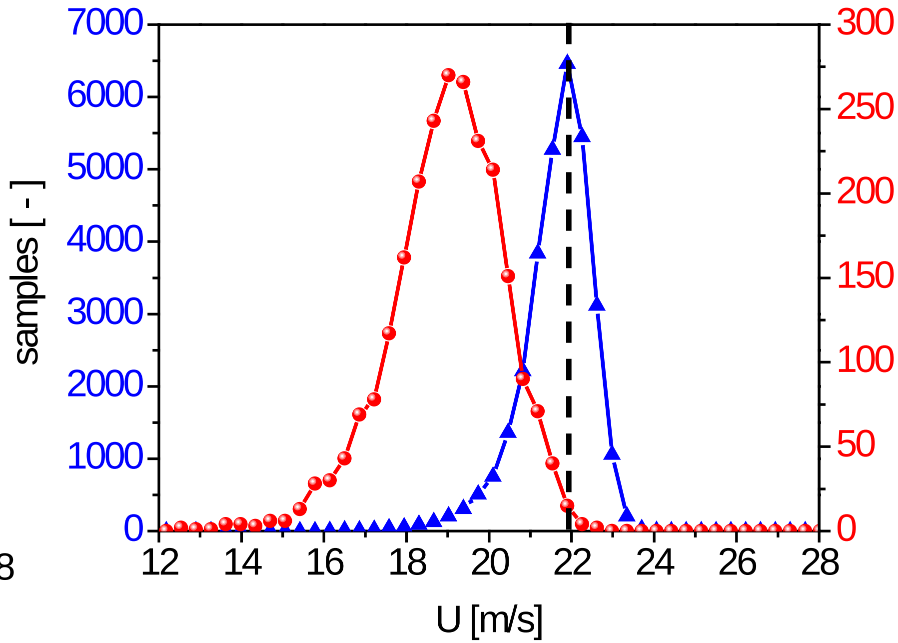
Validation of Measurement Procedure

☞ **For the validation of the measurement procedure the velocity distribution (stream-wise component) of tracer and quartz particles (185 µm) in the centre of the channel was analysed.**

Single phase flow



Two phase flow (η = 0.3)

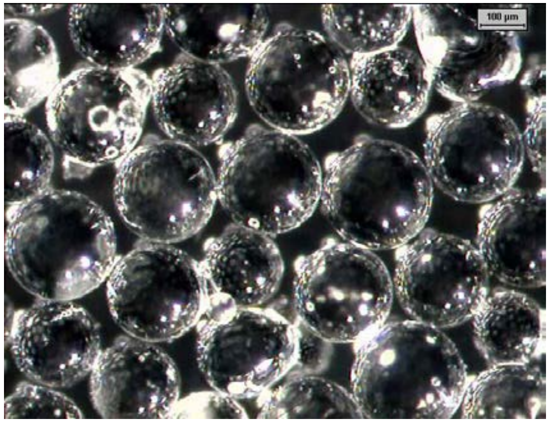


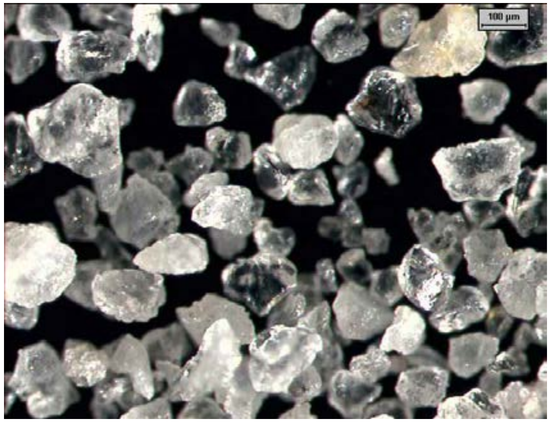
Particles 1

☞ **Properties of the considered particles:**

T_L = 3.66 ms

Particles	Glass beads	Duroplast I	Glass beads	Quartz sand	Duroplast II
Particle size	130 µm	180 µm	200 µm	185 µm	240 µm
Density	2450 kg/m^3	1480 kg/m^3	2450 kg/m^3	2650 kg/m^3	1480 kg/m^3
Relaxation time	81.1 ms	85.3 ms	143.3 ms	138.0 ms	123.1 ms
Stokes number	22.17	23.31	39.15	37.69	33.64



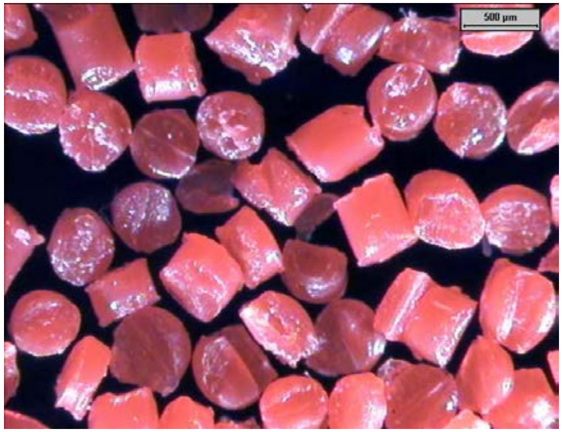


Particles 2

☞ Properties of the considered particles:

Particle	Cylinder	Polystyrene	Glass beads
Particle size	480 µm	660 µm	625 µm
Density	1120 kg/m^3	1050 kg/m^3	2450 kg/m^3
Relaxation time	216.8 ms	282.5 ms	461.1 ms
Stokes number	59.24	77.19	126.0

T_L = 3.66 ms



Euler/Lagrange Approach 1

Two-way coupling iterations (PSIC)

➢The **fluid flow** is calculated by solving the Reynolds-averaged conservation equations (steady or unsteady) by accounting for the influence of the particles (full two-way coupling).

Turbulence models with coupling:

✓ Reynolds-stress turbulence model

➢The **Lagrangian approach** relies on tracking a large number of representative particles (point-mass) through the flow field accounting for particle rotation

and all relevant forces like:

- drag force
- gravity/buoyancy
- **slip/shear lift (not)**
- **slip/rotation lift (not)**
- torque on the particle

Models for elementary processes:

- turbulent dispersion
- particle wall collisions (roughness)
- inter-particle collisions (spherical)

Particle properties and source terms result from ensemble averaging for each control volume

Euler/Lagrange Approach 2

Particle Phase: **simultaneous, time-dependent tracking of a large number of particles**

$$\frac{dx_{pi}}{dt} = u_{pi}$$

$$m_p \frac{du_{pi}}{dt} = m_p g_i \left(1 - \frac{\rho}{\rho_p} \right) + F_{Di} + F_{Li}$$

$$I_p \frac{d\omega_{pi}}{dt} = T_i$$

$$\vec{F}_D = \frac{3}{4} \frac{\rho}{D_p} m_p c_D (\vec{u} - \vec{u}_p) \left| \vec{u} - \vec{u}_p \right|$$

$$\vec{F}_L = \frac{1}{2} \rho C_L \frac{\pi}{4} D_p^2 \left| \vec{u} - \vec{u}_p \right|^2 \hat{n}$$

$$\hat{t} = \frac{\vec{u} - \vec{u}_p}{\left| \vec{u} - \vec{u}_p \right|} \qquad \hat{t} \cdot \hat{n} = 0$$

$$\vec{T}_P = \frac{1}{2} \rho C_T \frac{\pi}{8} D_p^3 \left| \vec{u} - \vec{u}_p \right|^2 \hat{n}'$$

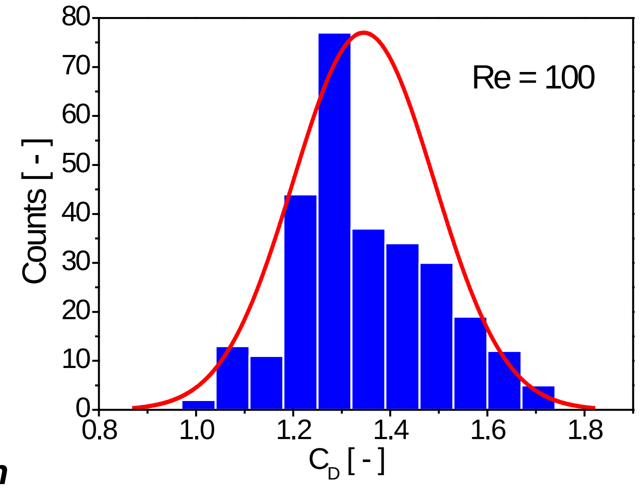
$$\hat{t}' = \frac{\vec{F}_{res}}{\left| \vec{F}_{res} \right|} \qquad \vec{F}_{res} = \vec{F}_D + \vec{F}_L$$

$$\hat{t}' \cdot \hat{n}' = 0$$

Stochastic Coefficients Determination

First approach: Gaussian random process

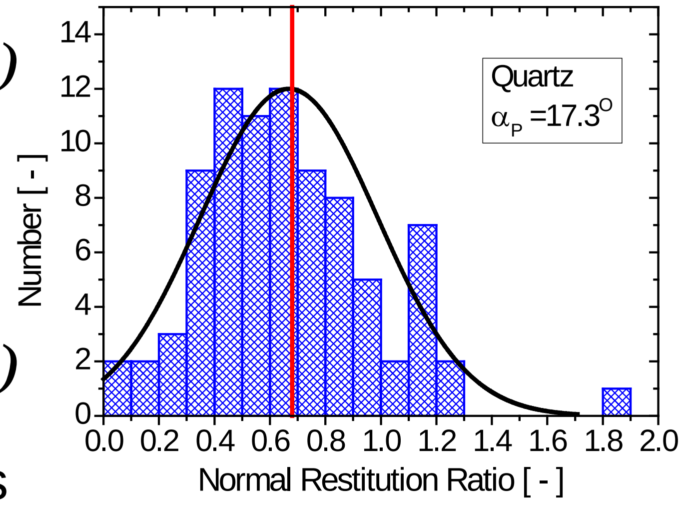
- Generate at each time step the instantaneous flow coefficients: C_D, C_L, C_T



$$C_x(Re_P,t) = C_x(Re_P) + \sigma_{C_x}(Re_P)\,N(0,1)$$

- Instantaneous normal restitution coefficient: ***e***$_n$

$$e_n(\alpha,t) = e_n(\alpha) + \sigma_{e_n}(\alpha)\,N(0,1)$$

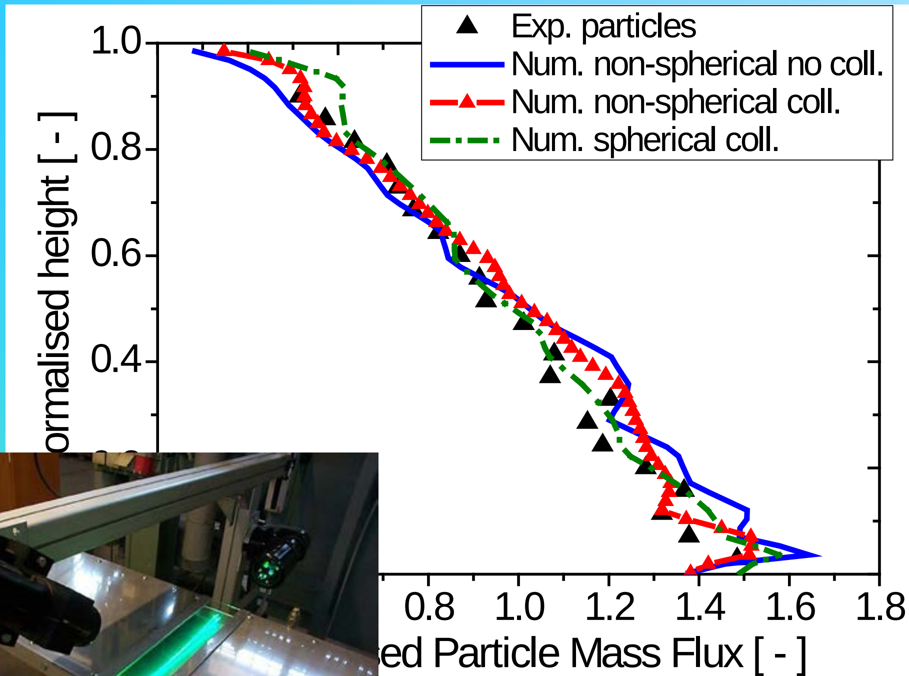


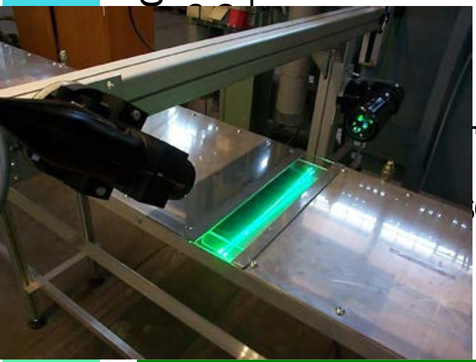
- Instantaneous tangential restitution coefficient: e_t

$$e_t(\alpha,t) = e_t(\alpha) + \sigma_{e_t}(\alpha)\,N(0,1)$$

- N (0, 1): standard Gaussian random process

Validation Horizontal Channel 1





Horizontal Channel:

Length: 6 m

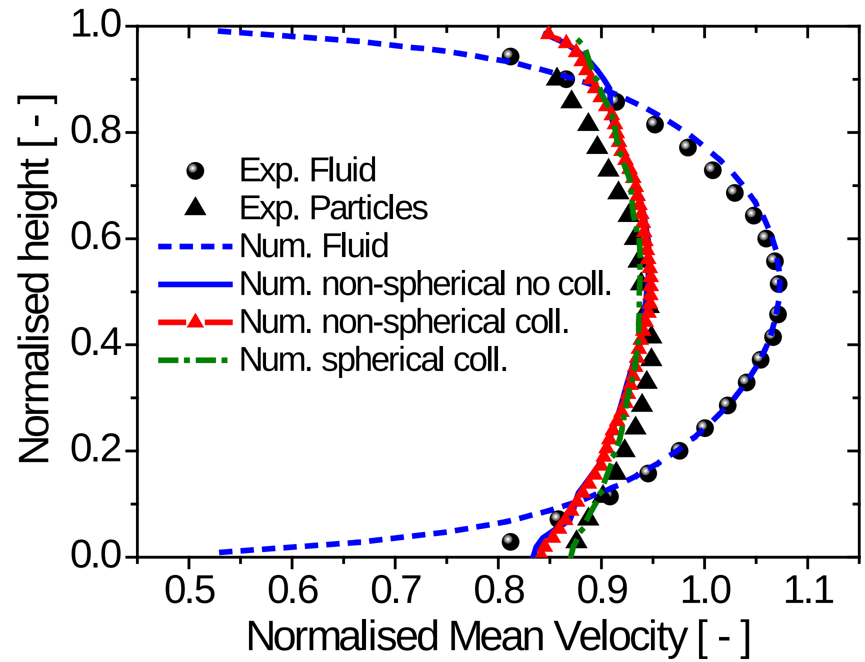
Width: 350 mm

Height: 35 mm

U_{av} = 20 m/s

Quartz sand: 185 µm

Roughness: 2.3 µm (1.5°)

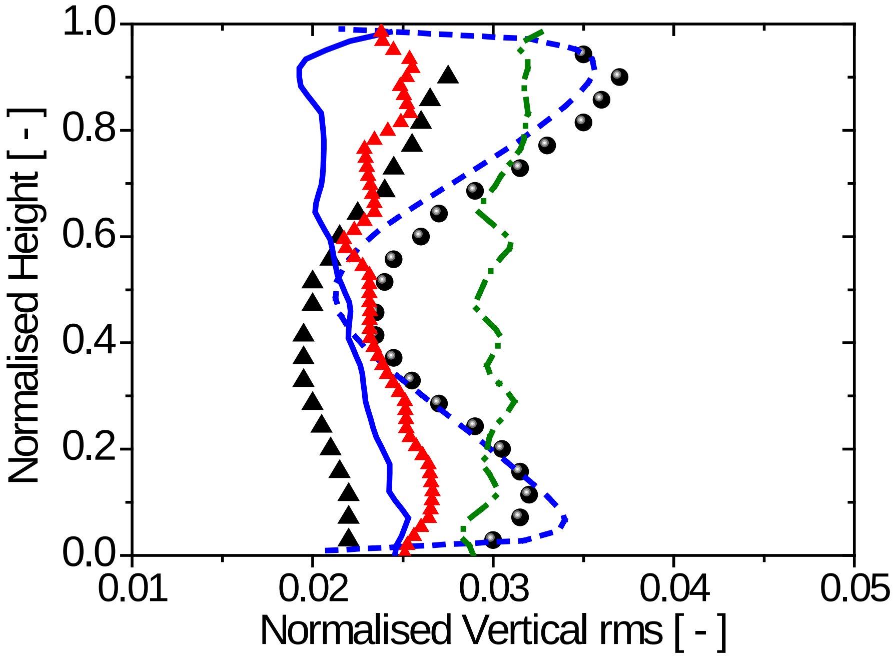


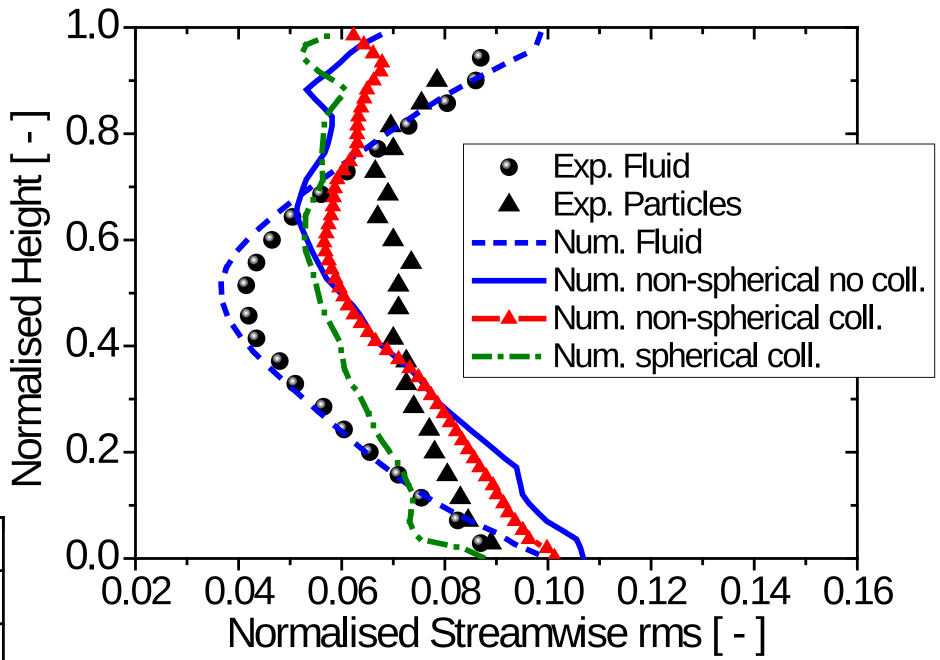
Euler/Lagrange computations (Lain and Sommerfeld 2008):

- **Reynolds-stress turbulence model**
- **Two-way coupling**
- **Wall collisions with roughness**
- **Inter-particle collisions**

Validation Horizontal Channel 2

- **Velocity rms values**

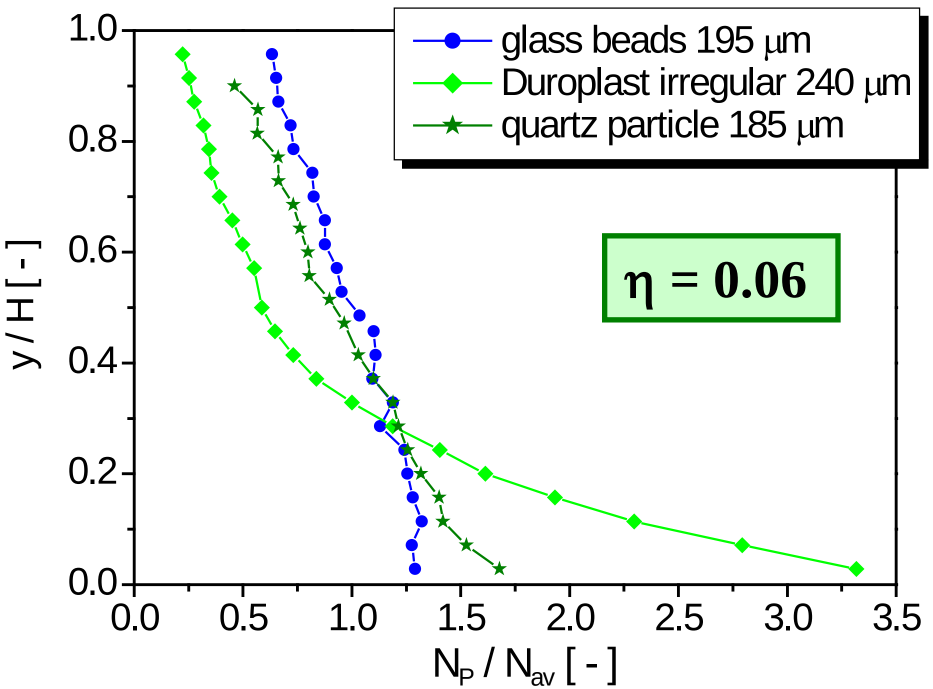


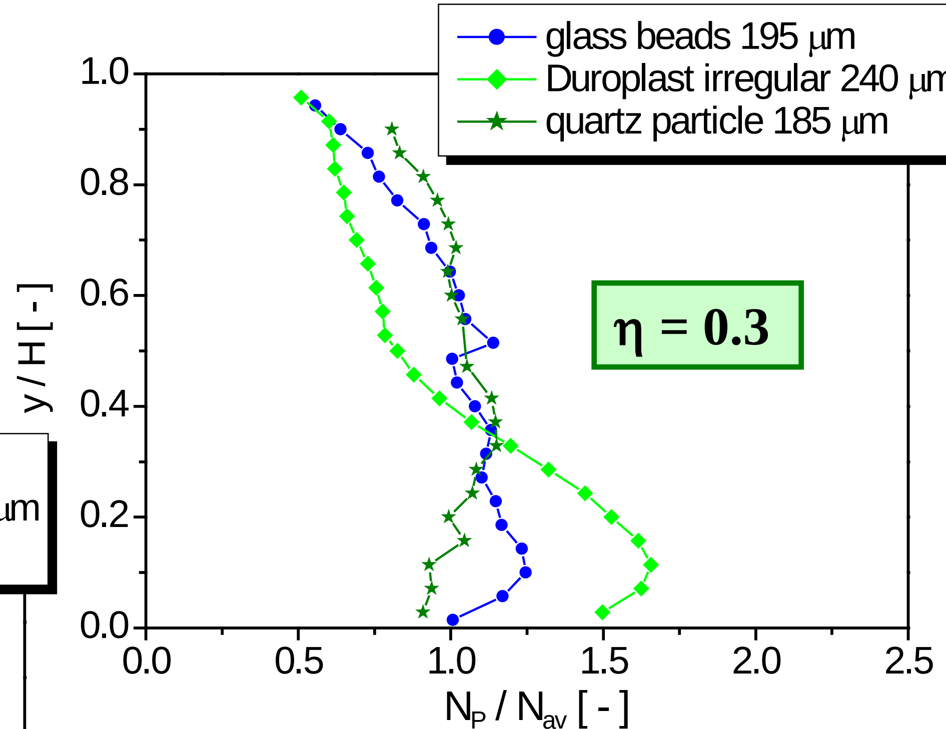


Properties of Different Particles 1

☞ **Comparison for different particles with almost identical Stokes number (St ~ 36.8):**

Normalised number flux



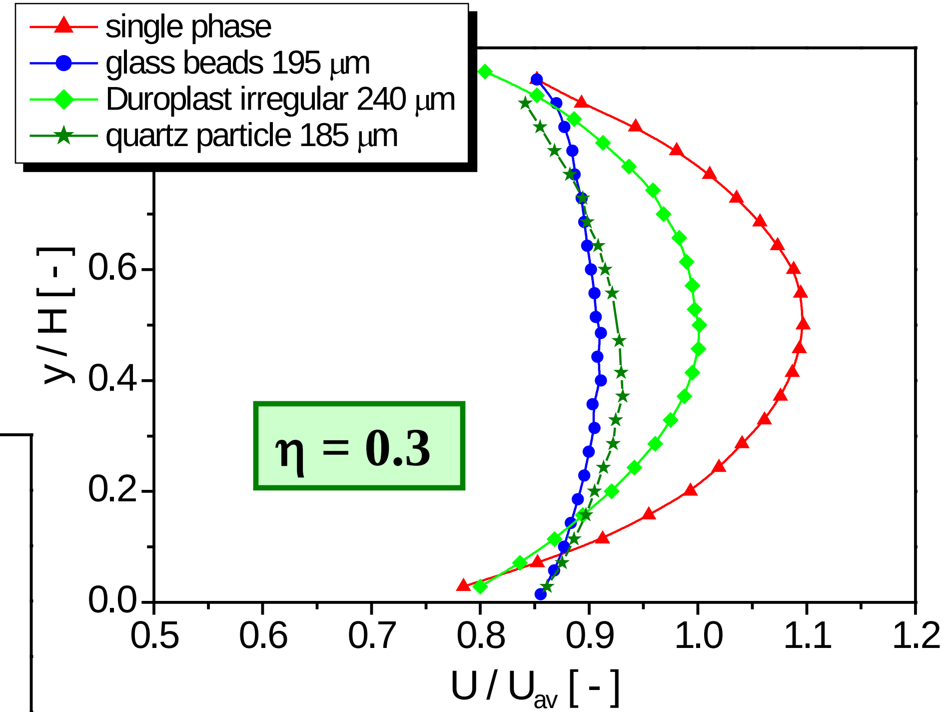


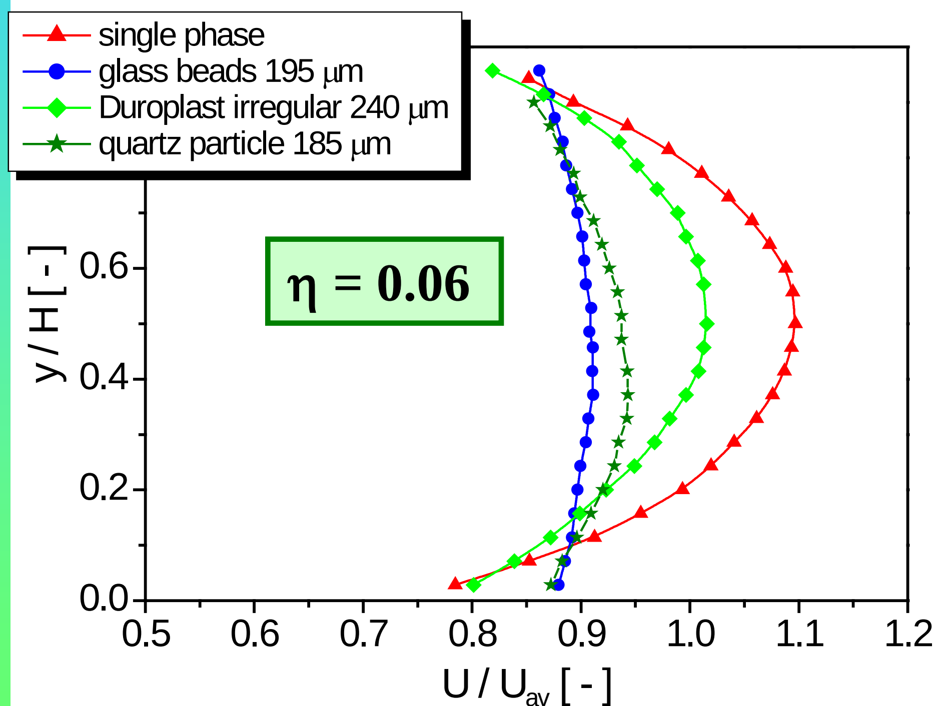
U_{av} = 19.7 m/s

Low roughness R0 = 2.2 μm

☞ **Comparison for different particles with almost identical Stokes number (St ~ 36.8):**

Stream-wise mean velocity





U_{av} = 19.7 m/s

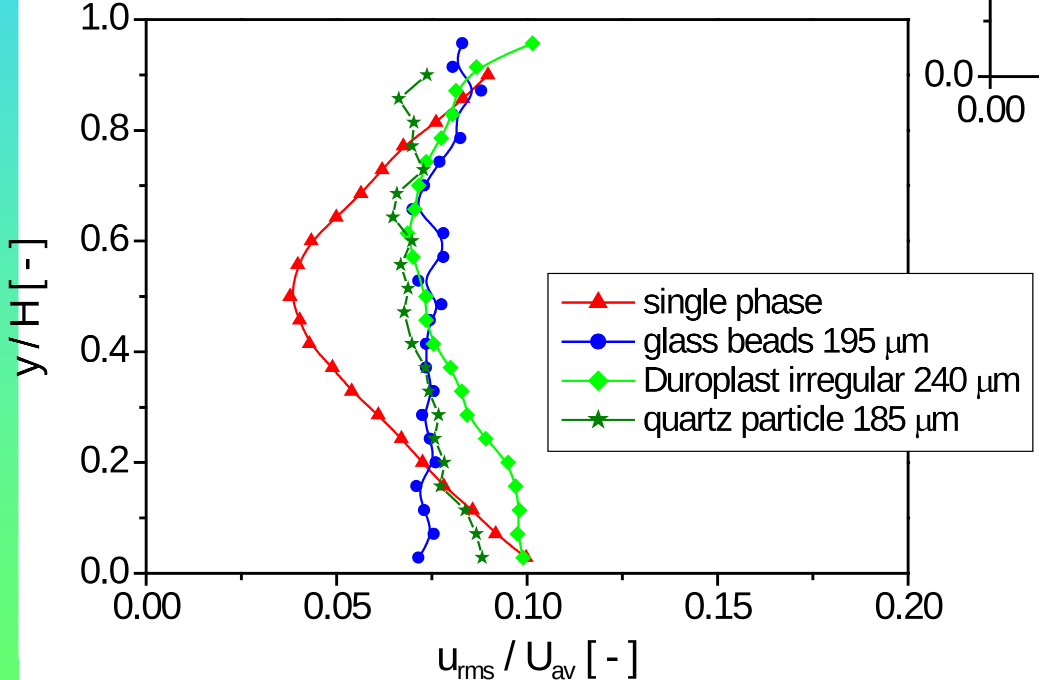
Low roughness R0 = 2.2 μm

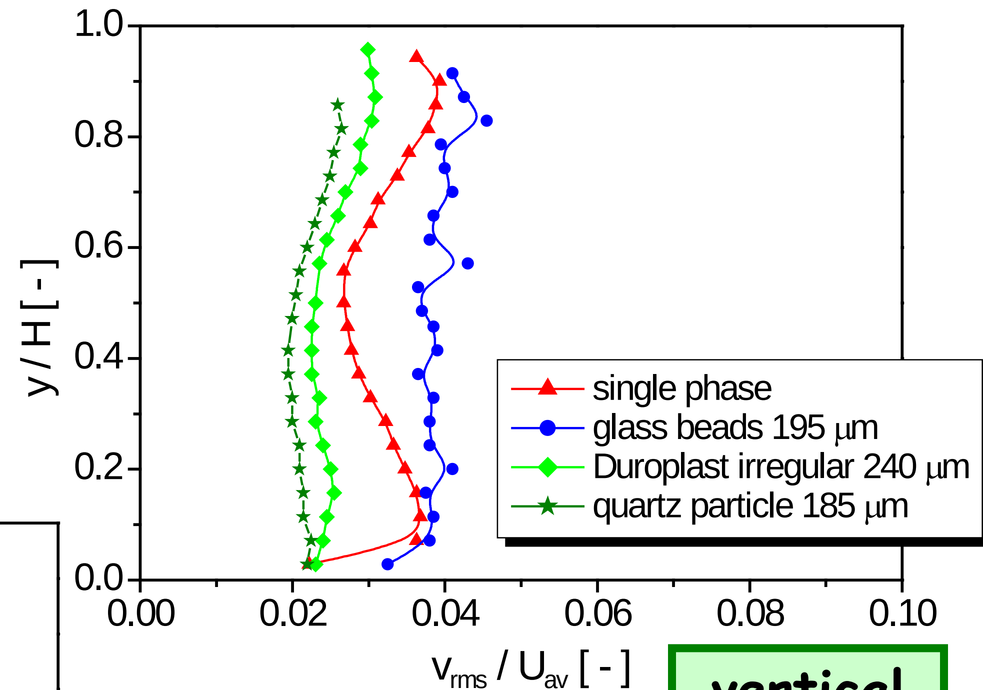
Properties of Different Particles 3

☞ **Fluctuating velocities:**

St ~ 36.8

horizontal





vertical

U_{av} = 19.7 m/s, η = 0.06
Low roughness R0 = 2.2 μm

Conclusions

- **A statistical Lagrangian model was developed in order to allow the numerical calculation of wall bounded particle-laden flows with irregular shaped particles was developed.**
  - Statistical generation of resistance coefficients along particle trajectories based on DNS by LBM
  - Statistical treatment of wall collisions based on experimental studies
- **In further studies slip-shear lift and slip rotation lift needs to be evaluated for irregular shaped particles by DNS**
- **Change of particle angular velocity through a wall collision ???**
- **An estimate of angular velocity change may be possible through a momentum balance**
- **The data base for the resistance coefficients and wall collision parameters will be further extended for other shapes of irregular particles**

Workshop 2015

ANNOUNCEMENT

14th Workshop on Two-Phase Flow Predictions

07. – 10. September 2015

Zentrum für Ingenieurwissenschaften
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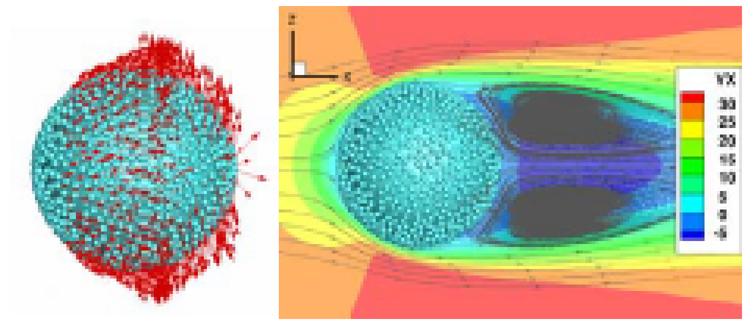

Lattice-Boltzmann Simulations: Flow about a particle coated with 882 drug particles at Re = 200, study related to drug particle detachment in an inhaler.