Czestochowa University of Technology
Faculty of Environmental Engineering and Protection
Department of Heating, Ventilation and Air Protection
Dabrowskiego 73, 42-200 Czestochowa, Poland
Phone/Fax: +48343250933

MODERN MODELING TECHNICS (DEM, POPULATION BALANCE, FRACTIONAL CALCULUS) IN THE ANALYSIS OF GRANULAR FLOWS

Jacek S. Leszczynski
E-mail: jaclesz@gmail.com
http://www.grmat.imi.pcz.pl

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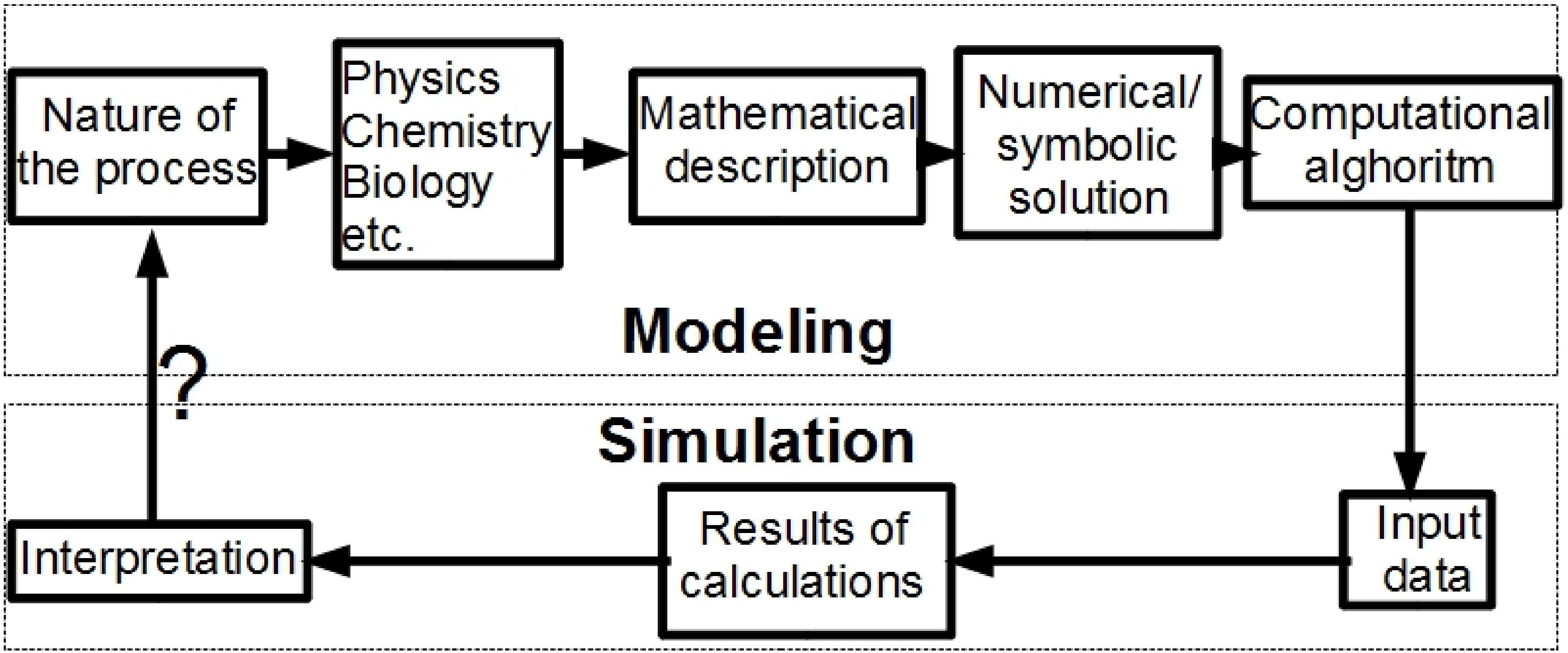
PART 0:

Introduction

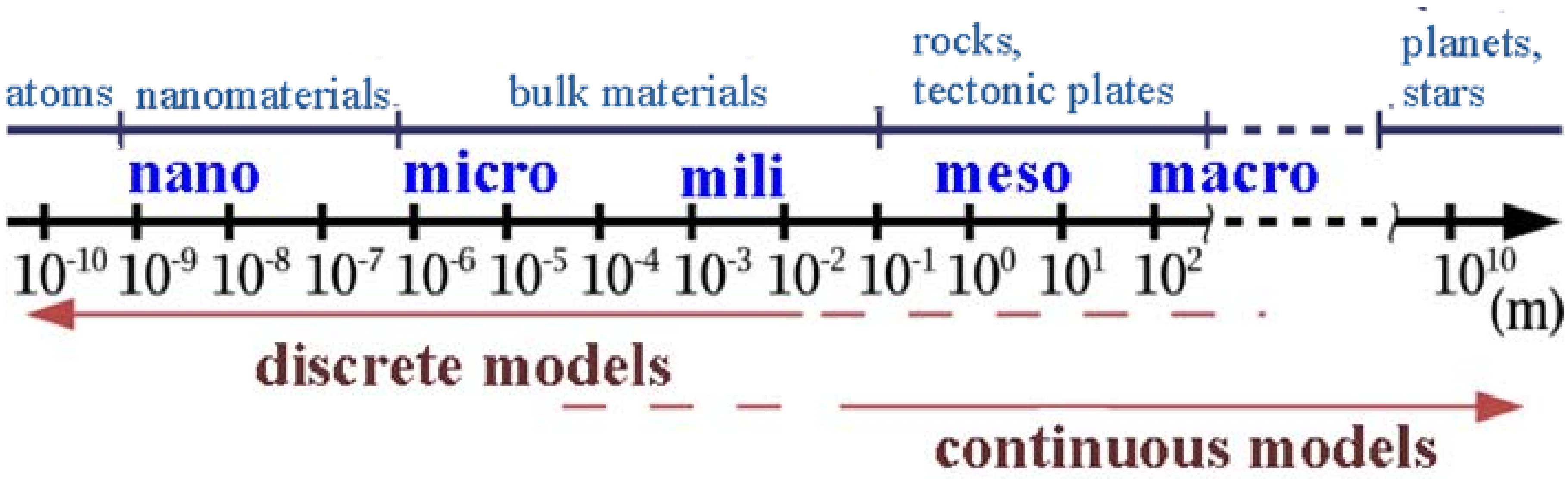
The origin of modeling and simulation[1]



[1] Leszczyński J.S., O modelowaniu i symulacji na maszynach cyfrowych, Materiały Sympozjum Naukowego Instytutu Matematyki i Informatyki, Częstochowa-Poraj, 2000, 69-74.

Granular matter is a set of objects called particles. From the multiscale point of view particles characterise by different: sizes, shapes and their physical properties and parameters describing their state of surface, i.e. the surface roughness, viscosity, etc. The existence of interparticle frictions, inelastic collisions between particles and thermal fluctuations in nanoparticles makes this granular matter to be defined as additional state of matter[1].

Granular materials[2,3]

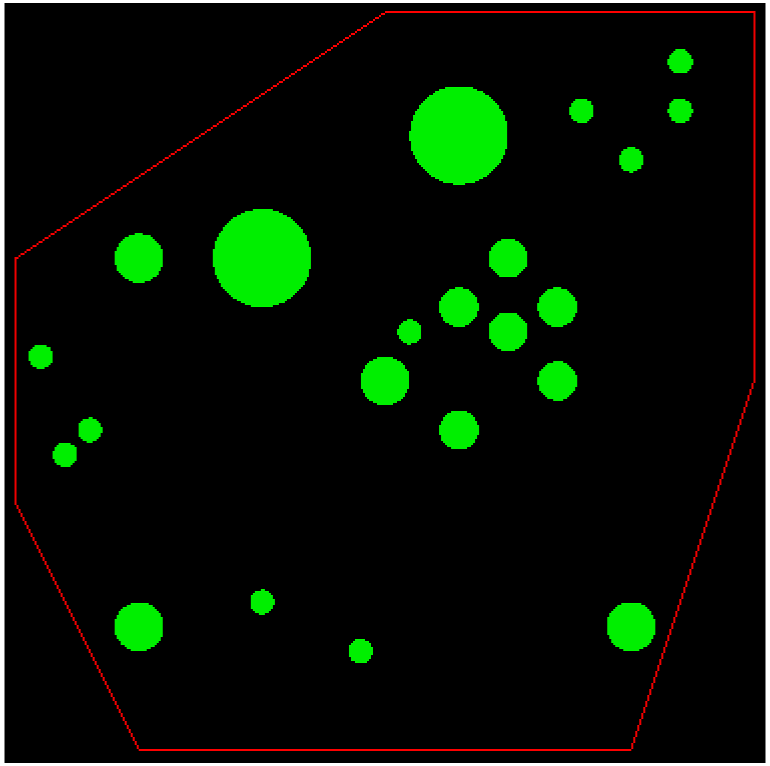


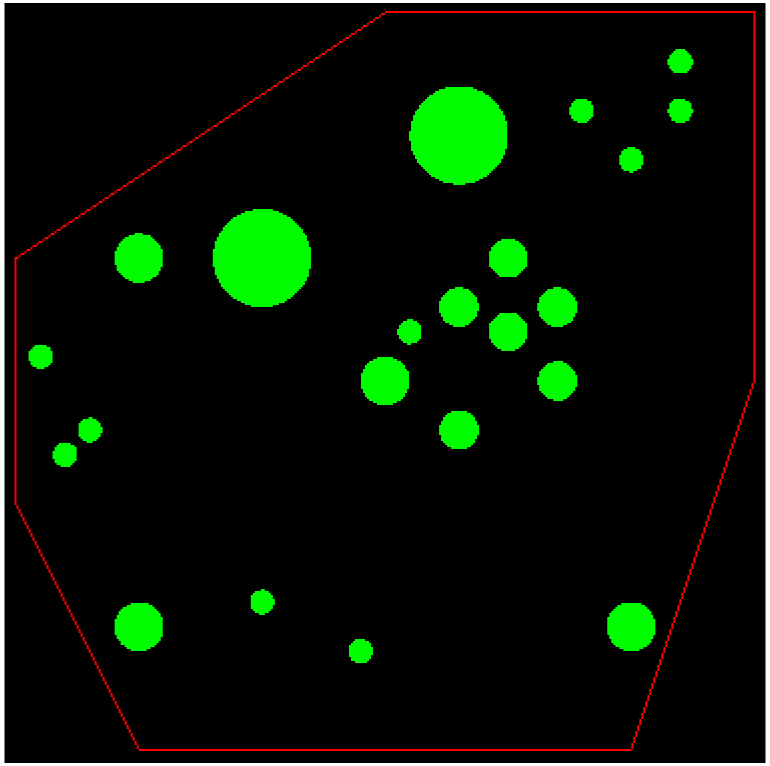
[1] Jaeger H.M., Nagel S.R., Behringer R.P., Granular solids, liquids and gases, Reviews of Modern Physics **68**(4), 1996, 1259-1273.
[2] Brady J., Computer simulation of viscous suspensions, Chemical Engineering Science **56**, 2001, 2921-2926.
[3] D'Adetta G.A. *et al*., From solids to granulates – Discrete element simulations of fracture and fragmentation processes in geomaterials, Lecture Notes in Physics **568**, 2001, 231-250.

The dynamics of granular material: Particles move individually under gas extortion and they exchange momentum and energy during mutual collisions.

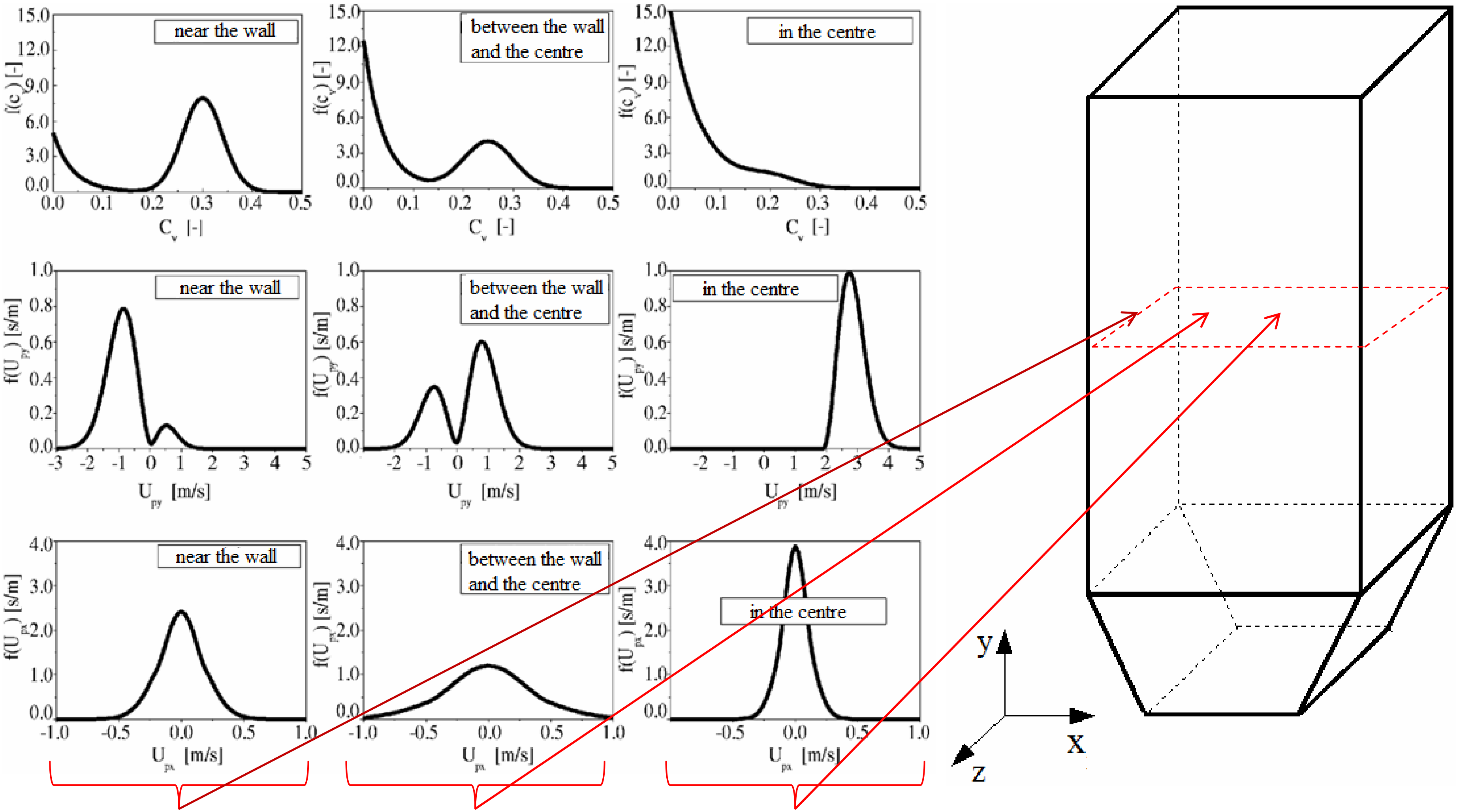
The dynamics of a two-particle collision: We can distinguish three phases of the collision process (impact, contact and the last phase being a result of a collision). One can observe phenomea which occur in the collision process: rebound, static contact, attrition, cohesion and fragmentation. Collisions may occur quickly or slowly in time.

The dynamics of multiparticle collisions: It occurs when the contact times between different pairs of colliding particles are larger than times of their individual motion.





Local structure of a granular material under fluidisation regime[1]



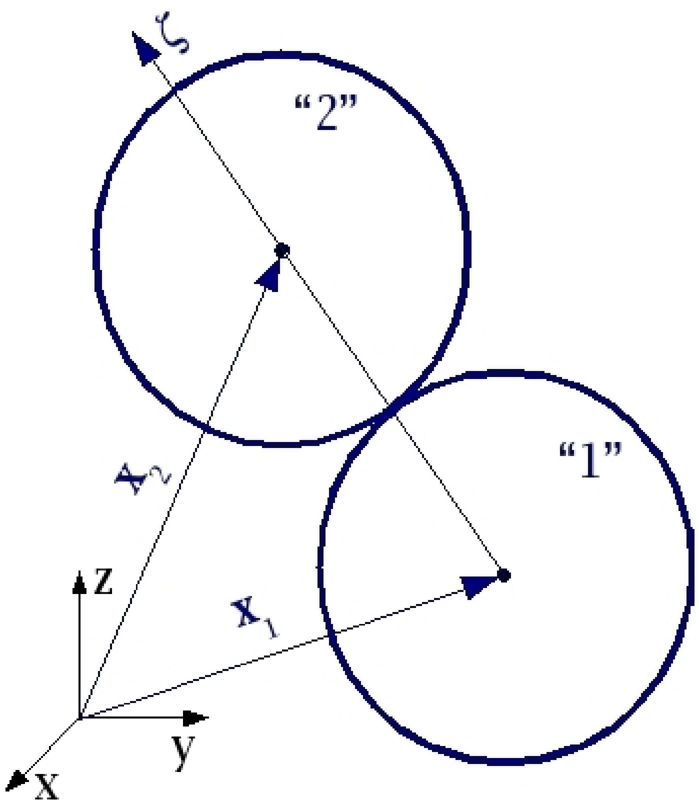
[1] Leszczyński J., Bis Z., Gajewski W., Evolution of structure and particle velocity distribution in circulating fluidized beds, Powder Techonolgy **128**, 2002, 22-35.

PART I:

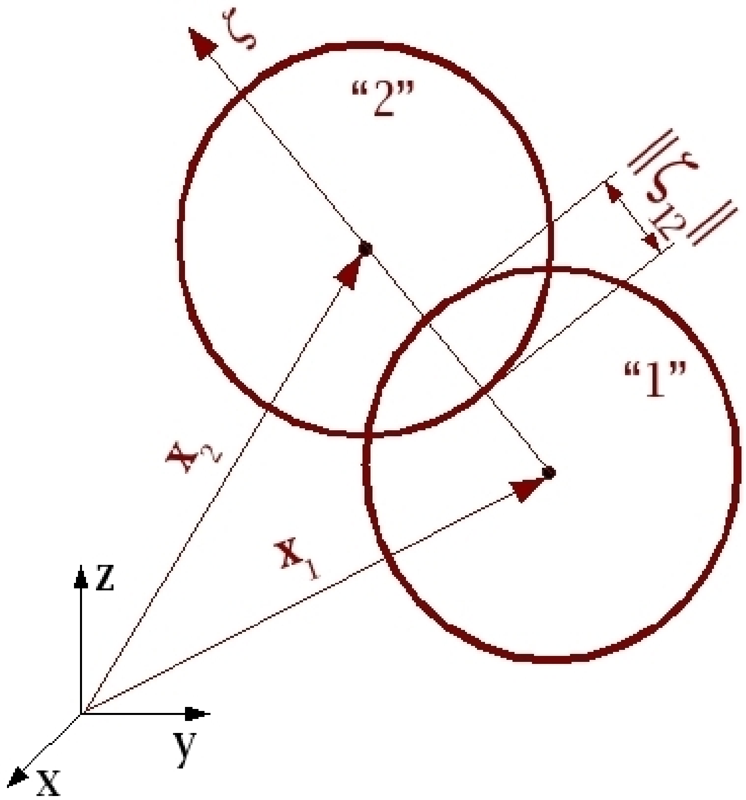
DEM

Modeling of particle collisions – the Discrete Element Method (DEM)

The hard sphere approach[1]
(particle contacts without deformation)



The soft sphere approach[2]
(particle contacts with deformation)



[1] Greenspan D., *Discrete numerical methods in physics and engineering*, Academic Press, New York 1974.
[2] Cundall P.A., Strack O.D.L., A discrete numerical model for granular assemblies, Geotechnique **29**, 1979, 47-65.

Let us consider to a set of spherical particles n_p. We introduce index $k=1,\dots, n_p$, denoting the particle number in the set of particles.

Motion equations of mass center of a particle in the global system of coordinates (x_1,x_2,x_3)

• particle motions without any collision

$$\begin{cases} m_{p_k}\ddot{\mathbf{x}}_{p_k} = \sum_l \mathbf{F}_{p_l} \\ \mathcal{I}_{p_k}\dot{\boldsymbol{\omega}}_{p_k} = \sum_l \mathbf{M}_{p_l} \end{cases}$$

$\mathbf{F}_{p_l}$ - long range forces

$\mathbf{M}_{p_l}$ - long range torque

• particle motions being in collisions with other particles (wall)

$$\begin{cases} m_{p_k}\ddot{\mathbf{x}}_{p_k} = \sum_{j(k),j(k)\neq k} \left(\mathbf{P}^{rep}_{j(k)} + \mathbf{P}^{att}_{j(k)}\right) + \sum_l \mathbf{F}_{p_l} \\ \mathcal{I}_{p_k}\dot{\boldsymbol{\omega}}_{p_k} = \sum_{j(k),j(k)\neq k} \left(\mathbf{M}^{rep}_{j(k)} + \mathbf{M}^{att}_{j(k)}\right) + \sum_l \mathbf{M}_{p_l} \end{cases}$$

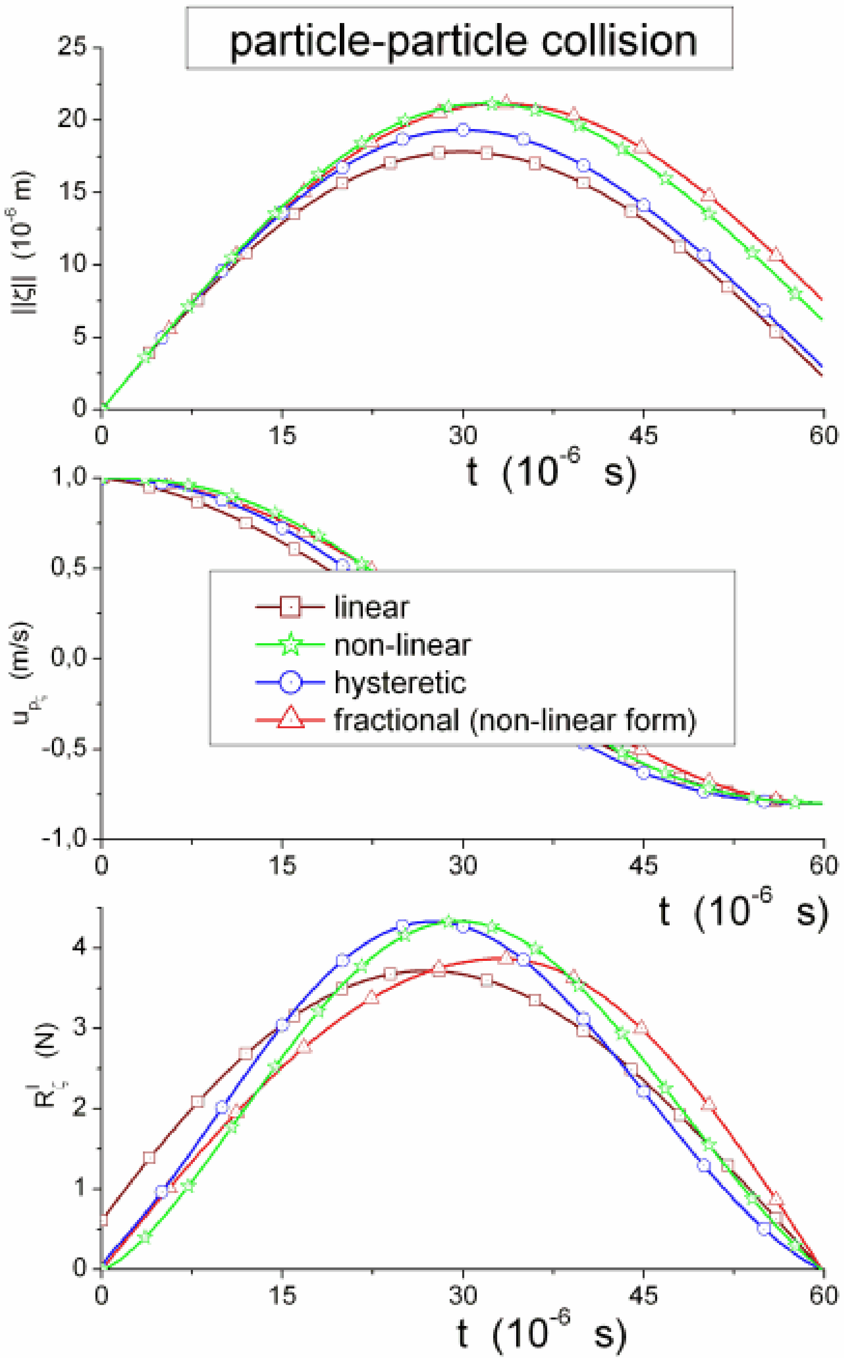
$\mathbf{P}^{rep}_{j(k)}$ - collisional force (repulsive force acting during collision)

$\mathbf{M}^{rep}_{j(k)}$ - collisional torque (acting during collision)

$\mathbf{P}^{att}_{j(k)}$ - attractive force (i.e. van der Waals force, liquid bridge force, etc.)

$\mathbf{M}^{att}_{j(k)}$ - attractive torque (arise from attractive force)

Comparison model-model



Full characteristics of particle-particle collision for assumed

t^{coll}=5,98·10^{-5} s, e_r=0,8.

Granular material: glass $\rho_{p1}=\rho_{p2}=2700\,\frac{\mathrm{kg}}{\mathrm{m}^3};\ r_{p1}=r_{p2}=0{,}0025\,\mathrm{m};\ u_{p\zeta}^{imp}=1\,\frac{\mathrm{m}}{\mathrm{s}}$	
Model of the repulsive force	Coefficients
linear	$k=206221{,}61\,\frac{\mathrm{kg}}{\mathrm{s}^2};\ c=0{,}608\,\frac{\mathrm{kg}}{\mathrm{s}}$
non-linear	$\tilde{k}=5{,}028\cdot10^{7}\,\frac{\mathrm{kg}}{\mathrm{s}^2\sqrt{\mathrm{m}}};\ \tilde{c}=191{,}021\,\frac{\mathrm{kg}}{\mathrm{s}\sqrt{\mathrm{m}}}$
hysteretic	$k=182932{,}79\,\frac{\mathrm{kg}}{\mathrm{s}^2};\ k^*=285832{,}48\,\frac{\mathrm{kg}}{\mathrm{s}^2}$ $\zeta^*=7{,}52\cdot10^{-6}\,\mathrm{m}$
fractional (non-linear form)	$\tilde{k}=5{,}028\cdot10^{7}\,\frac{\mathrm{kg}}{\mathrm{s}^2\sqrt{\mathrm{m}}};\ \tilde{c}=416{,}152\,\frac{\mathrm{kg}}{\mathrm{s}\sqrt{\mathrm{m}}}$ $\alpha=0{,}103$

Measure of impact energy dissipation over the number of particle contacts

$$\varepsilon = 1 - \left(e_r^{eff}\right)^2 = 1 - \left(\frac{\sqrt{\sum_{k=1}^{nc_p} \left(u^a_{p\zeta_k}\right)^2}}{\sqrt{nc_p}\left|u^{imp}_{p\zeta}\right|} \right)^2$$

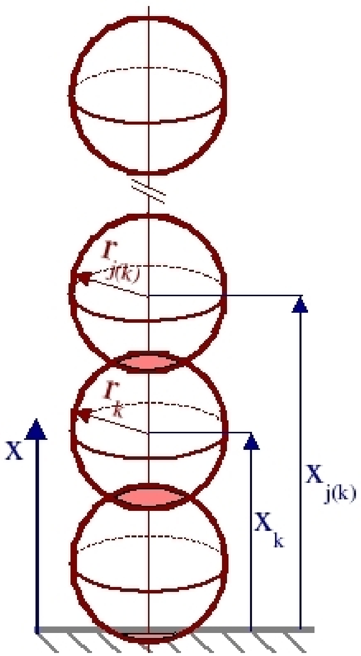
nc_p - number of particle contacts

$u^{imp}_{p\zeta}$ - velocity component of particle impact

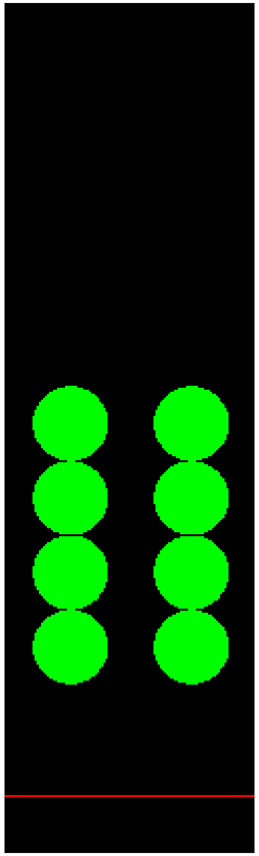
$u^{a}_{p\zeta}$ - velocity component of particle rebound

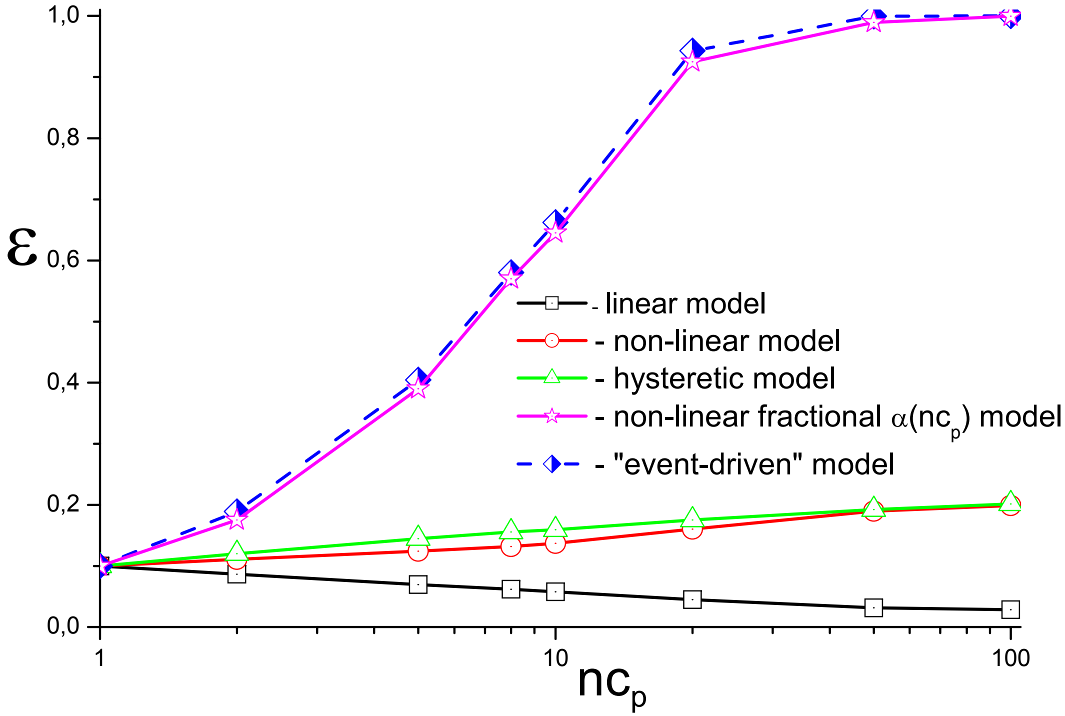
$r_p = 0{,}0015\ \mathrm{m};\quad m_p = 1{,}414 \cdot 10^{-5}\ \mathrm{kg};\quad u^{imp}_{p\zeta} = -0{,}5\ \frac{\mathrm{m}}{\mathrm{s}}$

we estimate $\alpha \sim 1 + e^{-nc_p}$ for fractional law



bottom plate





Comparison in global scale

Scheme of a container with notations and the distribution of particle sizes of a granular material used for simulations

COLUMN PARAMETERS

material: plexi $(E = 3 \cdot 10^9 \ \text{Pa};\ \nu = 0.35)$ $H_1 = 0{,}0425\,\text{m};\ H_{21} = 0.0425\,\text{m};$

$H_{22} = H_{12} = 0.073\,\text{m};\ H_{31} = 0.299\,\text{m};\ H_{32} = 0.399\,\text{m}$

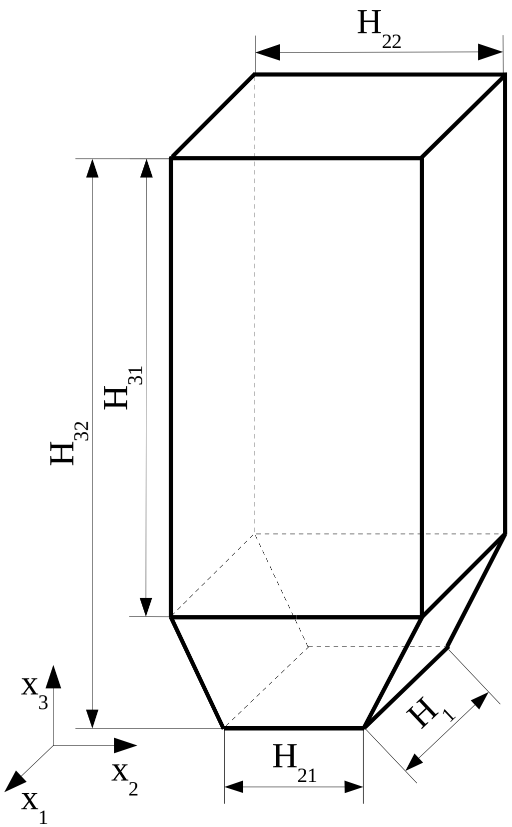
GAS PARAMETERS

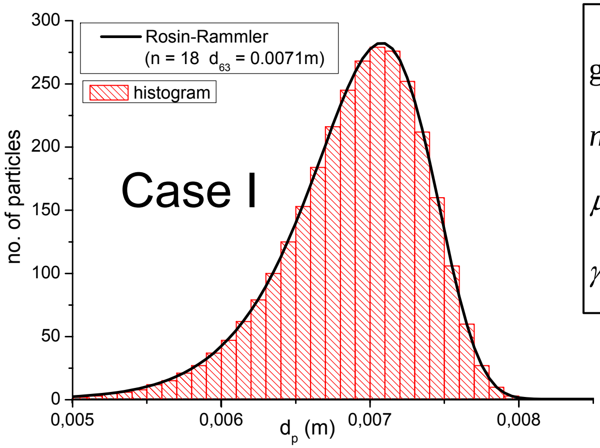
air; $\rho_g = 1.205\,\dfrac{\text{kg}}{\text{m}^3};\ \mu_g = 1.708 \cdot 10^{-5}\,\dfrac{\text{kg}}{\text{s}^2\text{m}};\ \bar{u}_{g\,x_3} = 0.0\,\dfrac{\text{m}}{\text{s}}$

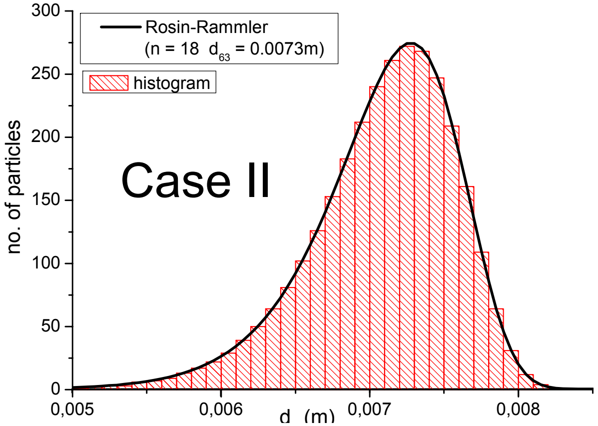
PARAMETERS FOR CALCULATIONS

cell dimensions: $\Delta x_1 = 0{,}0073\,\text{m};\ \Delta x_2 = 0{,}0073\,\text{m};\ \Delta x_3 = 0{,}00798\,\text{m}$

time step for calculations: $\Delta t = 2 \cdot 10^{-5}\,\text{s}$







PARAMETERS OF PARTICLES

granular material: pea

$n_p = \{3000, 4000\};\ \rho_p = 1300\,\dfrac{\text{kg}}{\text{m}^3};\ E = 4 \cdot 10^6\ \text{Pa};\ \nu = 0.2$

$\mu_{st} = 0.05;\ \mu_{dy} = 0.01$

$\gamma = 0.0725\,\dfrac{\text{J}}{\text{m}^2};$ water content $= \{0, 10, 20\}\,\%$

Comparison in global scale

Discharging of a container from dry pea particles

3000 dry particles

experiment

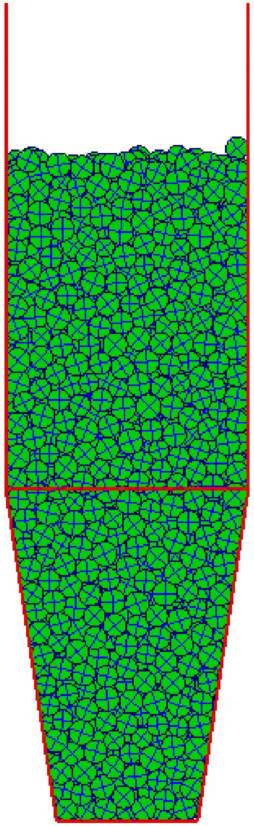
H_{bed}=21.0 cm

$T_{discharge}$=0.88 s±0.04

simulations

Case I

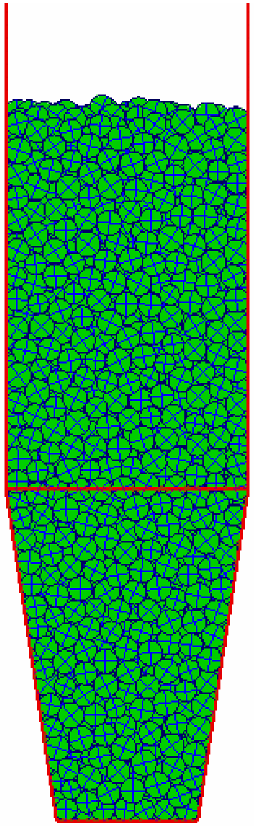
H_{bed}=20.5 cm



$T_{discharge}$= 0.77 s

Case II

H_{bed}=21.5 cm



$T_{discharge}$= 0.84 s

4000 dry particles

experiment

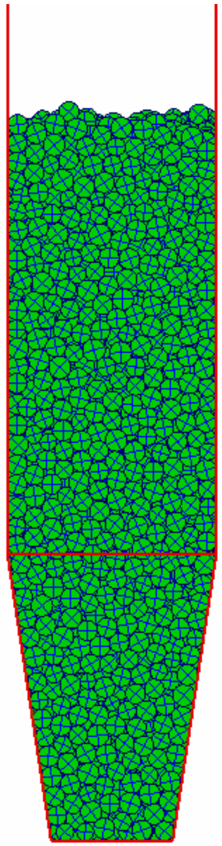
H_{bed}=26.8 cm

$T_{discharge}$=1.16 s ±0.04

simulations

Case I

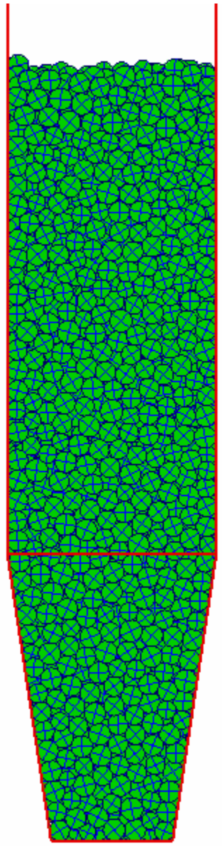
H_{bed}=25.8 cm



$T_{discharge}$= 1.01 s

Case II

H_{bed}=27.3 cm



$T_{discharge}$= 1.08 s

Discharging of a container from wet pea particles – 3000 particles

3000 wet particles

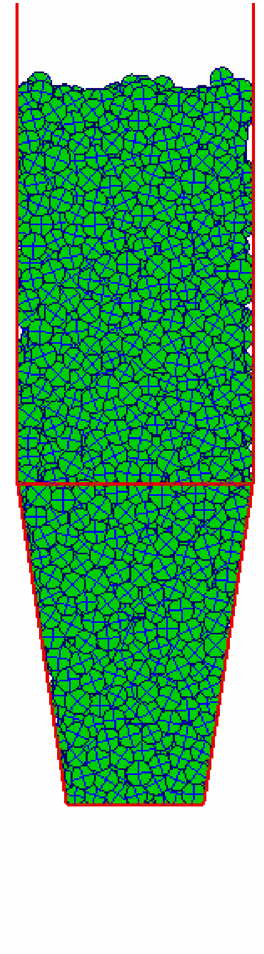
experiment

H_{bed}=23.0 cm

$T_{discharge}$=?

simulations

H_{bed}=22.5 cm



$T_{discharge}$=?

3000 wet particles

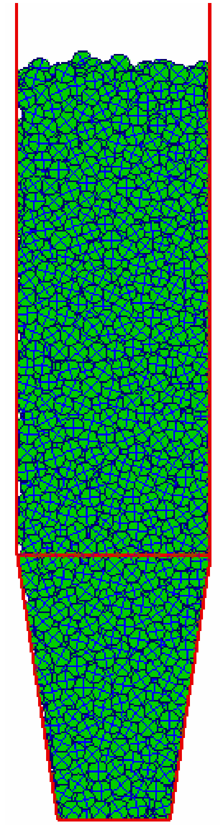
experiment

H_{bed}=31.0 cm

$T_{discharge}$=?

simulations

H_{bed}=29.2 cm

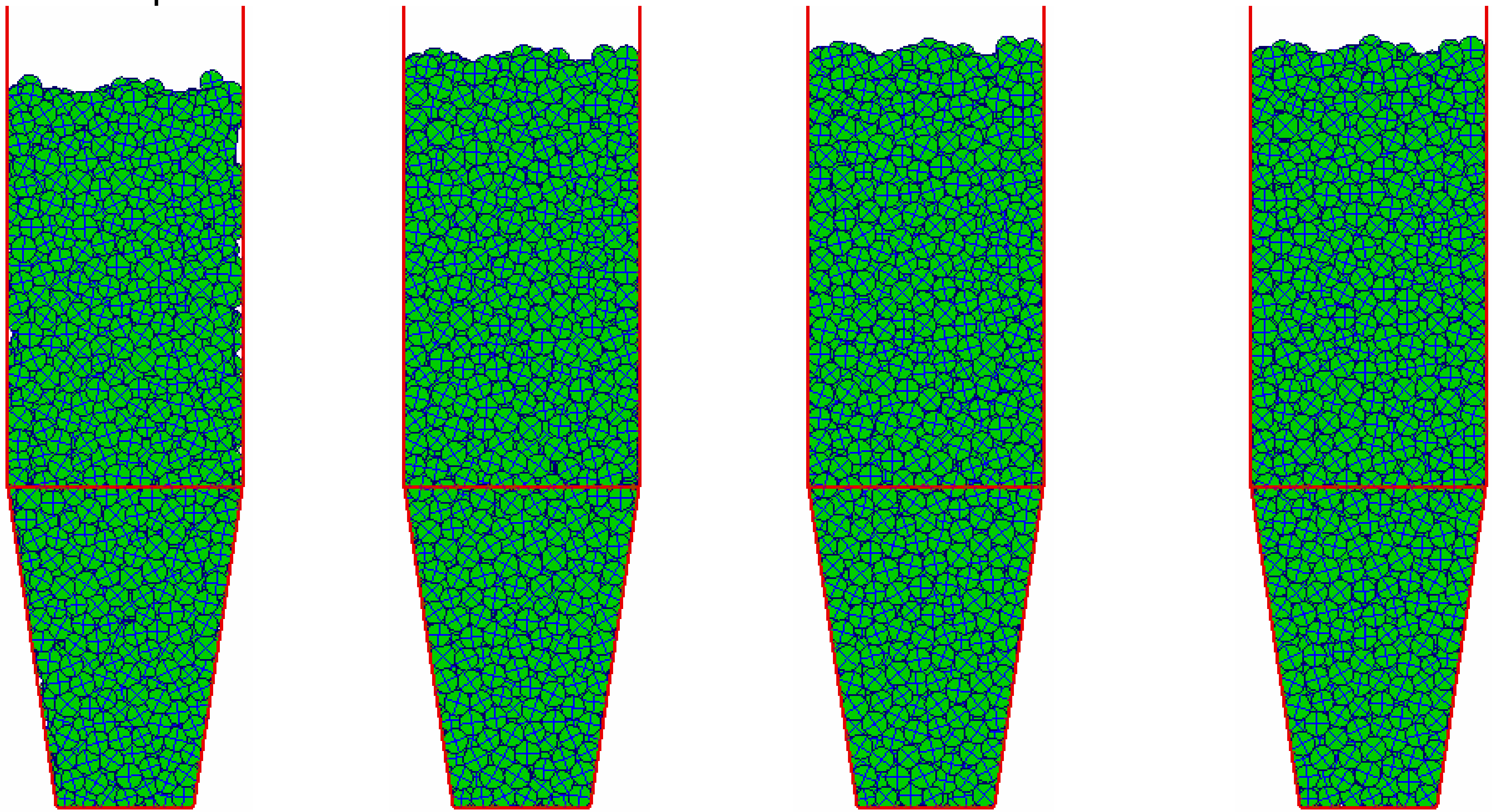


$T_{discharge}$=?

Simulations in global scale

An influence of the values of capilary forces for behavior of 3000 pea particles

H_{bed}=22.5 cm	H_{bed}=23.5 cm	H_{bed}=23.9 cm	H_{bed}=24.0 cm
The same as in the experiment	10 times smaller	50 times smaller	200 times smaller

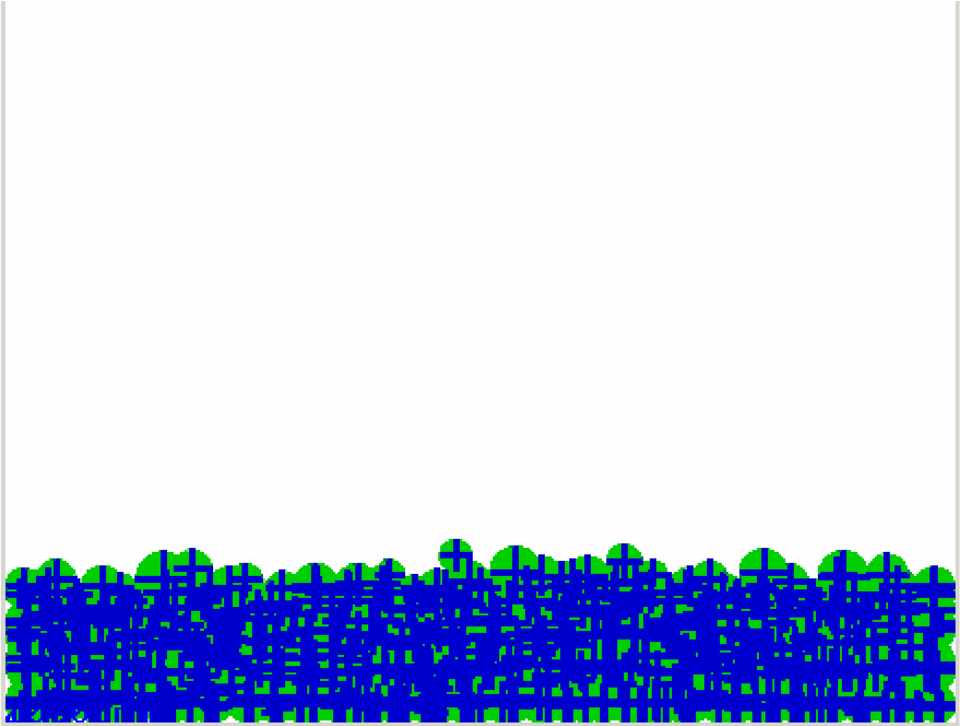


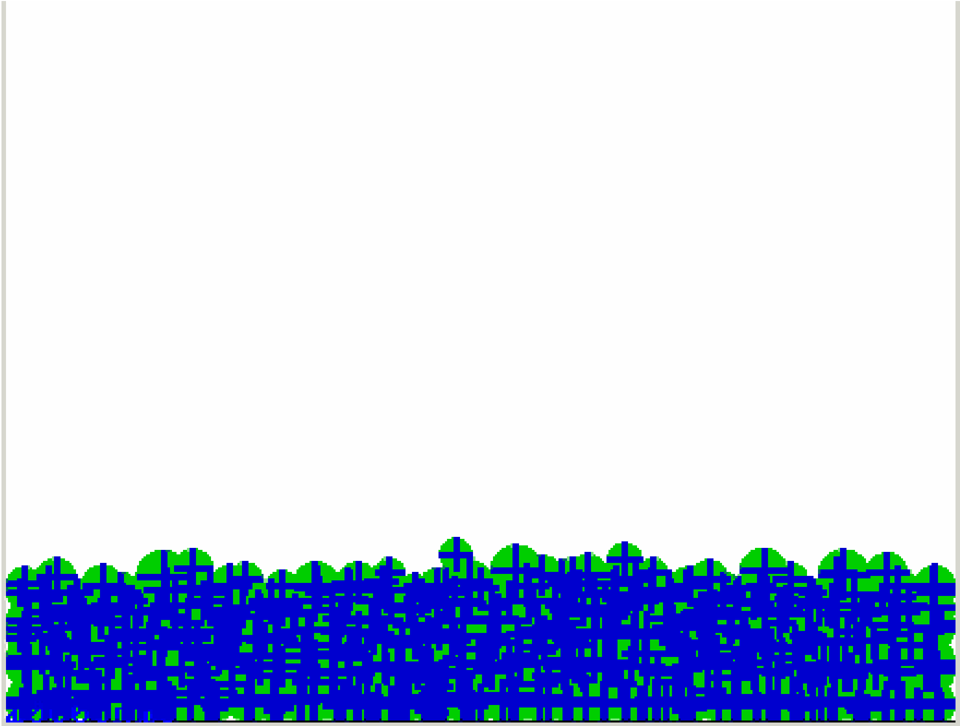
Granular dynamics of 5000 particles

Strong repulsive regime (α=0,1)

Without particle frictions: $\mu_{st} = \mu_{dy} = 0$

Particle frictions: $\mu_{st} = 0{,}3$; $\mu_{dy} = 0{,}1$

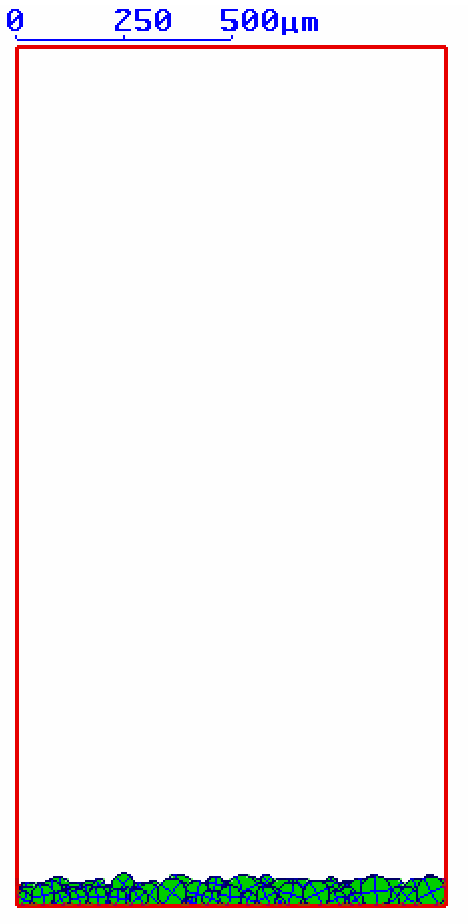




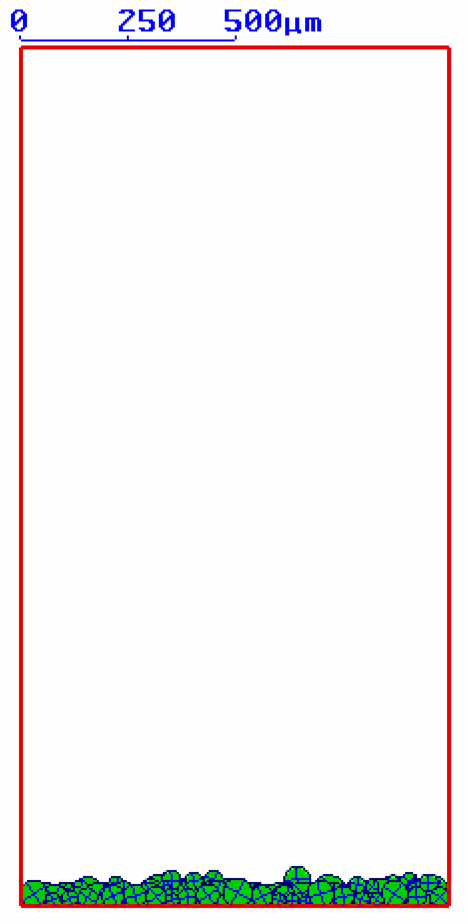
Particle elutrations from fluidised bed – 200 particles

ρ = 2500, E = $5*10^9$, ν = 0.28

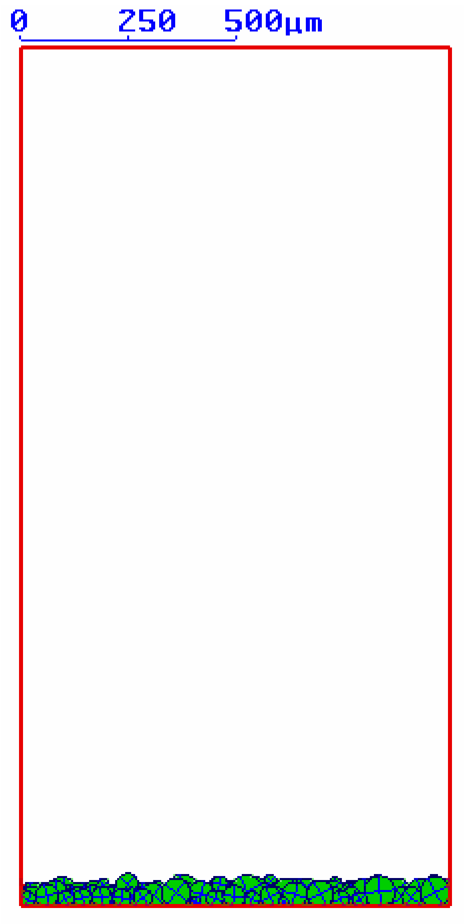
Without cohesion



Van der Waals cohesion



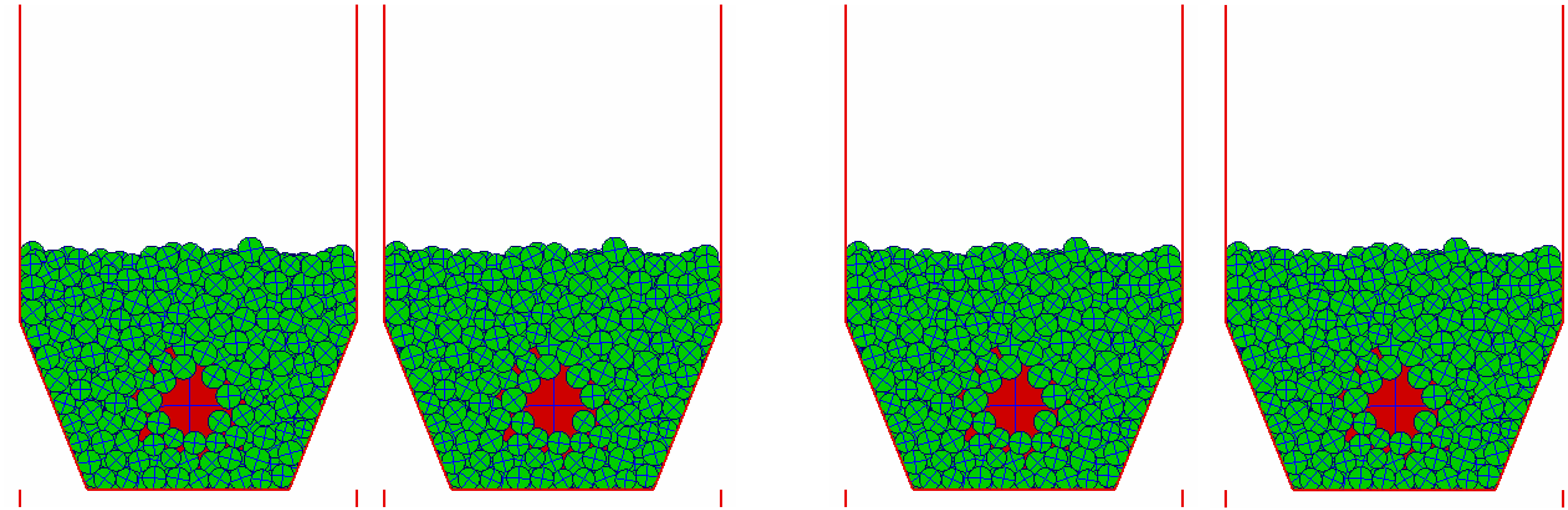
Van der Waals cohesion and capilary force



Mean value of air velocity at the bottom = 4 m/s

Simulations of „Brazil-nut effect „

without cohesion | Capilary force - 10% of moisture | without cohesion | Capilary force - 10% of moisture



$A=3*10^{-4}$ m
f=100 Hz

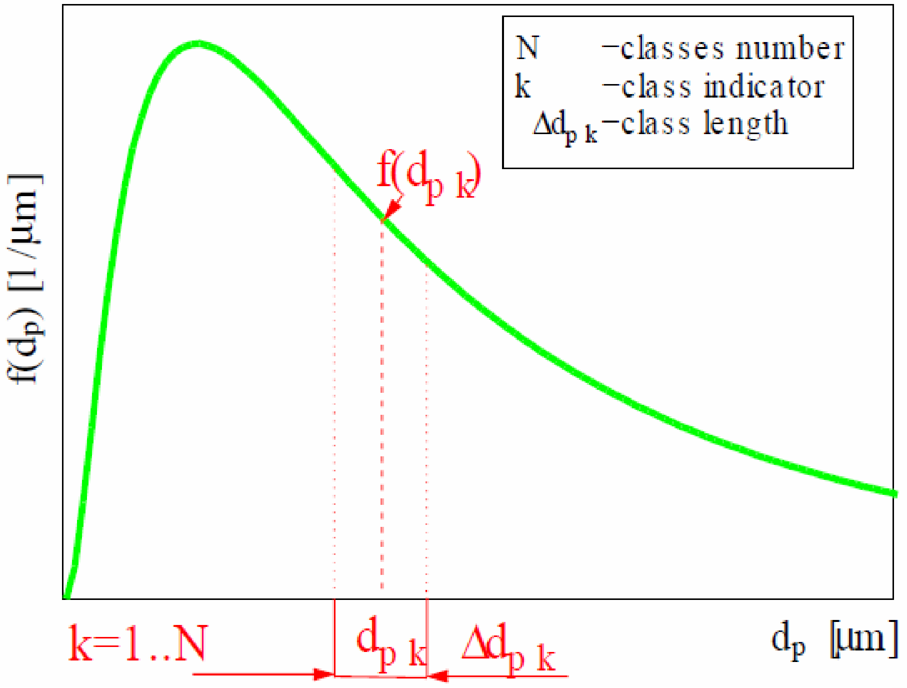
$A=4*10^{-4}$ m
f=100 Hz

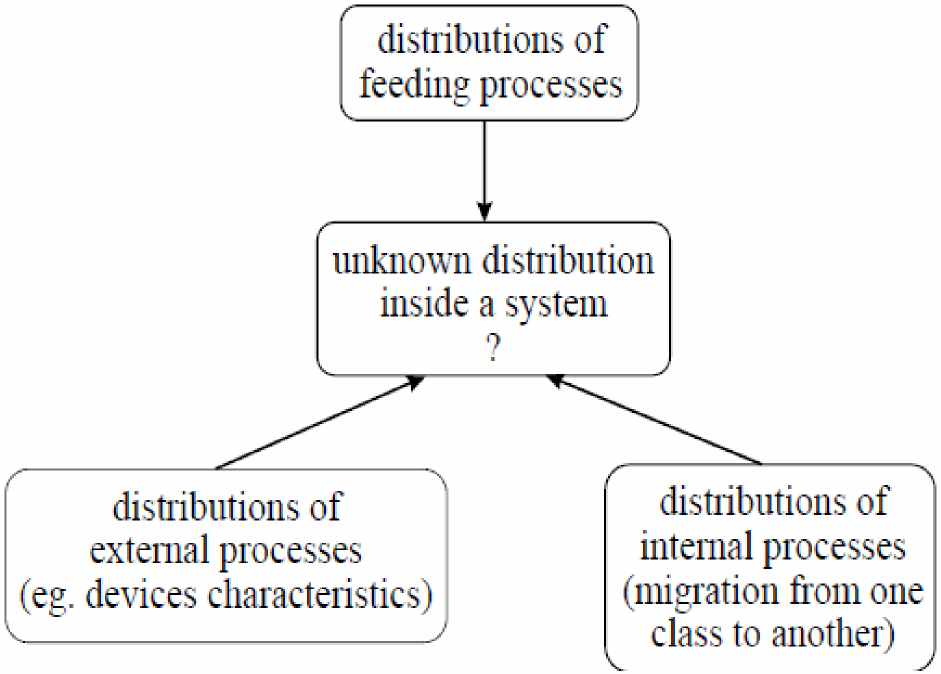
Hint: cohesion induced by capilary forces decreases „the Brazil-nut effect"

PART II:

Population balance

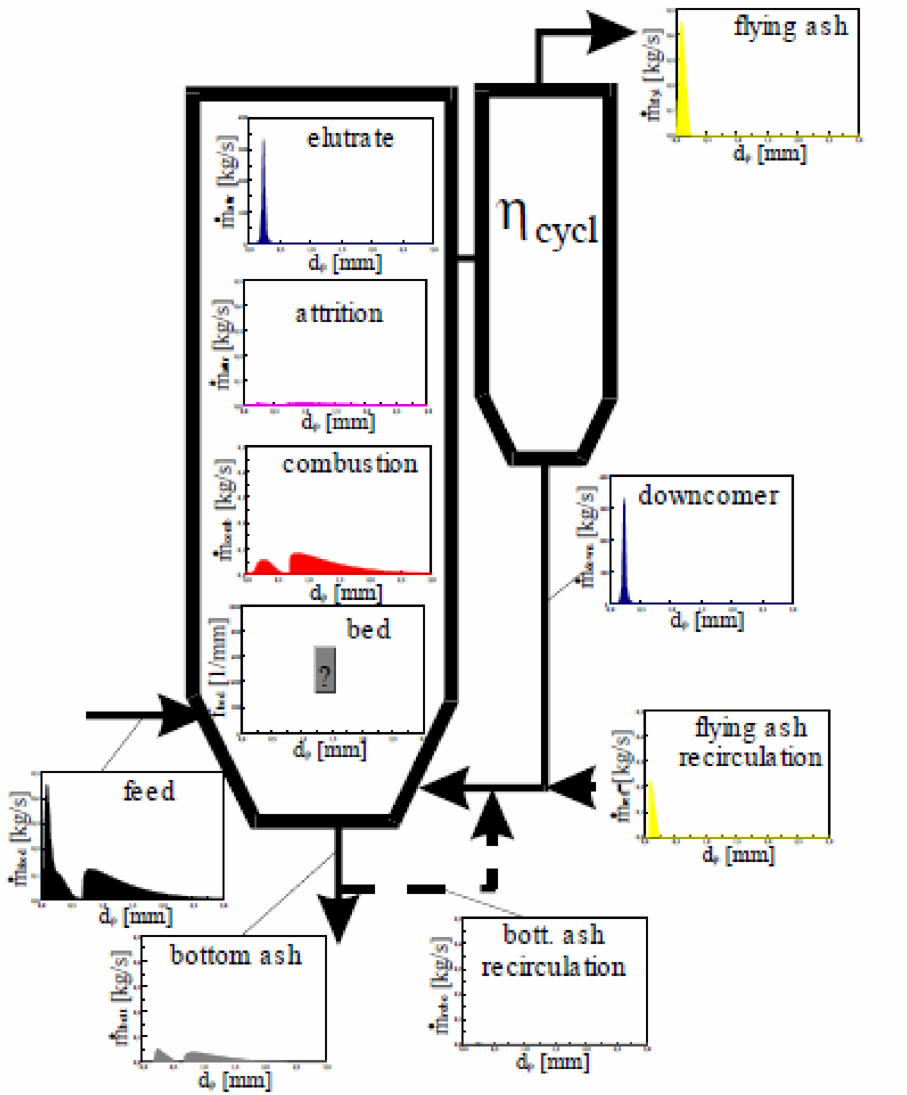
General idea of population balance[1]



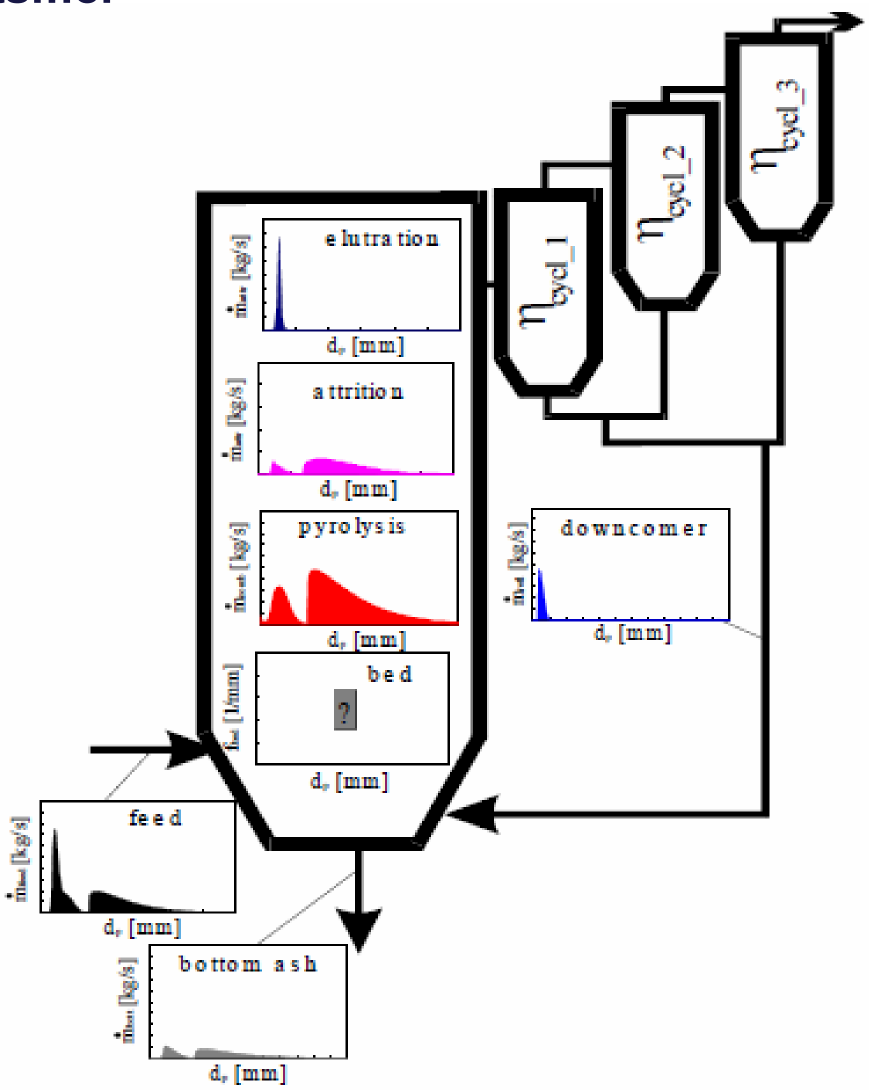


[1] Domański Z., Grzybowski A., Leszczyński J.S., Stationary regime modelling of industrial systems using granular materials, Proc. of the Fifth International Symposium and Exhibition on Environmental Contamination in Central and Eastern Europe, Prague, Czech Republic 2000, 7 pages (CD-ROM)

Topology of a circulating fluidized bed boiler[1]



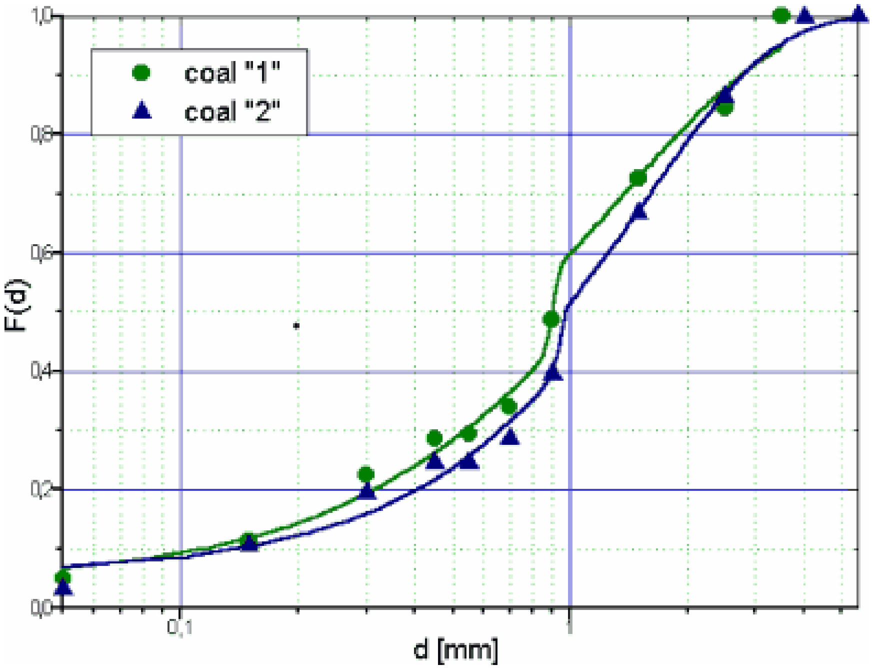
Topology of a circulating fluidized bed gasifier[1]



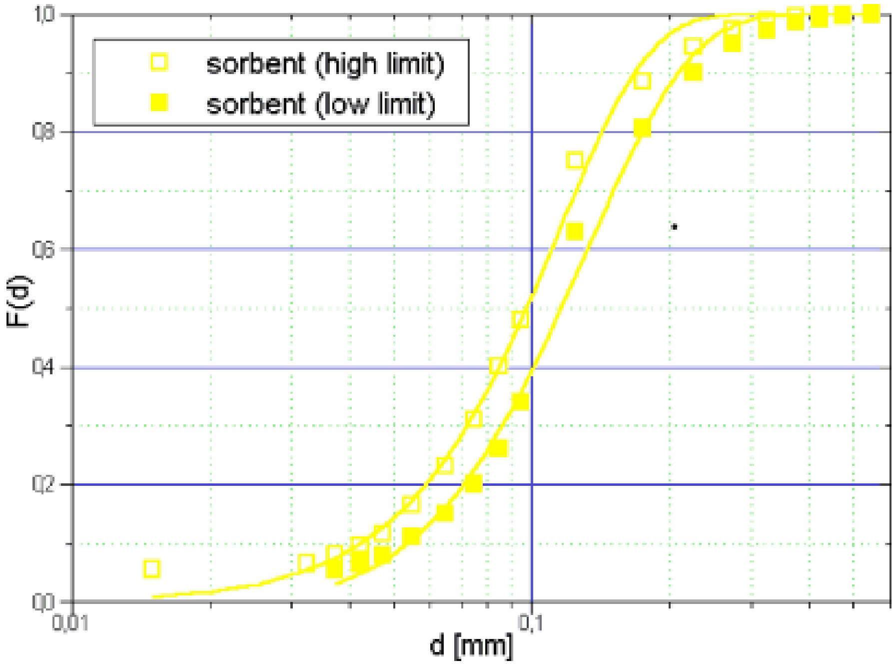
[1] Domański Z., Grzybowski A., Leszczyński J.S., Stationary regime modelling of industrial systems using granular materials, Proc. of the Fifth International Symposium and Exhibition on Environmental Contamination in Central and Eastern Europe, Prague, Czech Republic 2000, 7 pages (CD-ROM)

Granular materials feeding a combustion chamber[1]

Coal

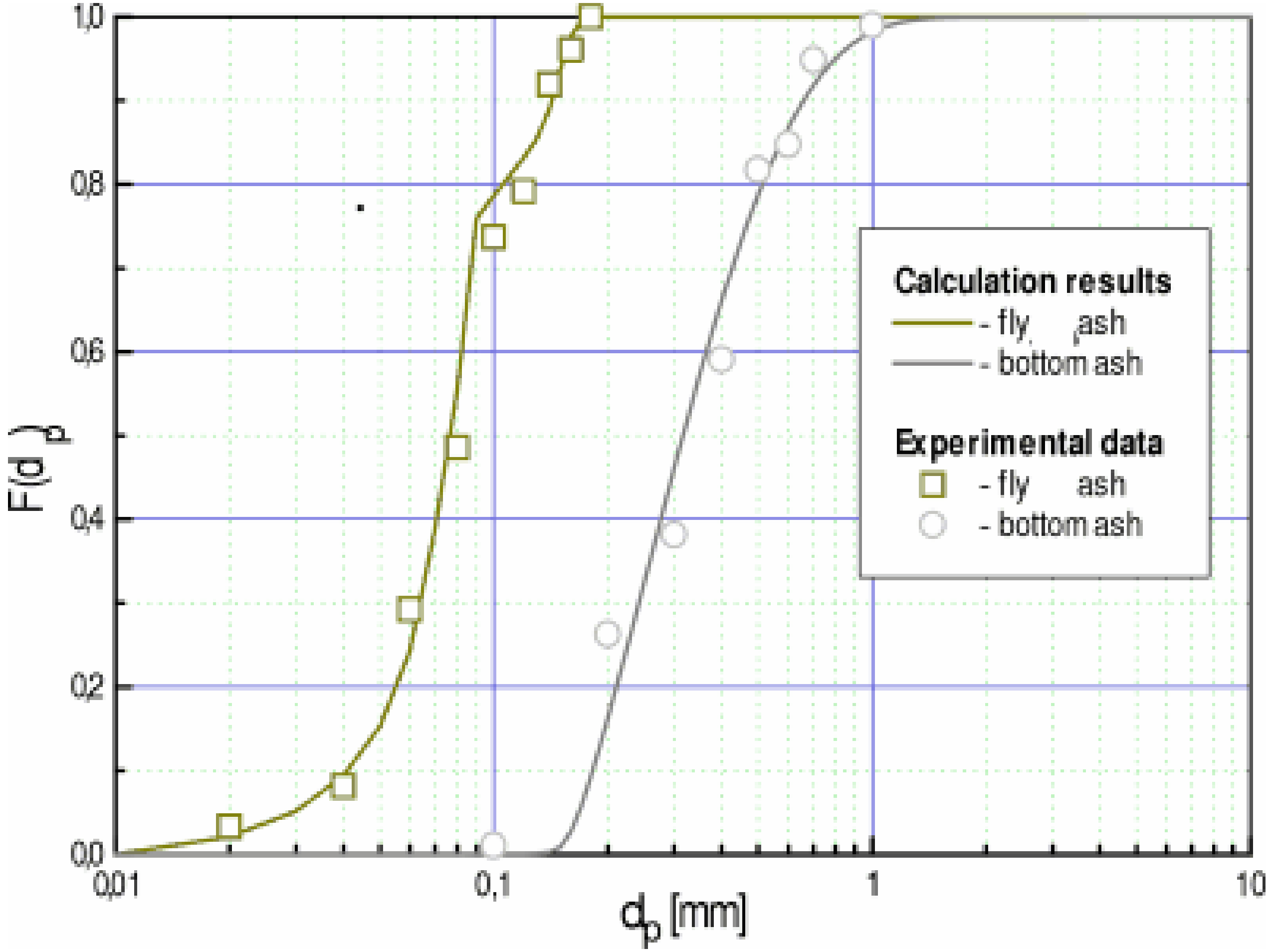


Limestone



[1] Kobyłecki R., Horio M., Bis Z., Leszczyński J.S., Nowak W., Analysis and optimization of solid particle distribution in the fluidized bed boiler OFz-450 in Zeran Power Station in Poland, Proceedings of the 4th SCEJ Symposium on Fluidization, Sapporo, Japan 1998, 302-309.

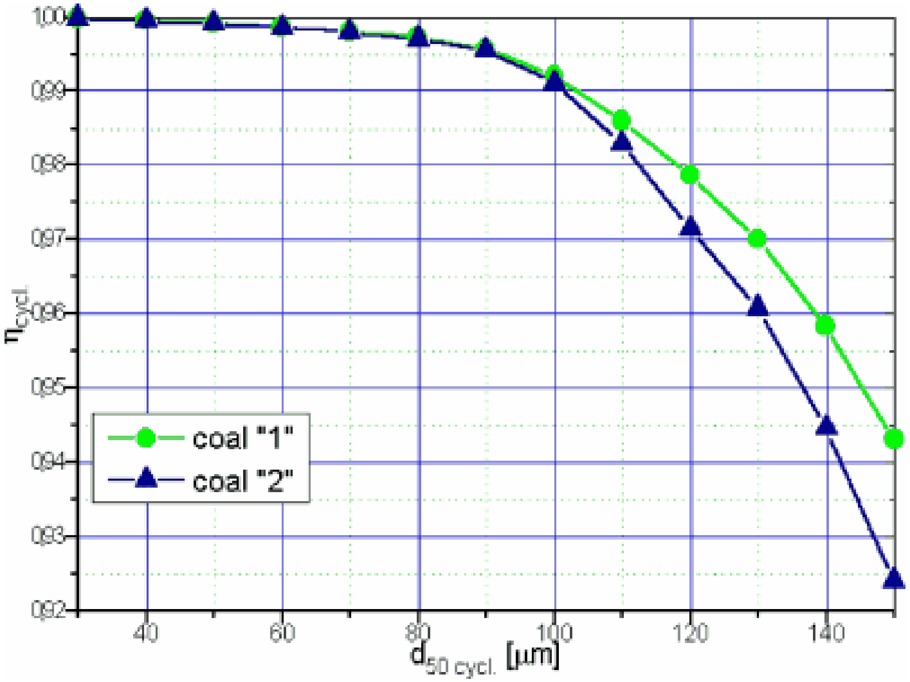
Comparison of cumulative distributions for fly and bottom ashes[1]



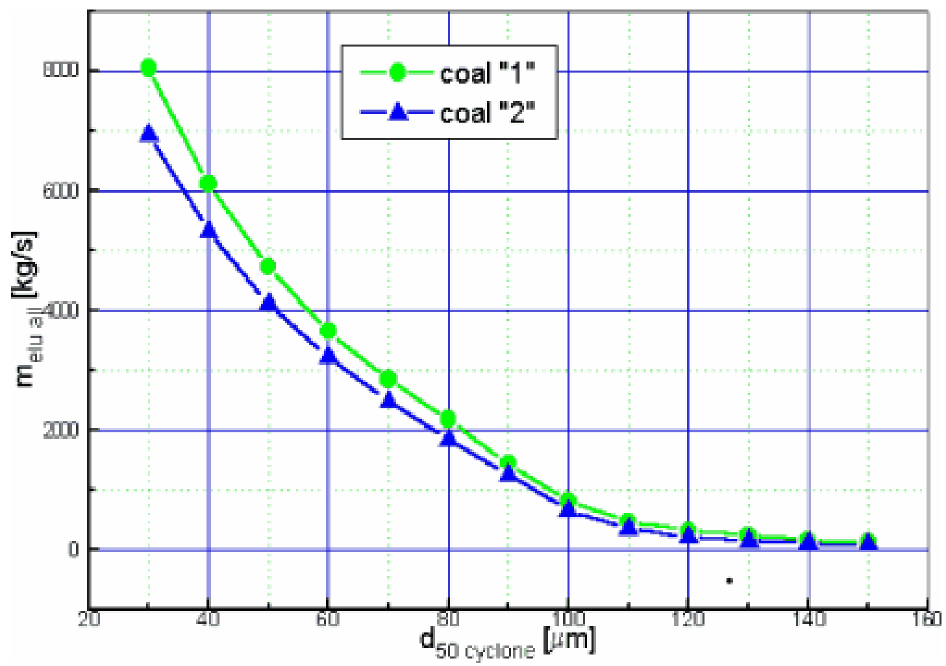
[1] Kobyłecki R., Horio M., Bis Z., Leszczyński J.S., Nowak W., Analysis and optimization of solid particle distribution in the fluidized bed boiler OFz-450 in Zeran Power Station in Poland, Proceedings of the 4th SCEJ Symposium on Fluidization, Sapporo, Japan 1998, 302-309.

Some sensibility study of the bolier[1]

Cyclone efficiency



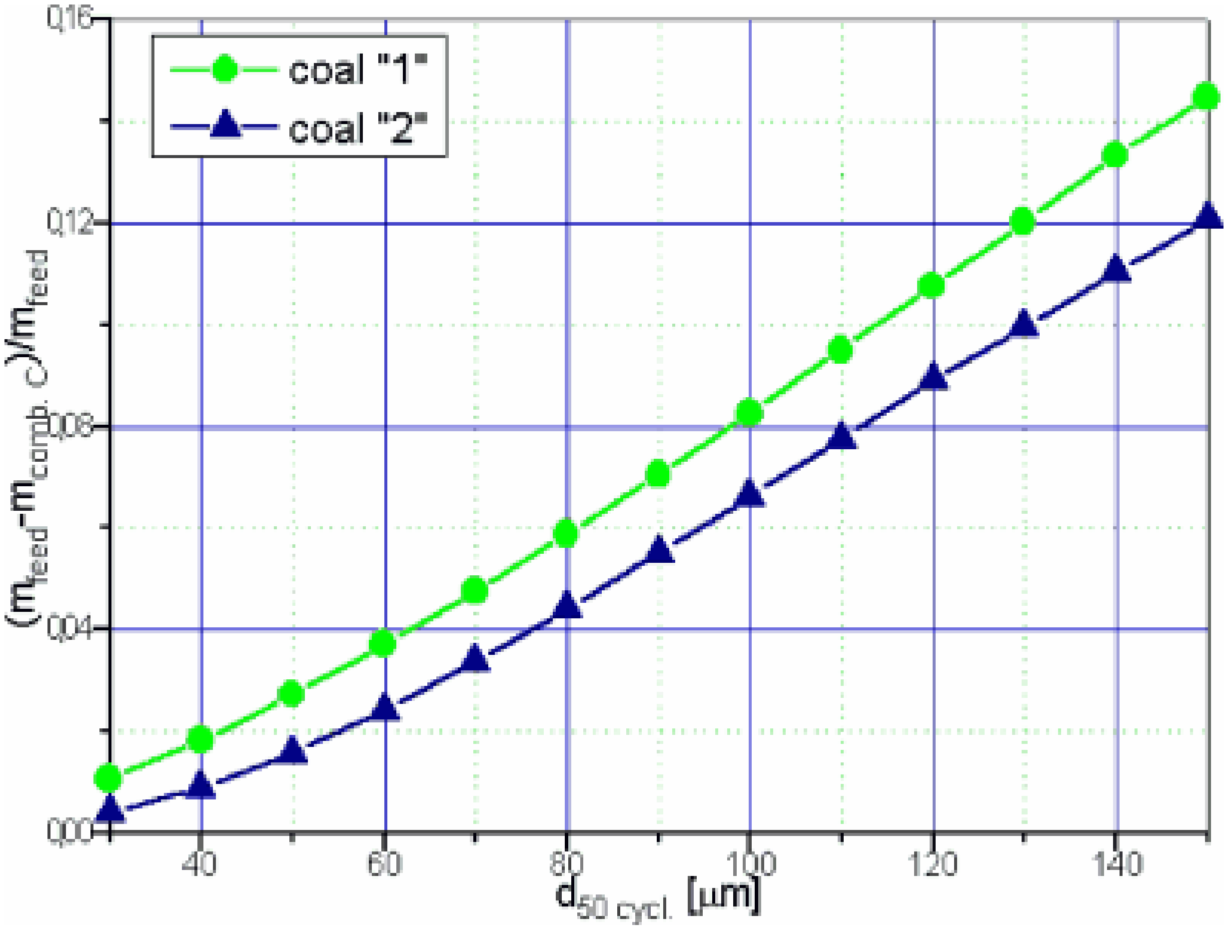
Mass flow elutrated from the bed



[1] Kobyłecki R., Horio M., Bis Z., Leszczyński J.S., Nowak W., Analysis and optimization of solid particle distribution in the fluidized bed boiler OFz-450 in Zeran Power Station in Poland, Proceedings of the 4th SCEJ Symposium on Fluidization, Sapporo, Japan 1998, 302-309.

Some sensibility study of the bolier[1]

Uncombusted coal particles vs. d_{50} of the cyclone



[1] Kobyłecki R., Horio M., Bis Z., Leszczyński J.S., Nowak W., Analysis and optimization of solid particle distribution in the fluidized bed boiler OFz-450 in Zeran Power Station in Poland, Proceedings of the 4th SCEJ Symposium on Fluidization, Sapporo, Japan 1998, 302-309.

PART III:

Fractional calculus

On some evolution of mathematical modeling

1. If our knowledge is limited to the theory of algebraic equations then we would solve only simple problems. We obtained only a simple class of mathematical solutions. This was the past.

2. If we know the integro-differential calculus, of course the ordinary order, then we can build mathematical models of many dynamical processes with some degree of their complexity. We obtained a complex class of mathematical solutions where the previous simple class is included. This is the past and the presents.

3. If we will extend the integro-differential calculus to fractional one – the calculus where the order of an integral or differential operator is real (comlex) then we will model hyper-complex dynamical processes as: multiscale phenomena, processes with memory or history, etc. In my opinion this is the future.

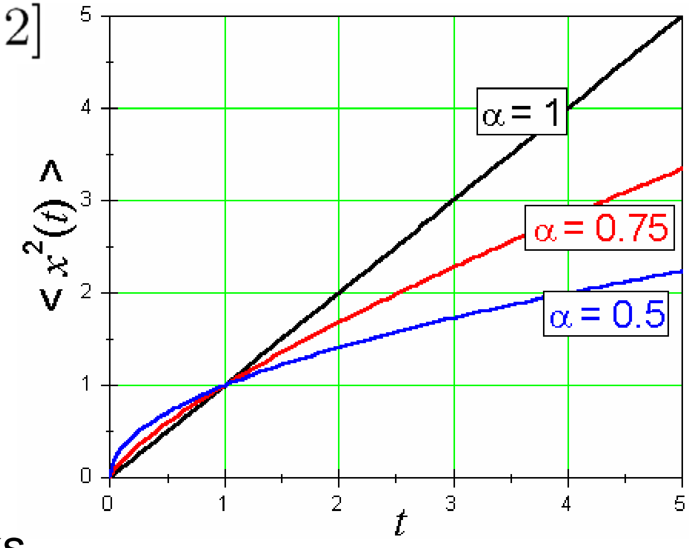
Continuous approach – partial fractional differential equations

We start from anomalous diffusion[1]

Anomalous diffusion is a phenomenon which is strongly observed in complex and non-homogenous systems.

- Classical diffusion $\langle x^2(t) \rangle \sim k_1 t$
- Anomalous diffusion $\langle x^2(t) \rangle \sim k_\gamma t^\gamma \quad \gamma \in (0, 2]$
  - subdiffusion $0 < \gamma < 1$
  - superdiffusion $1 < \gamma < 2$

or $\langle x^2(t) \rangle \to \infty$ Lévy's flights



One observes anomalous diffusion in:

- gas flows inside porous materials
- water diffusion in biological tissues
- molecular dynamics inside some polymer networks
- eddy flows
- ... and many others

[1] R. Metzler, J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Physics Reports **339**, 2000, 1-77.

Equations connected with anomalous diffusion[1]

- temporal fractional derivative $\beta = (0,2]$

$$\frac{\partial^\beta}{\partial t^\beta} C(x,t) = K_{2,\beta} \frac{\partial^2}{\partial x^2} C(x,t)$$

- spatial fractional derivative $\alpha = (0,2]$

$$\frac{\partial}{\partial t} C(x,t) = K_{\alpha,1} \frac{\partial^\alpha}{\partial |x|_\theta^\alpha} C(x,t)$$

- Generalized anomalous diffusion equation

$$\frac{\partial^\beta}{\partial t^\beta} C(x,t) = K_{\alpha,\beta} \frac{\partial^\alpha}{\partial |x|_\theta^\alpha} C(x,t)$$

$$t \geq 0, \quad x \in \mathbb{R},$$

where $C(x,t)$ is a well-known function (i.e. scalar field of particle concentrations, etc.), $K_{\alpha,\beta}$ is the coefficient of anomalous diffusion $[m^\alpha/s^\beta]$

[1] R. Metzler, J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Physics Reports **339**, 2000, 1-77.

Continuous approach – partial fractional differential equations

Mathematical forms of fractional derivatives[1]

- temporal fractional derivative defined in the Caputo form (for the function $\phi(t)$)

$$\frac{\partial^{\beta}}{\partial t^{\beta}}\phi(t) = {}_{0}^{C}D_{t}^{\beta}\phi(t) = \begin{cases} \dfrac{1}{\Gamma(m-\beta)}\displaystyle\int_{0}^{t}\frac{\frac{d^{m}}{d\tau^{m}}\phi(\tau)}{(t-\tau)^{\beta-m+1}}d\tau & \text{dla } \beta \notin \mathbb{N} \\ \dfrac{d^{m}}{dt^{m}}\phi(t) & \text{dla } \beta \in \mathbb{N} \end{cases}$$

where $m \in \mathbb{N},\ m-1 < \beta \leq m$

- spatial fractional derivative defined in the Riesz-Feller form (for the function $\phi(x)$)

$$\frac{d^{\alpha}}{d|x|_{\theta}^{\alpha}}\phi(x) = D_{\theta}^{\alpha}\phi(x) = \begin{cases} -\left(c_{L}(\alpha,\theta)\cdot{}_{-\infty}D_{x}^{\alpha}\phi(x) + c_{P}(\alpha,\theta)\cdot{}_{x}D_{+\infty}^{\alpha}\phi(x)\right) & \text{dla } \alpha \neq 1 \\ -\cos\dfrac{\theta\pi}{2}\dfrac{d}{dx}H\phi(x) + \sin\dfrac{\theta\pi}{2}\dfrac{d}{dx}\phi(x) & \text{dla } \alpha = 1 \end{cases}$$

where

$$c_{L}(\alpha,\theta) = \frac{\sin\frac{(\alpha-\theta)\pi}{2}}{\sin(\alpha\pi)},\quad c_{P}(\alpha,\theta) = \frac{\sin\frac{(\alpha+\theta)\pi}{2}}{\sin(\alpha\pi)} \qquad |\theta| \leq \begin{cases} \alpha, & \text{dla } 0<\alpha<1 \\ 2-\alpha, & \text{dla } 1<\alpha\leq 2 \end{cases}$$

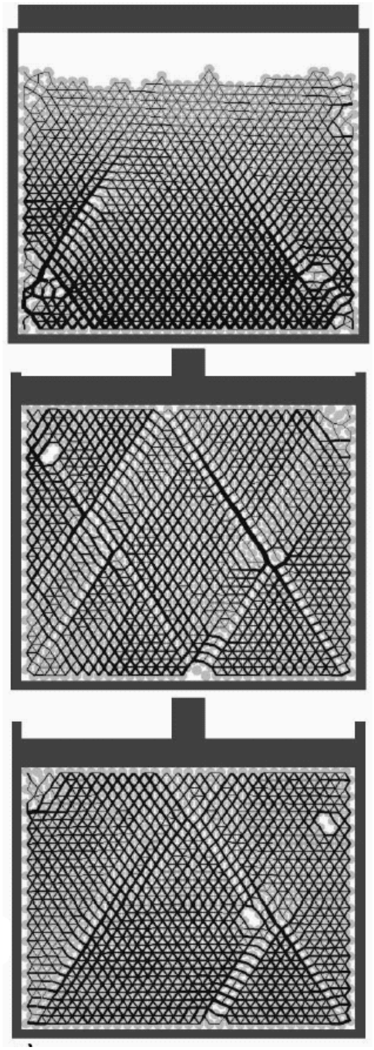
$$H\,\phi(x) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\phi(\xi)}{x-\xi}d\xi$$

[1] Samko S.G., Kilbas A.A., Marichev O.I., *Fractional Integrals and Derivatives. Theory and Applications*, Gordon and Breach, Amsterdam 1993.

Continuous approach – partial fractional differential equations

Comparison of numerical solution with experimental data[1,2]

Network of normal forces in particle-particle contacts under load

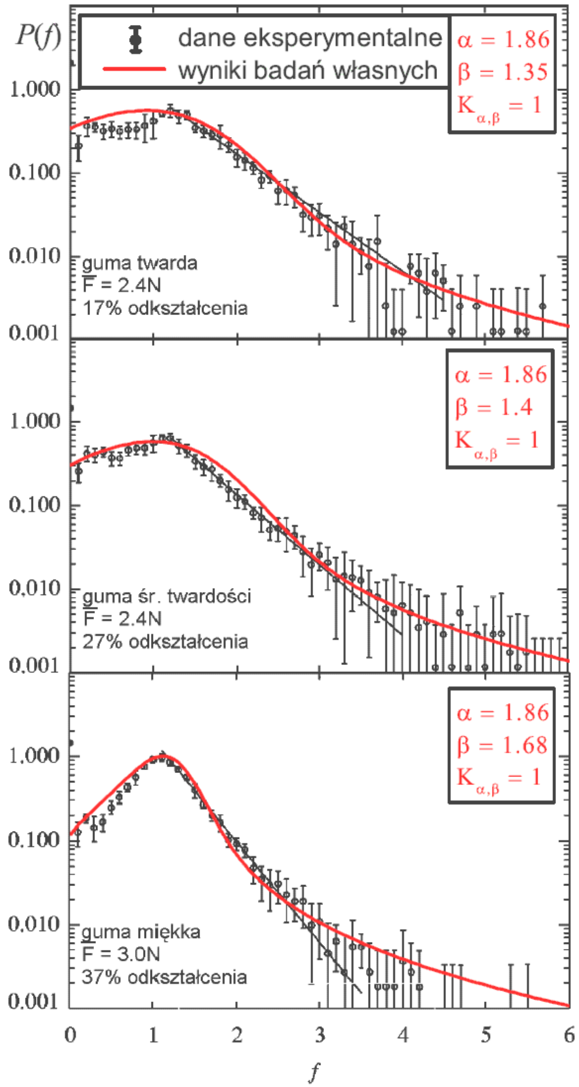


PDF of normalized inter-particle forces [1] – right side

$$\frac{\partial^\beta P}{\partial t^\beta} = K_{\alpha,\beta}\frac{\partial^\alpha P}{\partial |f|_\theta^\alpha}$$

$$P(f,0) = \delta(f)$$

$$f = F/\bar{F}$$



[1] Erikson J.M., Mueggenburg N.W., Jaeger H.M., Nagel S.R., Force distributions in three-dimensional compressible granular pack, Phys. Rev. E **66**, 2002, 040301.

[2] Ciesielski M., Fractional finite difference method applied for solution of anomalous diffusion equations with initial-boundary conditions, PhD thesis, Czestochowa University of Technology, Czestochowa, 2005.

Continuous approach – partial fractional differential equations

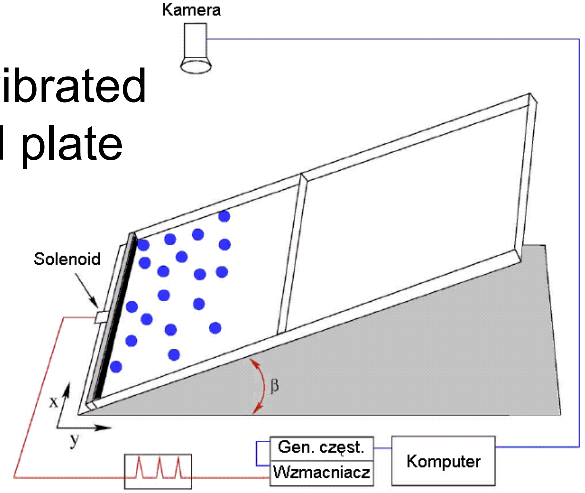
Comparison of numerical solution with experimental data[1,2]

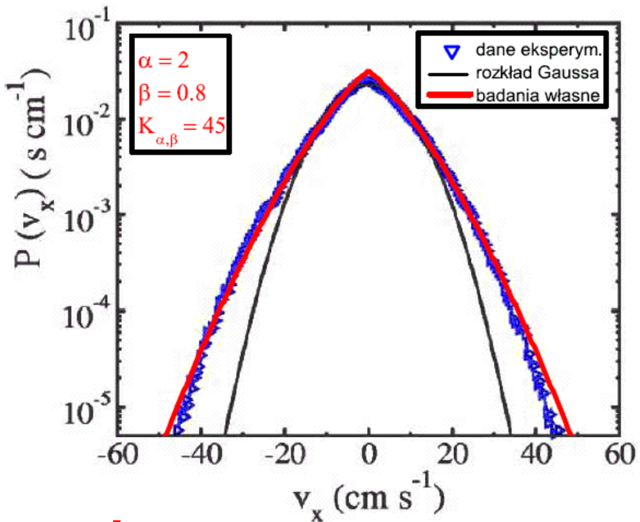
PDF of particle velocities registered in cross-section, according to Blair and Kudrolli [1]

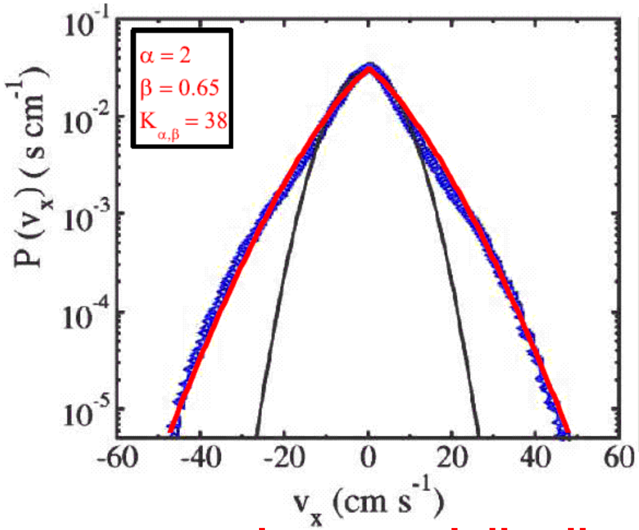
$$\frac{\partial^\beta}{\partial t^\beta} P(v_x, t) = K_{2,\beta} \frac{\partial^2}{\partial v_x^2} P(v_x, t)$$

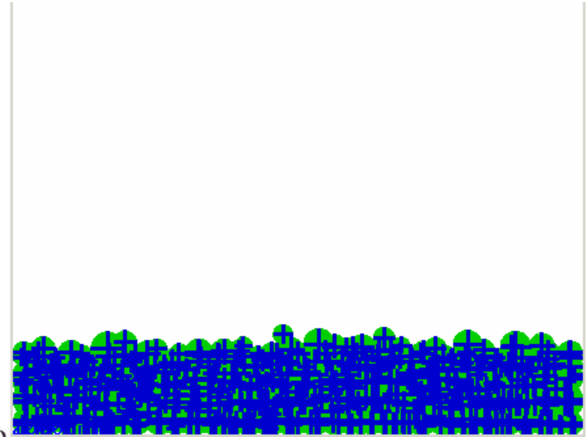
after t = 1s

Particles are vibrated on the inclined plate









Hint: ... but the kinetic theory assumes the normal distribution of particle velocities!

Kinetic theory = binary particle collisions, inter-particle frictions are neglected

[1] Blair D.L., Kudrolli A., Collision statistics of driven granular materials, Phys. Rev. E **67**, 2003, 041301.

[2] Ciesielski M., Fractional finite difference method applied for solution of anomalous diffusion equations with initial-boundary conditions, PhD thesis, Czestochowa University of Technology, Czestochowa, 2005.

Thank you