CD Lab - Particulate Flow Modelling

Quarterly report - VI - 2014

# Materials2Simulation2Application


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## 1.1 Jenike's Shear Cell tester

We have performed from 6 to 16 experiments per bulk material.

### 1.1.1 SCT simulation

The script has been modified to run on 32 cores over *Mach*. As of now each shear cell experiment is simulated approx. 250 times with different combinations of parameters. As can be seen in Fig. 1, a wall effect appears in the simulations, an the coefficient of internal friction decreases if the cell dimension grows. Since a bigger dimension means more particles and more computational demand, only a part of the simulations have been realized with a larger cell's diameter. The Neural Network, see section 3.2, will account also for this *wall* effect.

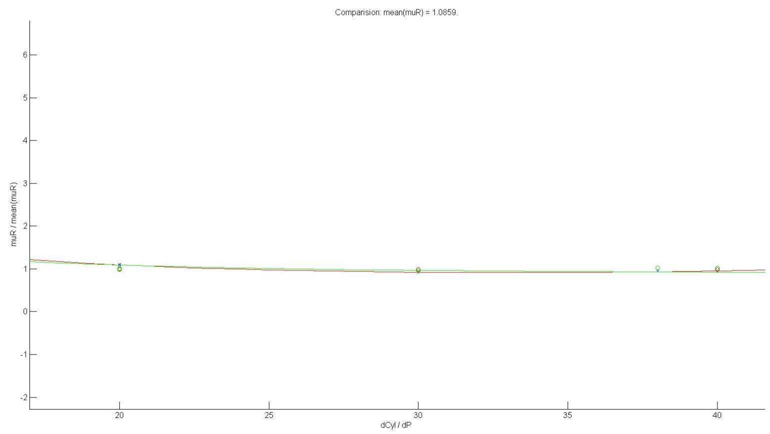


**Figure 1:** increased geometry effect

I received on the 10th of September this message from Mach: *qsub: Maximum number of jobs for group k3b02 already in queue std.q*, with 35 scripts in queue (of them 14 are running, occupying 512 cores), when I tried to add a new script to the queue. Now I have 18 scripts in queue (of them 7 are running, occupying 256 cores), but, since then, when I try to add a new script a receive the same error. Since I am yet the only one in the department using Mach, I will contact the Administrator ASAP.

## 1.2 Angle of Repose

For each bulk have been performed at least 2 experiments, of which the mean, median and variance values have been considered.

#### 1.2.1 AOR simulation

The script has been modified to run on 32 cores over *Mach*. As of now each material is simulated approx. 108 times with different combinations of parameters.

### 1.3 Granulometric curves

I have completed sieving of all materials (except from 0 to 1.25 mm iron ore) and I have for them:

- the granulometric curve;
- the mean radius (R);

### 1.4 COR characterization

A new system based on frequency has been suggested. I will start working on it ASAP.

### 1.5 Hollow spheres

This project will remain in stand-by until further notice.

### 1.6 Rolling drum

Both the experiment and the simulation manage to rotate the spheres at a given velocity. To identify the slope in the middle of the experimental drum have been suggested:

- to put a laser measurement system in the middle of the beam, that rotates together with the drum, but at least once per turn it registers correctly the slope's angle;
- an "unstable" system connected to a load cell: when in a steady-state the load on the cell will be 0, when in movement the load over the cell would allow to determine the mass of the "inclined" material;

To identify the slope in the middle of the numerical drum I will work with LIGGGHTS *compute crosssection*.

I will proceed and complete ASAP with the documentation for all these experiments.

## 2 CFDEM Characterization Workflow Coarse Particles

### 2.1 Pressure drop tester

I have completed the realization of a second pressure drop tester, with a diameter 50 % larger than the old one. The pressure drop registered is still not reliable, the main culprits should be leakages or a wrong void ratio.

### 2.1.1 Pressure drop tester simulation

The GUI of the simulation is up and running (thx Daniel Q). I have compared an old Nicolaus' experiment with both analytical and simulation in Fig. 2.

## 2.2 Venturi device

Initially conceived as an extension of the mass hopper flow tester, I am still stuck in the design phase and I am evaluating if dropping it completely.

# 3 Behavior Investigation

This is the third draft of what should be the main topic of my PhD Thesis. The **ToC** is developed accordingly and attached, at its end you can also find the **Bibliography** collected until now.

## 3.1 Investigation topcis

The scientific core of my PhD Thesis will investigate the following themes:

1. the influence of variations (distributions) of input parameters and poly-dispersity,

2. the possbility to extrapolate (e.g. given 3 different fraction distributions, with known behaviors, extrapolate the behavior of a fourth fraction distribution).

## 3.2 Micro - DEM parameters

The main micro parameters in a simulation are:

(A) the particle diameter distribution ($radii$ (R),%) (0.00025 - 0.05 $[m[$),

(B) the particle density ($\rho_p$) (2000-4000 $[kg/m^3]$),

(C) the Young modulus ($E$) (10 $[MPa]$),

(D) the Poisson ratio ($\nu$) (0.4 $[-]$),

(E) the coefficient of restitution ($e$) (0.1-1.0 $[-]$),

(F) the sliding friction ($sf$) (0.1-1.0 $[-]$),

(G) the rolling friction ($rf$) (0.1-1.0 $[-]$),

(H) the domain edge dimension ($D_{cyl}$), proportional to R (76, 100, 124 times bigger).

The parameter that drives the simulation time is $D_{cyl}$. The number of particles is cubically proportional to its size.
The simulations will be run with defined interval values.

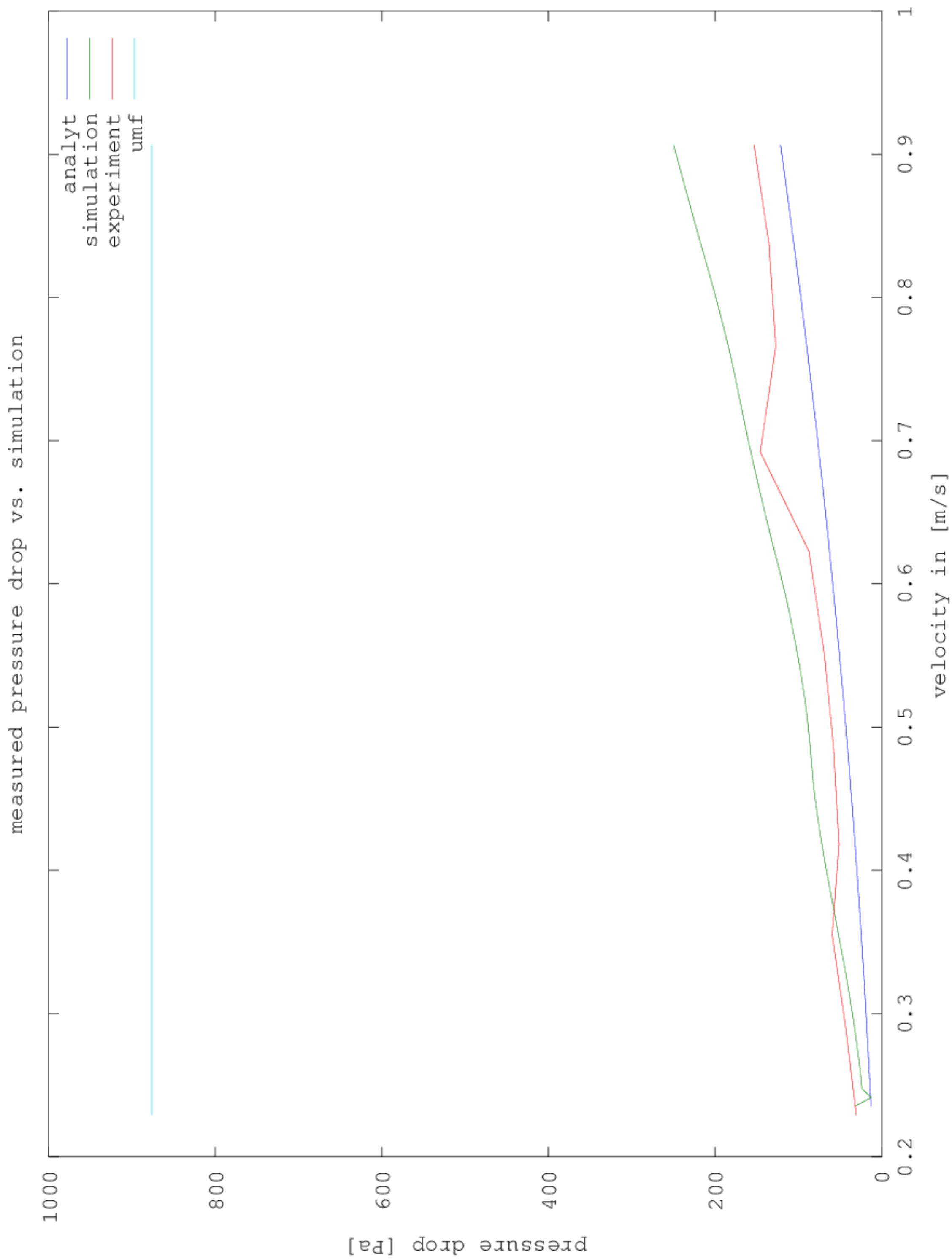


**Figure 2:** pressure drop: exp-an-sim: mono glass d2 h1300 v2 R02 xlsx 5

## 3.3 Macro - bulk parameters

The main macro parameters we experimentally determine for a bulk material are:

(a) the particle diameter distribution ($radii$) (0.00001 - 0.05 [$m$[),(%),

(b) the bulk density ($\rho_b$) (1000-3000 [$kg/m^3$]),

(c) the coefficient of restitution ($e$) (0.1-1.0 [$-$]),

(d) the internal friction angle in different loading and consolidation conditions ($\phi$) (25-50 [°]).

## 3.4 Defined intervals simulations

For the Angle of Repose simulation the individual contacts micro-DEM parameters will be:

- Sliding friction: from 0.05 to 1, 0.05 interval = 20 possibilities;
- Rolling friction: from 0.05 to 1, 0.05 interval = 20 possibilities;
- Coefficient of restitution: from 0.5 to 1, 0.1 interval = 6 possibilities;
- Particle density: e.g. from 2500 to 3500 $kg/m3$, 100 interval = 11 possibilities;
- (Particle to geometry ratio (p2g): 50, 100, 150 = 3 possibilities;)

$20 \cdot 20 \cdot 6 \cdot 11 \cdot 3 = 26400$ possible combinations of parameters. Each combination would require a simulation, each simulation requires 9 hours over 32 cores = 9900 days! All for only one material with a defined size distribution (e.g. from 3 to 10 mm)! We only consider p2g = 50, because otherwise with e.g. 100 the number of particles is 8 times higher, and so the time 8 times longer.

For the Shear cell simulation the individual contacts micro-DEM parameters will be the same of the AOR simulation, plus:

- Normal stress: 1, 2, 5, 10 kPa = 4 possibilities;
- Shear %: 40, 60, 80, 100% = 4 possibilities;

$20 \cdot 20 \cdot 6 \cdot 11 \cdot 4 \cdot 4 = 422400$ possible combinations of parameters. Each combination would require a simulation, each simulation requires 64 minutes over 32 cores = 18774 days! Again all for only one material with a defined size distribution (e.g. from 3 to 10 mm)!

## 3.5 Artificial neural network

Do we really need all these simulations? How to identify the effect (weight) of each parameter?
The representation of a multi-sphere experiment through a mathematical model presents numerous complexities. A different approach involves an artificial neural network, that can be realized to understand the relationship between the input and the output parameters. An artificial neural network is composed of many artificial neurons that are linked together according to a specific network architecture. The objective of the neural network is to transform the inputs into meaningful outputs. The inputs are:

1. *A*, from real data *a* but simplified,
2. *B,H*,
3. *C,D*, from literature,
4. *E*, from real data *e*,
5. *F,G*, the main calibration parameters,

The outputs are $b$, $f$ and $g$.
The idea would be to use a *feed forward Multilayer Perceptron Neural Network (MLPNN)*. A backpropagation reinforcement learning training algorithm has been used (scaled conjugate gradient).
A Neural Network (NN) has been created for each bulk parameter investigated ($\mu_{e,ps}$, $\mu_{e,s}$, $\rho_b$). This bulk parameters, or $target$, have been obtained by running a limited number of simulations (for each bulk), ≈ 600 for the shear cell and 81 for the angle of repose. Together with the corresponding inputs they have been used to train the networks.
15% of the simulations have been excluded from the training processes. They have been used to define per each NN the correct number of neurons in the hidden layer, based on an $R^2$ maximization. Now that the networks have been trained, we can feed the networks with all the combination we need and receive reliable macro-BULK parameters as response. Especially, we can increase the parameter that account for the geometry dimension, without paying completely the price for it.
The NN inputs will be defined interval values or random values.

### 3.5.1 Defined interval values

For the $defined\ interval\ values$ procedure each trained NN received as input the 422400 different combinations. Then we selected between them the valid $input - DEM - micro$ parameters combinations by fitting NN outputs to experimental data (within a 5% error). About 400 of them were selected. Next step will be to validate the DEM parameters by means of static angle-of-repose experiments and AOR simulations-trained NN (the 26400 combinations).

Let's say that between the 400 simulations remained, as hypothesis 20 of them are experimentally validated. At this point I should be able to *extrapolate the behavior of bulk with a volume too large to be simulated* with this complete neural network and to compare the results with the real scale experiments (Leoben).

The reliability of this work is deeply based on the already performed simulations: further numerical investigations as suggested in draft 1 could improve it.

### 3.5.2 Random values

For the $random\ values$ procedure each trained NN received as input the same as the $defined\ interval\ values$, except for the following:

- Sliding friction: from 0.05 to 1, 100 random numbers, and so 100 possibilities;

- Rolling friction: from 0.05 to 1, 100 random numbers, and so 100 possibilities;
- Coefficient of restitution: from 0.5 to 1, 50 random numbers, and so 50 possibilities;
- Particle density: e.g. from 2500 to 3500 $kg/m3$, 50 random numbers, and so 50 possibilities.

Together it makes 25 millions different combinations. Again we selected between them the valid $input - DEM - micro$ parameters combinations by fitting NN outputs to experimental data (within a 5% error). About 400 thousand of them were selected. From them we extracted of the *valid* input parameters the following values:

1. the minimum and the maximum,
2. the mean ($\mu$) and the standard deviation ($\sigma$),
3. the lines between $p_i$'s.

The lines connecting 1 and 2 can be seen in Fig. 3

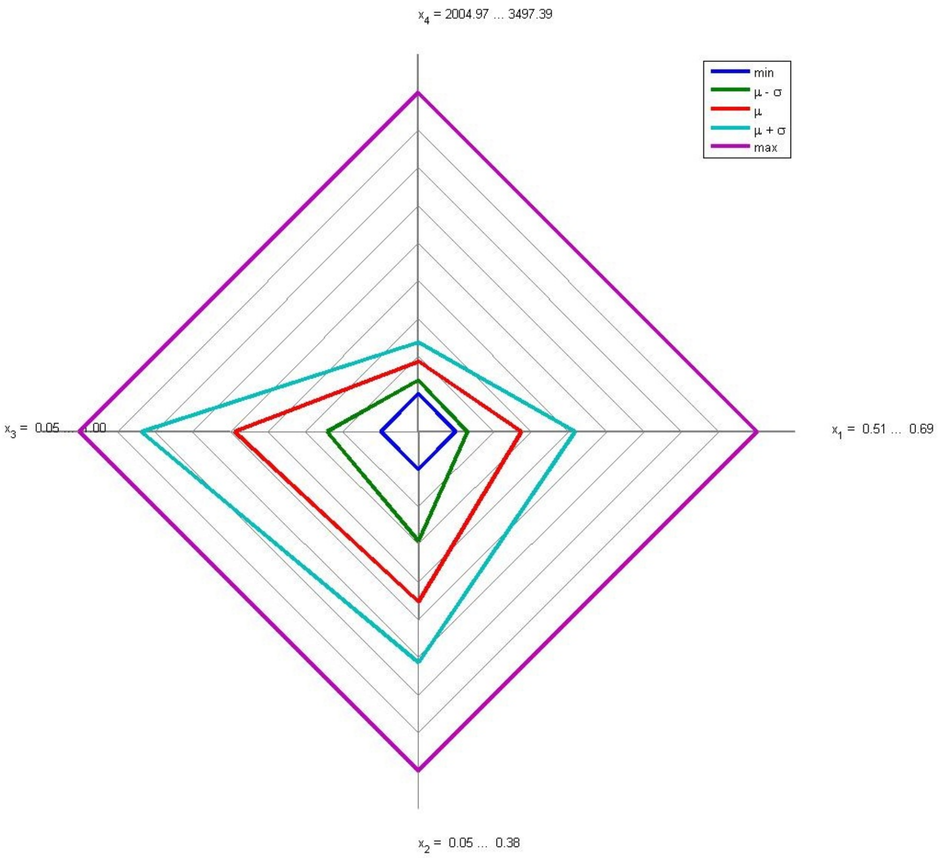


**Figure 3:** radar plot of random inputs: $X_1 = e$, $X_2 = sf$, $X_3 = rf$, $X_4 = \rho_p$

# 4 Elsevier Paper

I started to describe this NN work, together with the numerical *DEM* and the experiments in a paper for an Elsevier Journal (Powder Technology ?). You can find the abstract with the titles of the sections and the subsections, plus some random text for layout sampling, attached.