

Christian-Doppler Laboratory on Particulate Flow Modelling

CHRISTIAN-DOPPLER LABORATORY ON PARTICULATE FLOW MODELLING

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Front cover: Partial de-fluidisation in fluidised beds due to de-mixing of two particle classes: Large (black) particles form a packed bed just above the distributor plate; process gas channels to the upper part of the bubbling fluidised bed of small (gray) particles. Our hybrid simulation model is able to reproduce this critical behaviour. © S. Schneiderbauer & S. Puttinger

EDITORIAL

Dear Readers,

in 2013 our research group has experienced considerable growth for the fifth time in a row. By now we assemble a smooth mix of 26 postdocs, PhD-students and further scientific employees which are embedded into a new Department of Particulate Flow Modelling.

In the last year we received an excellent scientific evaluation by Professor Soldati from Udine, Italy. Furthermore, new mathematical models of our Dust 'n' Dirt group found their way into high impact journals triggering a collaboration with Princeton University. Our Rock 'n' Roll group, in turn, attracted two major European research projects. Finally, also our experimental group gained international visibility leading to joint research activities with Swedish colleagues.

In the upcoming year our research group will be challenged by transferring this scientific success to industrial application. Besides establishing a standardised simulation platform for industrial users, this requires joint efforts of mathematical and numerical modelling being substantiated by dedicated calibration experiments for simulation parameter identification and on plant measurements.

With these introducing words I wish you a pleasant reading!

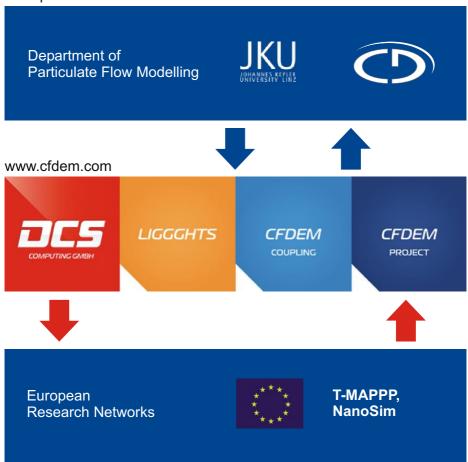
Sincerely,

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ORGANIGRAMM

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The new JKU Department of Particulate Flow Modelling, hosting the eponymous CD-Lab, represents the scientific base of CFDEMproject.

DCS Computing GmbH, guaranteeing for professional code development and consultancy, opened the door towards European research networks.

2013 | Particulate Flow Modelling

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ROCK 'N' ROLL

Dear Readers,

In 2013 the Rock 'n' Roll group has seen a phase of maturation. Our group with its expertise in model development for Discrete Element Method (DEM) and Computational Fluid Dynamics coupled to DEM (CFD-DEM) has achieved awareness and respect in industrial and academic communities. This resulted in several keynote lectures at international conferences, as well as invitations to joint research projects and development work at national and international level. While the previous years brought growth in group size and modelling diversity, this year the focus was on model applicability and validation:

The PhD thesis of **Luca Benvenuti**, which is dedicated to closing the gap between real material properties of granular media and its counterpart in the simulation tools, for instance shows how the group aims to provide applicable simulation tools.

In order to allow for the application of already existing models, they often have to be modified to make them more efficient, either on computational or model level. Here the PhD thesis of **Daniel Nasato** is an example where existing models for cohesion forces of fine powder particles are generalized to make them applicable for clusters of particles and thus making it applicable for large scale applications, in the context of die filling for powder metallurgy applications.

The necessity of profound code development as a basis for numerical modelling is being tackled by the PhD thesis of **Richard Berger**, who focussing on computational efficiency of simulation models and harnessing latest developments of hardware and parallelization paradigms.



Another example for validation work being performed is the PhD thesis of **Alice Hager** focussing on the comparison between fluid and granular flow simulations of a blast furnace and experimentally obtained data.

The Rock 'n' Roll group profits a lot from its diversity: **Stefan Amberger** (mathematician) is working on the mathematical basis of the interaction of non-spherical particles. **Daniel Queteschiner** (physicist) has been working on simulating the flow of fibres in a turbulent channel by coupling LIGGGHTS to a DNS (direct numerical simulation) flow solver.

An important factor for successful growth will be the availability of young researchers possessing the interest and the wide range of specific skills needed for modelling, simulation and experiments on fluid-granular systems. **Nikolaus Doppelhammer** has finished his bachelor thesis at our group and showed that young researchers can bring lots of motivation and persistence to accomplish their tasks.

Last, but not least, **Gijsbert Wierink** joined our group as a senior post-doc associate. Having worked with OpenCFD (London), the producer of the OpenFOAM® software, he brings along very profound experience in the field of open source CFD and will play a key role in the future of the Rock 'n' Roll group .

Confirmed by our success, we will follow the path of sustainable development and research.

Sincerely,

Christoph Jania

Christoph Kloss | Christoph Goniva





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ROCK 'N' ROLL MATERIALS2SIMULATION2APPLICATION

Gravels, corn seeds, pharmaceutical powders, sand and ore can not be easily characterized as for instance a steel beam.



To improve the range of applicability and reduce the bias of the characterization of particles properties we have set up a series of experimental devices and corresponding numerical simulations.

These calibration experiments are user friendly, as mechanised as possible and easy to set up.

After data collection (thanks to these devices) physical key parameters of particles are identified; this physical information allows the calibration of series of trustworthy numerical parameters for DEM (LIGGGHTS) and CFD (CFDEMcoupling) reliable simulations.

Accompanying numerical simulation is necessary to completely understand the flow and mechanical behavior of a defined particle in small scale, when the confrontation with another available lab's experiment could give indication about the correctness of the procedure, and in larger scale (if confronted to the lab's scale).

The knowledge gained so far should be applied to industrial processes, where handling and processing of bulk solids play an important role (metallurgical industry: sinter plants and blast furnaces).

Angle of repose

A digital protractor estimated the static angle of repose: once the particles are in position, the boundary is lifted up, allowing some particles to drop; once stabilized, the angle of repose is measured 8 times: the result is given as distribution of the measures.



Fig. 1: Angle of repose test



Shear cell tester

A simplified Jenike Shear Cell tester has been realized; a dc motor gives the tangential displacement: only the preshear force can be determined and used in simulations. In this case the coefficient of static sliding friction is the fraction of the Shear Force over the Normal Force.

A complete Jenike Shear Cell tester will be soon part of the devices available.

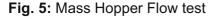
Maximum static angle

A sample of particles is placed on a plate: the inclination of the plate starts from 0° and is increased until the particles move.



Mass Hopper Flow

3 load cells are used to collect in real time the mass flow, given a diameter for the hopper's hole: the result is then used as comparison for the simulations.



Supervision: Christoph Kloss





Fig. 3: Shear cell simulation

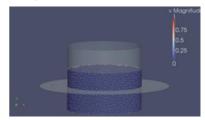


Fig. 4: Maximum static angle test





ROCK 'N' ROLL | DIE FILLING PROCESS

Simulating die filling process

Die filling process in powder metallurgy deals with a prohibitive number of particles to be simulated in most of the cases. Coarse graining allows reducing the computational effort by replacing individual particles by representative parcels, substantially reducing the required number of particles to picture a process. However, this procedure has to be accompanied by analytical considerations and verification in order to ensure that the physics is captured correctly.

Complex physics are usually involved in powder simulation and cohesive contact properties like van der Waals forces or liquid bridges are relevant in such scale. The usage of coarse graining methods considering correct physical behavior of such complex system is the object of study of this project.

To simulate die filling process discrete element method software LIGGGHTS is used. New cohesion models are implemented or adapted to have their physical effects modelled independent of system scale.

To validate simulation results an experimental device that mimics die filling process is used. Tests using dry and moisturized sand particles (to replicate cohesive behaviour of certain powders) were performed. Also metallic powders are currently tested in the experimental device. Preliminary simulation results indicates a good initial correlation but there is still room for improvement.

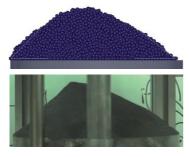


Fig. 1: Metallic powder simulated (top) and experimental (bottom).

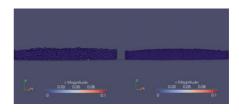


Fig. 2: Big (left) and small (right) particle exhibit same behaviour due to coarse graining.

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CFDEMcoupling allows to couple DEM and CFD methodologies and calculate void fraction distribution in a defined region. A homogeneous field is important for final product quality in die filling process.

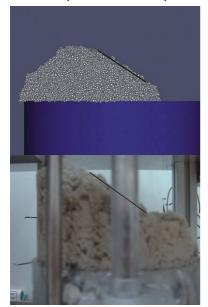


Fig.3: Simulation (top) and experimental (bottom) result using sand.

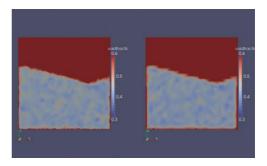


Fig. 4: Void fraction distribution in the die region filled with particles.

Figure 3 depicts the effect of cohesive forces. Water was added to sand to generate liquid bridges among particles. To simulate the liquid bridges forces a numerical model was implemented in software LIGGGHTS.



Supervision: Kloss

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ROCK 'N' ROLL SERVO WALL AND COHESION

New DEM boundary condition: Servo wall

The name 'servo wall' stands for a new feature of our open-source, DEM code LIGGGHTS. This new wall style uses a force or torque controller in order to prescribe the motion of a triangulated mesh.

Initially, it was designed to enable the simulation of shear testers for material characterisation purposes. As shown in figure 1, the top lid, which applies a constant normal stress to the bulk material, is modelled by the 'servo wall'. By measuring the required force for the motion of one ring with constant velocity, the coefficient of static friction can be determined.

In the meantime the 'servo wall' is used by members of our institute and of the very active, open-source community throughout the world. Potential applications range from raceway simulation in blast furnaces to material compression in sintering processes.

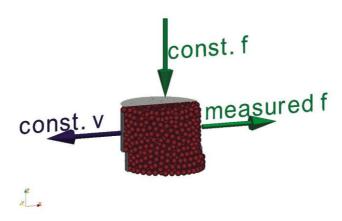


Fig. 1: Simulation of a simplified Jenike shear tester; the top lid ('servo wall') applies the constant force on the bulk solid

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Modelling of cohesive material

Industrial processes work with a wide range of material scales. Since the influence of cohesion on the behaviour of granular flow increases as the material size decreases, thoroughly modelling of cohesive forces is a very important issue.

Therefore, several models are implemented in our simulation tool LIGGGHTS. On the one hand this includes non-contact forces like the Hamaker constant model that takes the van-der-Waals into account. On the other hand cohesive contact forces, which can be caused by numerous physical effects, are considered with simplified Johnson-Kendall-Roberts (JKR) model or a piecewise linear model according to Stefan Luding. The most recent feature is a implementation of the original JKR model including latest research results.

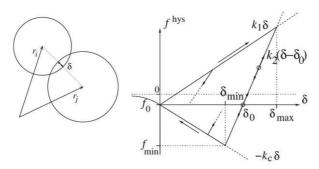


Fig. 2: (left) Two particles in contact with overlap d in normal direction. (right) schematic graph of the piece-wise linear force-displacement model (cf. Luding, 2008)



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Supervision: Schneiderbauer

ROCK 'N' ROLL MODELLING NON-SPHERICAL PARTICLES

Contact Modelling of Non-Spherical Particles

Worldwide, several approaches on how to handle non-sphericity are currently developed and tested for viability. While since 2011 our lab has the means to derive multi-sphere objects from real samples (the approximation-by-spheres algorithm) and then do non-spherical simulations using the multi-sphere method which is implemented in LIGGGHTS, this year we have been strategically pushing into exploring other methods to handle non-spericity in yet another way.

One of those methods is the use of polygonal surfaces. To simplify, we concentrate on the Minkowski sum of a so-called margin-sphere with convex hulls of sets of points in 3-space. Figure 1 (left) shows the Minkowski sum of a margin-sphere with the vertex-coordinates of a cube, Figures 1 (right) shows the Minkowski sum of a margin-sphere with the convex hull of those vertices, highlighting the connection to Figure 1 (left).

Within this framework we can calculate overlap and model collisions of said convex hulls. Figures 2 to 4 show examples of configurations, and two series of snapshots from modeled collisions.

Future efforts will be directed to improving the contact model, and implementing all algorithms in LIGGGHTS 3.

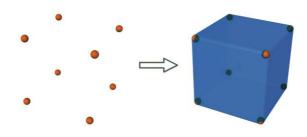


Fig. 1: Minkowski sum of a margin-sphere with the convex hull of 8 vertices.

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Fig. 2: Tetrahedron bouncing off a cube (partial surface-surface contact)

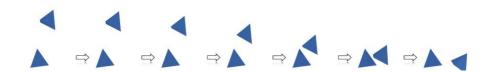


Fig. 3: Tetrahedron bouncing off another tetrahedron (edge-edge contact)



Fig. 4: Testing stability of algorithms by "balancing" tetrahedron on cube

Supervision: Kloss



Stefan Amberger | stefan.amberger@cfdem.com

ROCK 'N' ROLL BLAST FURNACE SIMULATION

Blast furnaces play an important role in steel production. Even though they have been in use for smelting for decades now, processes taking place in the inside are still not known in every detail. The flow system of a blast furnace is very complex, involving multiphase flows of Eulerian and Lagrangian nature as well as chemical reactions due to the high temperatures.

In the present study we concentrated on one specific detail, namely the formation of raceways. As can be seen in Fig. 1 blast air enters the blast furnace through tuyeres. Due to the impact of the air jet, cavities are formed – the raceways. In this area the combustion takes place.

The presented project is a combination of experiment and simulation: a cold, downscaled, pseudo 2D model was set up both in the laboratory and as numerical test case. The simulations were carried out with the Open Source toolbox CFDEMcoupling. The software combines the Discrete Element Method (DEM) code LIGGGHTS and Computational Fluid Dynamics (CFD) solvers that are based on OpenFOAM®.

As illustrated by Fig. 2 the container is first filled with granular material and then the surface is adjusted to the material level in the experiments. These two steps are pure DEM calculations. Finally, the coupled calculation is launched.

The experimental test rig is made of acrylic glass, which deforms slightly due to the burden of the material bed. Consequently, the large side-plates exert a pressure force onto the particles, leading to stresses inside the bed. In order to simulate this effect, the concept of servo walls (developed by Andreas Aigner) has been applied: the rigid simulation box was equipped with servo walls that are able to impose a pressure force in a given direction (cf. Fig. 3).

In the diagrams in Fig. 4 and 5 experimental results are compared against simulation results, for a case, where the inlet velocity is first increased step wisely and then decreased again. In Fig. 4 no servo walls were used in the simulations, leading to a strong over prediction of the raceway size. Furthermore, the hysteresis observed in the experiments cannot be depicted. Fig. 5 shows the comparison of the same experiment against a simulation with servo walls. Here the results are in far better accordance.



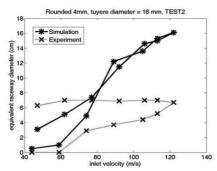


Fig. 4: Comparison of the results Sim./Exp. (no servo wall)

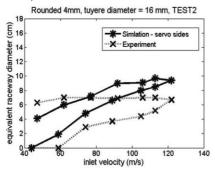


Fig. 5: Comparison of the results Sim./Exp. (servo wall)

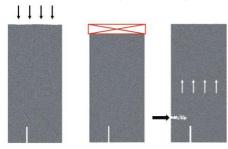


Fig. 2: Case setting: Filling, adjustment of the bed and coupled calculation.



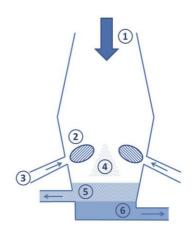


Fig. 1: Sketch of a blast furnace. (1) entering iron ore, coke, limestone, etc. (2) raceways (3) blast air (4) "dead man" (5) slag and (6) molten iron leaving the furnace.

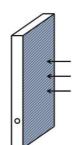


Fig. 3: Servo walls can be used to exert a pressure onto the bed.



Alice Hager | alice.hager@jku.at

ROCK 'N' ROLL PARTICLES IN FLUID TURBULENCE

Simulating fibres in turbulent channel flow

Dynamics of non-spherical particles in fluid turbulence is an important field of research addressing a range of industrial sectors. This includes conventional paper manufacturing as well as any processes involving the transport of fibres as a water suspension such as the production of microfibrillated cellulose.

Starting from this motivation, a cooperation between the University of Udine and the CD-Lab was initiated in an effort to combine their expertise in Direct Numerical Simulation (DNS) of turbulent channel flow and the know-how behind LIGGGHTS.

The DNS solves the Navier-Stokes equations numerically based on a Fourier-Chebyshev pseudo-spectral method. The use of a finely resolved computational mesh renders any turbulence model redundant. The fluid velocity field thus obtained can be used to compute and apply a drag force to the particles simulated in LIGGGHTS.

In a first approach this one-way coupling was established using spherical particles only and applying a drag force according to the Schiller-Naumann model. A snapshot of a test case consisting of 100.000 spheres driven by a turbulent channel flow is shown in Fig. 1. Note how the particles get trapped in low speed streaks near the walls at the top and the bottom, respectively.

Building on this code base, the functionality was extended to simulate ellipsoidal particles. To this end the applied drag force was adapted to take into account the particles shape and complemented with a torque calculated from the well-known Euler's equations.

Analogous to the case of spherical particles simulations to testify this model have been performed (cf. Fig. 2). Particle statistics like the mean streamwise and wall-normal velocities (cf. Fig. 3) support the validation of the implementation.



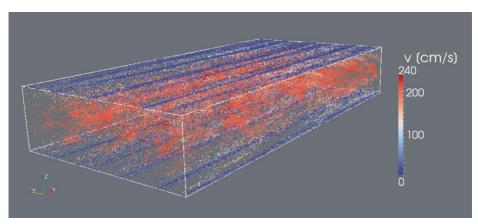


Fig. 1: Spherical particles carried by a turbulent channel flow (colored according to their velocity).

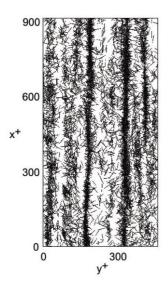


Fig. 2: Close-up ellipsoidal particles (aspect ratio $\lambda = 50$) near the wall.

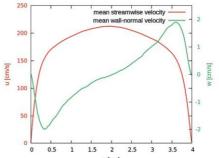


Fig. 3: Mean streamwise (red) and wall-normal (green) velocities of particles.



ROCK 'N' ROLL MULTITHREADING IN LIGGGHTS

LIGGGHTS uses MPI to parallelize simulations and distribute work among multiple CPUs. Each CPU obtains a subdomain. Inflowing and outflowing particles are communicated. While this domain decomposition works well in evenly distributed systems, simulations with varying particle densities will create load imbalance among the processors. This reduces the reached maximum speedup on many-core machines. Load-balancing mechanisms in LIGGGHTS dynamically adapt domain decomposition, however this approach is non-trivial and limited in 3D.

To better leverage the available resources in today's hardware, LIGGGHTS was extended with multithreading capabilities. Instead of relying solely on domain decomposition and MPI processes, each MPI process can now spawn multiple threads using OpenMP. The workload of each MPI process is dynamically partitioned and then distributed among these threads (see Fig 1).

This MPI/OpenMP hybrid approach allows organizing groups of threads to work on an optimal set of CPU cores, leveraging the underlying L1, L2, L3 caches. E.g. a 32-core AMD Opteron system may actually consist of two 16-core CPUs, each consisting of two 8-core teams sharing the same caches. By using the hybrid each of the four 8-core teams can be assigned to an MPI process and spawn 8 threads with shared caches. This can lead to vastly improved speedups compared to a MPI-only simulation (see Fig 2 & 3).

Adding multithreading to LIGGGHTS involved rethinking the structure of the current LIGGGHTS code base. These changes will also improve maintainability and will be seen in the upcoming LIGGGHTS 3.x release. Because of the usage of a test harness with 200+ examples, this will also be one of the most tested versions of LIGGGHTS prior to release.



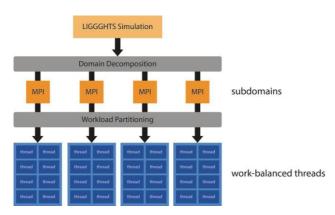


Fig. 1: Overview of the MPI/OpenMP hybrid approach



Fig. 2: 50,000 Particles dropping onto a cube. Simulation with 4 MPI processes (2x2x1), each with 8 threads. All particles are colored based on local thread ID (0-7). Illustrates how the workload is dynamically distributed over time.

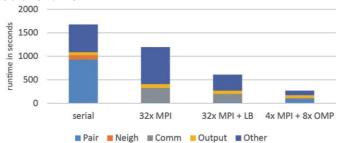


Fig. 3: Runtime comparison of the above example. The 32x MPI run uses a static 4x4x2 decomposition. Performance degenerates because of communication overhead and cache contention. MPI Load Balancing cuts this time in half. Our hybrid further improves performance because of dynamic load balancing, minimal communication and teams of threads working together on shared caches.



ROCK 'N' ROLL LATERAL MIGRATION IN CHANNEL FLOW

Lateral migration of particles in narrow channels is a well-known phenomenon that has received much attention by researchers for several decades. There are two effects associated with this behaviour: The decrease of apparent blood viscosity with capillary diameter due to the formation of a cell-free layer near the capillary wall is known as Fåhræus-Lindqvist effect (fig. 1) and the lateral migration of rigid spheres in pipe flow to an equilibrium position at about 0.6 pipe radii distance from the axis is called Segré-Silberberg effect (fig. 2).

In a first step to understand these phenomena, a coupling between a lattice Boltzmann (LB) solver and a discrete element (DEM) solver in two dimensions was realized. We used it to study the behaviour of a single circular particle in plane Poiseuille flow. A Segre-Silberberg-like migration pattern was also found in this reduced geometry, with a shift of the equilibrium position towards the axis for higher channel Reynolds numbers (fig. 3). In addition to this already well-known phenomenon, we investigated the trajectory of the particle. For higher Reynolds numbers, we found that the migration pattern changes. A particle can migrate towards the center and then be pushed back towards the wall. At Re=600, we even found that the particle crosses the centerline and comes back. The reason for this is the strong particle rotation which causes a negative lift force that drives the particle back across the centerline (fig. 4).

Further goals are an implementation of this method in three dimensions using the open source LB package *Palabos* (*www.palabos.org*) and a coupling to the DEM code *LIGGGHTS*. The insights gained in the course of this project, both physical and algorithmic, will be valuable in pursuing this. Once the coupling is created, we will aim at investigating the behaviour of deformable particles like red blood cells or fibres in different flow situations. A proof of concept for this is shown in figure 5: A particle is created from a ring of overlapping primary particles which are connected by springs. This system behaves similar to a red blood cell (*Pan et al., Soft Matter 6(2010), 4366-4376*) and shows a much more complex migration pattern.



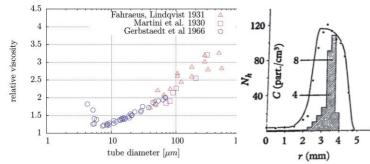
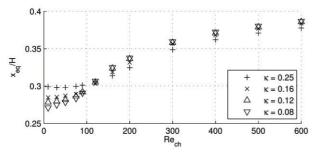


Fig. 2: Segré-Silberberg effect. Most spheres in a channel are found at an off-center e quilibrium position. Source: J.Fluid.Mechanics 14, 1962, p. 136-157.

Fig. 1: Blood viscosity as function of capillary diameter.



Re = 20
Re = 80
Re = 60
Re = 600

Fig. 3: Equilibrium position of particles of various diameters as function of channel Reynolds number.

Fig. 4: Lateral position (tio) and rotational velocity over time for different Reynolds numbers. The centerline is at x/H=0.5.

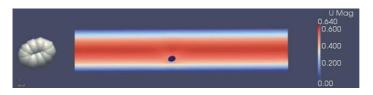


Fig. 5: Proof of concept for a deformable multisphere particle in channel flow.

Supervision: Pirker Philippe Seil | philippe.seil@jku.at

DUST 'N' DIRT

Dear Readers.

This year I want to take the opportunity to introduce you to my research group, that is the Dust & Dirt group. As the name suggests, my group deals with fine particles, where the number of particles is extremely large. Thus, it is impractical to study such fluid-particle (fluid-droplet) systems using discrete particle methods. In fact, in this case the granular phase can be considered by local averaged variables, i.e. by continuum approach. Basically, the Dust & Dirt group consists of three PhD students and three senior researchers dealing with a wide range of subjects.

Mahdi Saeedipour studies the high-pressure die-casting process in detail. In the first year of his PhD he made remarkable progress by developing a numerical hybrid model, which pictures the jet instability appearing during the casting process (Figure 1).

Afsaneh Soleymani will examine the pneumatic conveying of coal and cement within the scope of her PhD. In the starting phase of her work she has already been able to considerably improve the granular Eulerian solver delivered with OpenFoam by including boundary conditions for the solid phase, which distinguish between sliding and non-sliding collisions (Figure 2).

Finally, Gerhard Holzinger investigates flotation using gas-liquid bubble columns experimentally (Figure 3) and numerically. During the last year he was able to validate his numerical models against his bubble column experiments.

Finally, the effort has been honoured by a series of Journal publications and conference contributions, which manifests our international visibility.

Sincerely,

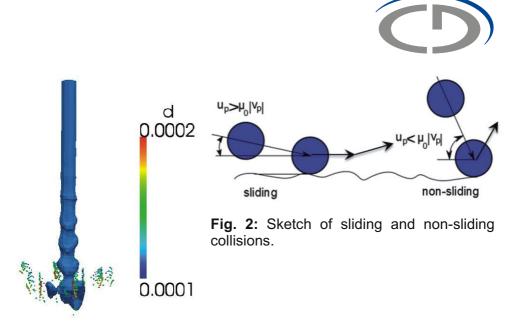




Fig. 1: Entrainment of water droplets from an instable turbulent jet with U = 20 m/s. The colourbar corresponds to the diameter of the entrained droplets.



Fig. 3: Detail view of the inlet section of the bubble column. Bubbles of similar size are rather uniformly distributed in lateral direction.



DUST 'N' DIRT

MODELLING PNEUMATIC CONVEYING

In many industrial processes, powdery dust (like coal or cement) has to be conveyed from a feeding vessel towards its processing point. The associated gas-particle flow should be studied carefully in order to optimize the design and operation efficiency of such an industrial system.

What's important in such a system?

- Formation of dust slugs in the conveying line
- Process of feeding particles from a feeding vessel into the conveying line
- The effect of bends or pivoting distributor elements
- The effect of an interconnected distributor or an interconnected buffer fluidised bed

Steps towards the target:

- Theory and analysis (literature review)
- Tools and implementation (OpenFOAM)
- Computations and validation

Accordingly, the following flowchart shows the studies at the start of the project:

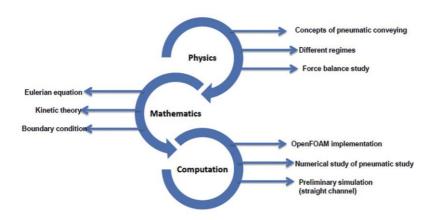


Fig. 1: Working Chart

2013 | Particulate Flow Modelling



Dealing with the first simulations:

At the starting point of the simulation, a straight simple channel was considered to compare the computed particle velocities with experimental data. The simulation is performed in the framework of a kinetic theory based Two-Fluid Model (TFM) using the open source CFD toolbox OpenFOAM®. The results show that the fast-moving particles at the channel center migrate towards the lower wall under the influence of gravity (Fig.2).

Fig. 2: Predicted streamwise particle velocity profile

To make the velocity profile of particles more realistic, the following measures should be adopted to modify the solver:

- Including wall-friction:
 - The boundary condition of Johnson-Jackson (1987).
 - Revisiting of Johnson-Jackson boundary condition (2011).
 - The boundary condition of Schneiderbauer (2012).
- Including wall-roughness and shadow effect, by Sommerfeld's virtual wall angle model (1999)

Including the wall-friction results in damping the momentum and decreasing the velocity of particles at the walls, however the velocity profile is still asymmetric. Wall-roughness has a strong effect on particles' rebound and re-dispersion, especially on transferring the horizontal momentum to the vertical direction. Currently, the modification of the solver is under development.



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DUST 'N' DIRT | MODELLING FLOTATION

Simulating bubble columns

In a variety of industrial processes bubbles are introduced into liquids for certain tasks, e.g. bubble induced stirring of liquid metal, flotation of minerals or waste water treatment.

For simulating bubble columns the open source CFD toolbox OpenFOAM® is used. Due to the availability of the source codes the solvers can be modified to fit certain needs. OpenFOAM® offers a great number of standard solvers which cover a huge range of physical fields.

To validate simulation results a small bubble column was built to be able to conduct validation experiments. This bubble column features interchangeable aerators and the possibility of introducing external flow. The interior of the bubble column is completely visible through its transparent walls.

Figure 2 shows the bubble column in operation with an active external pump. The incoming flow displaces the ascending bubbles. Thus a nearly bubble free zone forms.

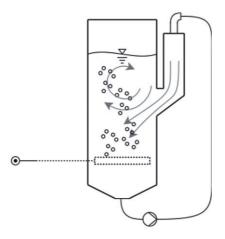


Fig. 1: Schematic experimental setup



Fig. 2: Experimental setup in operation

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A good accordance of simulation and experiment with respect to the size of the zone influenced by the cross-flow has been accomplished.

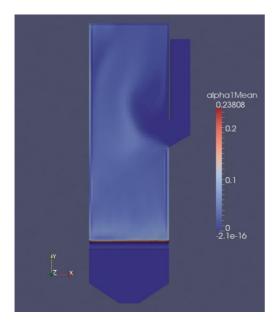


Fig. 3: Mean volume fraction of the gas phase.

Fig. 4: A single photo of the experiment. 1/10 s exposure.

In Figs. 3 and 4 the zone influenced by the incoming flow is clearly visible. In the experiment more bubbles are conveyed into this zone from above by the downward flow. This may be due to the polydisperse bubble generation in the experiment. Obviously, our mono-disperse simulation is not able reproduce this phenomenon.



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DUST 'N' DIRTHIGH PRESSURE DIE CASTING

High pressure die casting (HPDC) process is one of the most important but yet little known manufacturing methods. It is extensively used for mass production of different metal components in automotive and aerospace industries based on aluminum, magnesium or zinc alloys. Higher efficiency, accuracy and strength in final products are the main advantages of this method. However, the turbulent nature of flow during liquid metal injection and filling causes different problems. On the one hand, wavy disintegration of the jet might result in cold shut defect in the final product, on the other hand a high degree of atomization may strongly increase the porosity defect.

A threefold investigation is conducted in order to study this process. Analytical studies are done to characterize the turbulent behavior of liquid metal jet dispersion, breakup and atomization. The filling behavior, heat transfer and solidification should also be studied analytically. The HPDC is a challenging process for numerical simulation because it involves several simultaneous sub-processes with different time and length scales. Detailed knowledge in modelling of flow instability and breakup, turbulence, multiphase flow, heat transfer and solidification is of great importance.

A hybrid numerical framework is proposed and is currently under development using CFD open source toolbox OpenFOAM, to simulate the whole HPCD process from injection phase to solidification. The turbulent primary breakup during injection and the multiphase process are modeled by an Eulerian-Lagrangian approach. This numerical framework and one of the simulation results are shown in figures 1 and 2, respectively.

An experimental study based on water analogy is conducted to capture the flow instability and dispersion of hot water jet with different Reynolds and Weber numbers during mold filling. The experimental setup is designed and built in our laboratory (figure 3). Next steps include the analytical and numerical study of droplets behavior and their interaction with the continuum phase and the confining walls





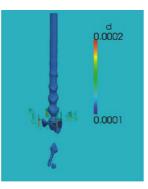


Fig. 2: Numerical simulation of liquid jet injection for Re=1.8e5 in comparison with experiment.



Fig. 3: Experimental setup for water analogy experiments.

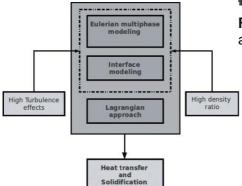


Fig. 1: The proposed framework for numerical simulation.



Supervision: Schneiderbauer Mahdi Saeedipour | mahdi.saeedipour@jku.at /

DUST 'N' DIRTEULERIAN SOLID PHASE MODELLING

Fluidized beds are widely used in a variety of industrially important processes. During the last decades the analysis of the hydrodynamics or the efficiency of fluidized beds through numerical simulations has become increasingly common. However, due to computational limitations a detailed simulation of poly-disperse reactive industrial scale reactors is still unfeasible. It is, therefore, common to use coarse grids and average particle properties to reduce the demand on computational resources. Such a procedure inevitably neglects on the one hand small (unresolved) scales. On the other hand, mixing, segregation and chemical reactions, which are triggered by the individual particle properties (diameter, particle porosity, ...), cannot be pictured appropriately.

Therefore, we have developed a computationally efficient hybrid model. The main idea of such a modeling strategy is to use a combination of a Lagrangian discrete phase model (DPM) and a kinetic theory based Eulerian continuum model to take advantage of the benefits of those two different formulations. On the one hand, the local distribution of the different particle diameters, which is required for the gas-solid drag force, can be obtained by tracking statistically representative particle trajectories for each particle diameter class. Further, chemical reactions can be evaluated on a discrete particle base. On the other hand, the contribution from the inter-particle stresses, i.e. inter-particle collisions, can be deduced from the Eulerian solution. Figure 1 demonstrates that the hybrid model yields (including bed expansion, segregation and channeling) fairly good agreement with experiments.

Secondly, figure 2 shows that neglecting the unresolved part of the particle frictional stresses yields to an overestimation of the bubble rise velocity. We, therefore, augmented the sub-grid drag modifications (presented last year) with two different types sub-grid stress correction. Both are able to predict the correct rise velocity of the bubbles (Models A and B in figure 2).



Next steps will concentrate on further testing and validating of the hybrid model in the case of cyclones and reactive fluidised beds of industrial scale.

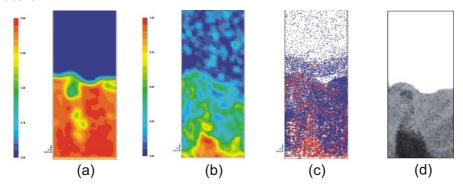
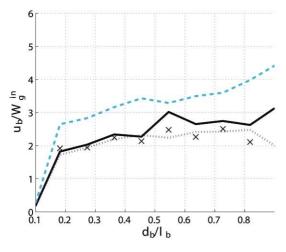


Fig. 1: Bidisperse fluidised bed: a) computed particle volume fraction, b) computed fraction of 2.6mm particles, c) diameter of tracer particles (blue: 500 m, red: 2.6mm), d) experiment (light gray: 500 m, dark: 2.6mm).

Fig. 2: Computed bubble rise velocity as a function of the bubble diameter: **x** fine grid simulation, - w/ sub-grid stress correction (Model B), w/ sub-grid stress correction (Model A), - - - w/o sub-grid stress correction





EXPERIMENTS

Dear Readers,

the last year has brought a lot of experimental activities. Our powder injection experiments have drawn some international attention, we have been asked to provide lance tests for an RFCS project (Fig. 1). Likewise our high-speed videos from the blast furnace raceway have gathered high interest.

While the last years were dominated very much by gas-particle experiments this year **Bernhard König** started a new project on gas driven liquid flows to investigate turbulence and mass transport in steel ladles and mould flows. A new water basin for such experiments is currently under construction (Fig. 2).





Fig. 1: The proposed framework for numerical simulation.

Fig. 2: New bubble column test rig.

To put our fluidised bed experiments on the next level **Lukas von Berg** redesigned our test rig for closed loop operation. We are now able to investigate segregation in fluidised beds and can also use fine particles which leave the bed and are separated by a cyclone and fed back at the bottom of the fluidised bed.



Roland Winkler has built a hopper outflow test rig for the test of mass flow measurement systems (Fig. 3). This test rig is designed for operation with real particles (e.g. pulverized coal) under industrial conditions.

With the particle characterization experiments of **Luca Benvenuti** (Fig. 4) we make another step forward from purely spherical particles to non-

spherical real world materials.



Fig. 4: Angle of repose experiment with non-spherical particles.

Fig. 3: Large scale hopper outflow test rig.

Lukas Fiel is conducting systematic experiments with a particle feeding injector to convey particles against an increasing pressure level. As quite often in science things turned out more complicated than expected and it will be a nice challenge to analyse all the data we gather from this test rig.

Finally we started a cooperation with the Technical University Graz to jointly develop a three-dimensional reconstruction of pneumatic conveying and fluidised bed experiments by use of an electrical capacitance tomography system (ECT). This will allow us to go from pseudo 2D setups to three-dimensional geometries.

Sincerely,

Style Rullan

EXPERIMENTSSEGREGATION IN FLUIDISED BEDS

In many industrial fluidised bed applications (e.g. coal combustors and gas-phase polymerisation), the fluidised particles are not homogeneous, but a mixture of particles with different phyiscal properties (e.g. size or density). Depending on the superficial gas velocity, this leads to an equilibrium of particle mixing and segregation. In order to understand and improve the processes for the various applications inside the bed, it is important to be able to predict the particle size distribution throughout the bed.

Experiments were done for a series of bi-disperse mixtures of differently sized and coloured glass spheres in a small pseudo two-dimensional rectangular fluidised bed. The experiments were recorded with a highspeed camera and the image sequences were processed in Matlab to observe the segregation process. A calibration curve which describes the correlation between pixel-intensity and particle mass fraction was created. Each picture was split in small cells and the calibration curve allowed to calculate the mass fraction of small particles inside each cell. A measure to describe the degree of segregation was calculated for each image. This allows to observe the extent of segregation over the duration of each experiment (Fig.1).

The bed pressure drop was measured in different heights above the distributor plate. When segregation occured, the pressure drop declined until segregation was complete and then remained at a constant level (Fig.2). This is because the mixed bed at the beginning of the experiment has a much smaller voidage and therefore a higher pressure drop.

Additional experiments were performed in a circulating fluidised bed (CFB) where the smaller particles leave the bed at the top, are separated from the gas by a cyclone and are then conveyed back into the bed at the bottom via pressurised air. Basic feasibility tests have been successfully performed. In future work, more experiments need to be done to understand segregation in a CFB better.



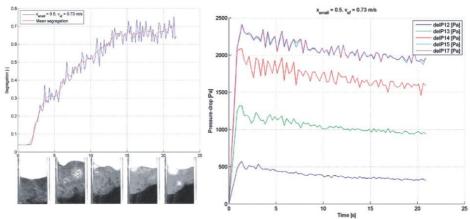


Fig. 1: Segregation for 1:1 mixture of 500 and 2600 micron particles.

Fig. 2: Pressure drop for 1:1 mixture of 500 and 2600 micron particles.

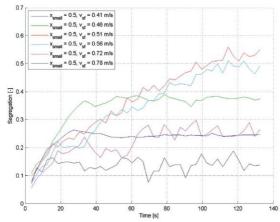


Fig. 3: Effect of increasing superficial velocity on segregation. When the minimal fluidisation velocity is reached, the bed does not segregate very well. For higher superficial velocities segregation gets more important until a certain velocity is reached. From there on, mixing processes are stronger and the segregation declines.



EXPERIMENTS | INDUSTRIAL DUST RECYCLING

Industrial burners for solid materials require a particle feeding injector. Quite often the combustion process takes place at a higher pressure than the surrounding environment. Therefore the injector system must be able to feed particles against an increasing pressure level.

The CDL has set up an 1D engineering tool to design the whole loop of a dust recycling system including cyclone, particle injector and feeding lines (Fig. 1).

To validate the 1D tool and 3D CFD simulations we have designed a modular lab-scale test rig (Fig. 2 and Fig. 4). In a first phase particles are fed via a vibrating chute to the injector box. After the conveying line the particles are collected on a weight balance in a box with adjustable pressure level.

With this setup we are able to do parameter studies on the behavior of the injector and the pneumatic conveying in the supply pipes (e.g. Molerus diagram in Fig.3).

In a second project phase the feeding injector can be included in our pneumatic test rig to form a closed loop system.

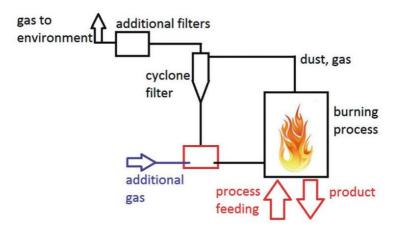


Fig. 1: Schematic outline of an industrial dust recycling system.

2013 | Particulate Flow Modelling



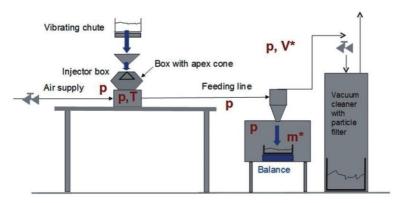


Fig. 2: Outline of the lab-scale experiment

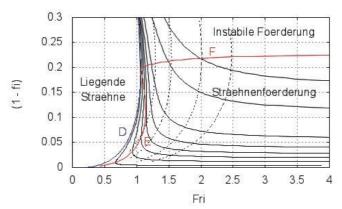


Fig. 3: Molerus diagram for particle feeding injector.

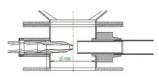


Fig. 4: Detail of labscale particle feeding injector







Stefan Puttinger | Damir Kahrimanovic | Lukas Fiel

EXPERIMENTS | BUBBLE STIRRED FLOWS

Bubble stirred flows or bubbling beds are commonly known for several industrial processes in multiple fields. They are used in chemical industry for material homogenisation in reactors to evite thermal hotspots or for mining purposes where the flotation process is driven by the rising bubbles

However, the essential field for this work is the steel production, where the hot metal desulfurisation represents the main background. This process is a major step in refining hot metal and is situated between the tapping of the blast furnace and the converter process. Dr. More's patent on hot metal desulfurisation describes a two step procedure. In a first stage rawiron desulfurisation occurs while enriching sulfur in a synthetically slag. To omit the slag disposal More postulates the oxidation of sulfur in a regeneration step which facilitates the slag to be reused several times.

The implementation of the first step comprises rinsing of both liquid phases with nitrogen inducing the transition of sulfur from the liquid metal into the slug-phase. This process is obviously realized by a bubbling bed where the forced convective flow and turbulences therein directly contribute to the effectiveness and are therefore the main focus of this work.

Howbeit, this process accommodates fascinating phenomena where the most important ones could be separated in the following three:

- Phase boundary interaction of liquid and overlaying phase (slag)
- Convective flow triggered by the rising bubbles
- Interaction between liquid and container walls (shear forces)

While the first and second point are related to the effectiveness of the process, the third one origins in the need of minimizing refractory erosion. Due to the core area of this work is an experimental one, measurement techniques delivering an insight into the correspondent quantities are developed.



Recent investigations aim at resolving the unsteady, three dimensional velocity field for further insight in the turbulent nature of such fields.

To seperate the liquid and gas phase a Light Induced Fluorescence (LIF) setup was used (Fig. 2). Image post-processing algorithms were implemented and applied, leading to phase discriminated vector fields like depicted in Figure 1.

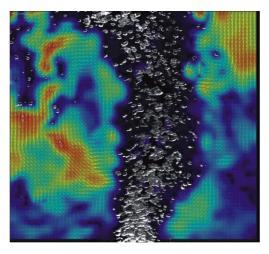


Fig. 1: Velocity vectors of the fluid phase (colored by magnitude) in the midplane of a small rectangular bubble column.

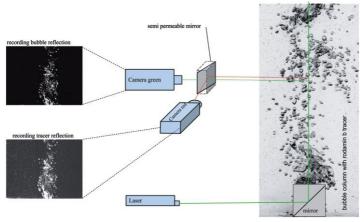




Fig. 2: PIV setup used for phase discrimination.

Bernhard König | bernhard.koenig@jku.at

EXPERIMENTS PRESSURE DROP IN PACKED BEDS

Determination of the Hydraulic Diameter of Irregular Shaped Materials by Pressure Drop Measurements

The Ergun equation is commonly used to express the pressure drop in any packed bed with spheres of the same size. Most of the real applications, however, work with irregular shaped particles (e.g. pellets, coke, and ore). It is difficult to predict the pressure drop for this kind of material because an important coefficient, contrary to spheres, is undetermined — the particle diameter. Aim of this work was to experimentally find a (fictive) diameter, which we call hydraulic diameter, for any testing material to apply known pressure drop equations correctly. Once the hydraulic diameter has been determined for a specific material, one can predict the pressure drop for any fluid velocity and material arrangement. A sketch of the test setup is shown in Figure 1.

At first, experiments with glass spheres (d = 2,3,4 mm) have been conducted to proof if the measurement apparatus works accurate and without errors. In a second step, the pressure drop of irregular shaped particles has been determined. Then, the parameter for the particle diameter in the theoretical pressure drop equations (e.g. Ergun's Equation) was adjusted as long as the theoretical pressure drop function fit best with the measurement data (Fig. 2).

Temperature Measurements in Packed Beds

The test rig was designed in a way to perform another, completely different, experiment. Dealing with the topic of material characterization it is of great significance to know the temperature profiles in packed beds when heated gas flows through a (cold) packed bed. Therefore, a power controlled heating element has been mounted to control the temperature of the gas flow. Sensors mounted in different distances detect the temperature of the packed bed locally (Fig. 1).

Until now experiments with glass spheres have been conducted (Fig. 3). For the future, materials with irregular shaped particles will be tested. The results will be used to validate e.g. simulation results.



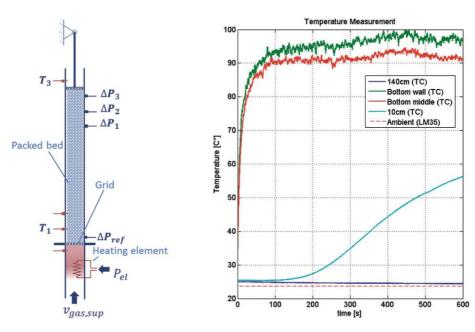


Fig.1: Experimental setup

Fig. 3: Heat transfer measurements

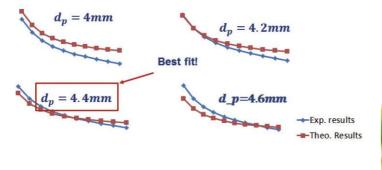


Fig. 2: Pressure drop measurements for the determination of equivalent particle diameter



EXPERIMENTS | PNEUMATIC CONVEYING

Laboratory studies of Bulk Material Pneumatic Conveying

Various industrial processes, such as the blast furnace process, require large quantities of powdery bulk material to be conveyed. Albeit its widespread application pneumatic conveying is a complex process and depends on numerous parameters, for example, load ratio, gas velocity, and particle diameter. An optimal transport state can only be achieved if the parameters are set in the correct ratios.

One goal of this project consists of designing and erecting a multifunctional test rig for pneumatic conveying and flow detection of different bulk materials and operating conditions (see Fig. 1,2).

With this experimental set-up we intend to generate reproducible pneumatic conveying regimes, which should be detected by different measuring devices. Thereby, we will focus on flow situations beyond homogeneous and steady state conveying.

In a series of conveying tests we will produce characteristic disturbances (e.g. by operating a plate slider) and study their influence on the quality of overall measurement results of different mass-flow detection devices.

The output will be compared with the literature and will provide an in-depth understanding of the flow conditions and behaviour in industrial pneumatic conveying lines.

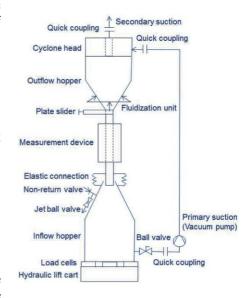


Fig. 1: Schematic of experimental setup





The test rig covers an area of 1 m² and is 4.5 m high. The illustrated outflow hopper has a volume of approx. 67 litres without the cap, where a cyclone is installed.

In the blue field a variety of measurement devices can be installed

To determine mass flow, different measurement systems, such as flow meters, load cells, and a high-speed-camera, are implemented.

Furthermore, an ECT (Electrical Capacity Tomography) system will be implemented in the test rig.

First measurement results of a special flow meter are shown in Fig.3. These results are output signals from current

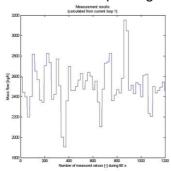


Fig. 3: Measurement of mass flow during conveying

Fig. 2: Test rig in the CD-Lab

With special thanks to the sponsor of this project: **Voestalpine steel GmbH**

Supervision: Puttinger Roland Winkler | roland.winkler@jku.at

EXPERIMENTS | PULVERISED COAL INJECTION

Pulverised coal is used as a fuel substitute to reduce the amount of coke necessary in iron making. The pulverised coal is injected through lances in the tuyere sections. A proper dispersion of these highly laden particle jets is crucial for efficient combustion. Within this collaboration project with voestalpine Stahl Donawitz a lot of lab scale experiments and numerical simulations with various lance tip designs were performed.

Finally we decided to test some of the most promising designs on the real blast furnace and observe the behaviour of the PCI flame with the high-speed camera. The quality of the obtained images was a surprise even for us and have gained some international attention (see also last years cover page).

Nevertheless the goal was to extract some quantitative information about the burning of coal. Therefore I did some digital image processing to analyse the flame size and dynamics of the various lance tips.

The alternative dead end lance which can be seen in Fig.1 showed 50% larger flame spots and better coverage of the visible raceway area. This can be interpreted as a better dispersion of coal particles.

However, the experiments so far contain no information on the overall mass flow rates, so the next step would be to couple the high-speed camera with a mass flow sensor in the conveying line.







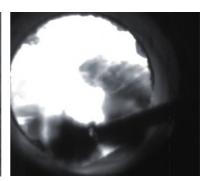


Fig. 1: PCI flame of standard lance (left), alternative dead end lance (center) and PCI flame of dead end lance tip.

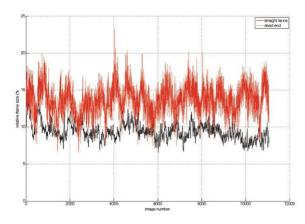


Fig. 2: Histogram of the relative flame size obtained by digital image analysis. The dead end lance shows an increase of 50% in flame size.

Fig. 3: Measurement setup at voestalpine Stahl Donawitz.





COLLABORATING SCIENTISTS | LCM | MARKUS SCHÖRGENHUMER

Fluid-structure interaction

Flexible multibody dynamics and smoothed particle hydrodynamics

The interaction of fluids with mechanical systems – fluid-structure interaction (FSI) – plays an important role in a variety of scientific fields and a wide range of real-world applications. Think, for example, of biomechanics (e.g. blood flow in flexible vessels, blood cells, aortic valve), structural engineering and offshore applications (e.g. bridges subject to strong wind, wave impact against dams, offshore wind farms), or industrial problems (e.g. flexible parts in machines, deformable tubes or valves, fibers or particles immersed in a fluid).

Due to the complexity of typical FSI problems, accurate, efficient, and versatile numerical approaches for modeling, simulation, and optimization are of significant interest from both the scientific as well as the industrial perspective. The current challenges in computational FSI are diverse, but particularly involve large rigid-body motion (with superimposed small deformation) or even large deformation of the mechanical components in contact with the fluid.

Our computational approach to FSI is based on the coupling of flexible multibody systems with fluid dynamics (cf. Fig. 1) via an explicit cosimulation between the two open-source simulators HOTINT (www.hotint.org) and LIGGGHTS (www.liggghts.com). The multibody code HOTINT provides a versatile framework for modeling and simulation of complex mechanical or mechatronical systems, including rigid and flexible bodies, loads, constraints, contact, and control. The parallel particle simulator LIGGGHTS includes an efficient implementation of the particle-based meshfree method SPH (smoothed particle hydrodynamics) which is well suited for handling fluid dynamics in complex moving or changing domains.

We are steadily testing, improving, and validating our approach, currently especially with respect to the coupling scheme and the SPH implementation. For a few numerical examples and applications, see Figures 2-4; further details can be found, for instance, in

M. Schörgenhumer, P. G. Gruber, J. Gerstmayr: Interaction of flexible multibody systems with fluids analyzed by means of smoothed particle hydrodynamics. *Multibody Syst. Dyn.*, **30**:53-76, 2013.



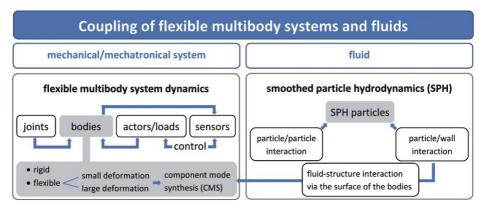


Fig. 1: Coupling of flexible multibody dynamics and fluid dynamics.

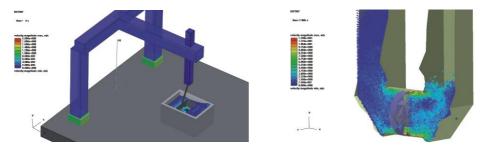


Fig. 2: Flexible linear robot scooping fluid out of a pool.

HOTINT

Fig. 3: Elastically supported axial pump.

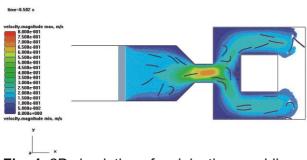


Fig. 4: 2D simulation of an injection moulding process with flexible fibers in highly viscous fluid.



COLLABORATING SCIENTISTS | TU-GRAZ | BEGONA CAPA GONZALES & STEFAN RADL

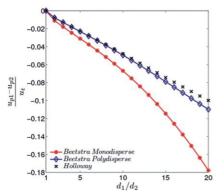
It is well known that simulations of dense fluid-particle systems are extremely challenging and often inaccurate in case a too coarse computational grid, or an inappropriate fluid-particle interaction force model is used. The situation is even more delicate in case a polydisperse particle population needs to be modelled. We have addressed these key challenges by implementing a new generation of fluid-particle drag models into the Euler-Lagrange simulation tool *CFDEM*.

In a first step we have implemented a novel drag model (Holloway et al., AIChE J 56:1995-2004) into Matlab® to compute the average fluid and particle velocities of a freely sedimenting suspension. These calculations were based on a simple force balance and a homogeneous dispersion of the particles. Specifically, we considered a bi-disperse particle population with diameter ratios d_1/d_2 between 1 and 20. We compared the Holloway drag model with the "standard" Beetstra model (AIChE J 53:489-501; designed for monodisperse systems), as well as a variant of the Beetstra model for polydisperse models (see Fig. 1). The drag model has then been transferred to the code *CFDEM*.

Our Matlab calculations indicate that there are significant differences in the segregation rate depending on the drag model and the density ratio of the systems (Fig. 1). We anticipate, that our Matlab® tool will be helpful for testing future drag models for polydisperse systems. The *CFDEM* simulations indicate that particle clustering can increase or decrease the segregation rate depending on the particle volume fraction (see Fig. 2). This indicates, that the currently available drag (and particle-particle interaction) models might need to be improved for future application in coarse-grid simulations.

Finally, we have applied the new drag model for the simulation of a pseudo-two-dimensional bubbling bed. First results indicate that especially for bubbling beds the drag model formulation is of key importance. This is due to the complex interplay between bubbling-induced re-mixing, wall effects and the segregation process driven by forces on individual particles (see Figure 3). Currently, we focus on the analysis of the particle packing close to the walls (e.g., using Voronoi tesselation, see Fig. 4) to reconstruct the local porosity.





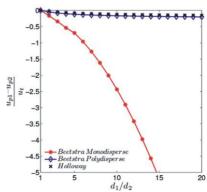
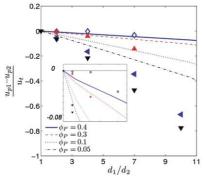


Fig. 1: Segregation rate of homogeneous dense gas-particle suspension (left), as well as a liquid-particle suspension (right; $_{\rho}$ = 0.4).



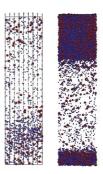


Fig. 2: Segregation rates of homogeneous and clustered gas-particle suspensions (left), as well as corresponding particle distributions (right).

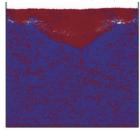


Fig. 3: Segregation in a bubbling bed.

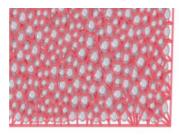


Fig. 4: Voronoi tesselation to analyze voidage near walls.



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SEMINAR | TSUNAMI MODELLING

Research is a creative process. Lateral thinking and a flexible and open mind are important ingredients of successful research and development. Last but not least, work should be fun as well. With this in mind PFM organizes an annual "lateral" seminar, where various groups work together on a topic that is new to all. This year the topic is the dynamics of a tsunami.

The seminar participants choose to join one of the three main teams; Analytics (Simon Schneiderbauer and Michael Krieger), Numerics (Gijsbert Wierink), and Experiments (Stefan Puttinger).

The analytical group focuses on shoaling, how the amplitude of a tsunami changes as it approaches the shore. The frightening results show that amplitude A increases with the fourth root of water depth ratio. A Tsunami triggered in the deep ocean of an amplitude of 1 m hits the beach with an amplitude of at least 10 m! With a wave speed of several hundreds of km/h and a wavelength of over 100 km, the destructive force is clear. A subgroup further tries to solve the Shallow Water Equations (SWEs) by using the Lax-Wendroff method with reflective boundary conditions.

The numerical groups consists of two sub-groups; one team applying Smoothed Particle Hydrodynamics (SPH) simulations and one picturing a tsunami using the Volume Of Fluid (VOF) method. The VOF team created a small scale tsunami case that corresponds to the wild plans of the experimental group.

Now, what would colourful diagrams be without and actual tsunami? Our experimentalists built a 3 m scale model of a tsunami, where the wave is triggered by releasing a spring mounted plate. Image recognition, floaters and lego villages helped the experimental team to successfully measure wave speed and impact on a beach. All this is work in progress and so far it has been a great opportunity to think out of the box and work together on an exciting topic!







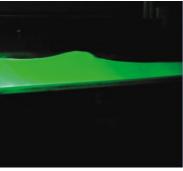


Fig. 1: Laboratory scale tsunami (left), lit by green light for contrast (right)

t = 40.80, tv = 21.32

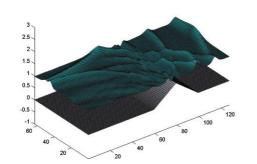


Fig. 2: Results of the Shallow Water Equations of wave interaction with a sub-marine hump.

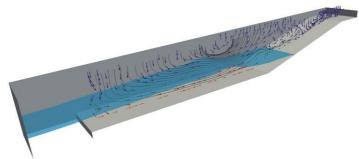


Fig. 3: Volume Of Fluid solution of the wave travelling through the scale model.

Supervision: Simon Scheiderbauer

SELECTED PUBLICATION

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