

Christian-Doppler Laboratory on Particulate Flow Modelling

Annual Report | **2012**

CHRISTIAN-DOPPLER LABORATORY ON PARTICULATE FLOW MODELLING

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Front cover: Pulverized coal dust is injected into an industrial blast furnace (voestalpine Donawitz) at temperatures above 2.000°C. The image was taken from a high-speed video at 2.000 frames per second (fps) which reveals that the incoming hot gas causes a local fluidization of the burden material. At 10.000 fps even the dynamics of the combusting flame (dark region in the lower part) could be resolved. © S. Puttinger

EDITORIAL 1

Dear Readers,

in 2012 our research group on Particulate Flow Modelling has experienced considerable growth for the forth time in a row. By now we assemble a smooth mix of 20 postdocs, PhD-students and further scientific employees which are embedded into a well defined research environment.

The elapsed year might be characterized by pronounced internationality: We organized dedicated mini-symposia at conferences, delivered international lectures and hosted visiting scientists. We continuously collaborate with partner universities, participate in EU-level research programs and due to our international visibility we are able to attract top PhD-students from all over the world.

In the upcoming year our CD-Lab will be transformed into a new Johannes Kepler University Department on Particulate Flow Modelling. Siemens VAI, voestalpine and the Upper Austrian government will provide a start-up funding before JKU is going to take over. This structural transformation paves the way towards a persisting place for our group within an exciting research environment.

With these introducing words I wish you a pleasant reading!

Sincerely,



EDITORIAL 2 | ROCK 'N' ROLL

Dear Readers,

Another year has passed for the CD-Lab on Particulate Flow Modelling, reason enough to have a look at the past, but also the future:

From a small group of “young guns” in the field of particulate flow modelling we have developed to a well established research centre of international reputation. This can be seen as the success of the coordinated work of bachelor-, master-, PhD-students as well as post doc seniors working in the fields of analytics, numerics and experiments. As an outstanding success we would like to emphasize the teaching activities of our group, which has proven to be a core requirement to continuous growth. Participants from nearly all continents found their way to the CD-Lab on Particulate Flow Modelling and thus enforced our international reputation and network. This consequent growth enables profiting from synergies and establish groups dedicated to sub-topics. Assuring a successful future for this group new challenges are to be tackled. As a clear commitment to sustainability of our DEM and CFD-DEM modelling tools (www.cfdem.com) we successfully launched a spin-off company early 2012. Further we try to acquire long-term funding schemes, especially on EU level. Greatly supported by our industrial partners we look forward to convert this short term platform to a persistent research centre.

Sincerely,

Christoph Kloss | Christoph Goniva



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EDITORIAL 3 | DUST 'N' DIRT

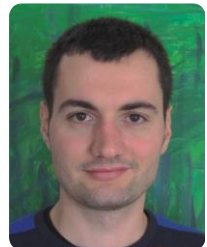
Dear Readers,

This year the Dust 'n' Dirt group once again grew by one PhD student. Our Iranian colleague Mahdi Saeedipour will study the high-pressure die-casting process in detail by following the three main pillars of the CD-Lab, i.e. (1) analytical analysis of the problem, (2) numerical modelling and (3) experimental validation.

During this year I have observed remarkable progress, which I want to emphasize by the following examples. (1) Our hybrid particle laden flow model has been augmented by particle agglomeration. Sub models account for the formation of particle strands and clusters yielding significant improvement of the computed separation efficiency of a cyclone compared to measurements. (2) The performance of the continuum particle models at industrial scale application has been significantly improved by developing sub-grid models. (3) The hybrid turbulence model has been successfully applied to characterize the short-cut-flow in cyclones and its impact to the separation efficiency.

Finally, our efforts has been honoured by several high impact Journal publications and a plenty of conference contributions, which tremendously improves the international visibility of our group.

Sincerely,



EDITORIAL 4 | EXPERIMENTS

Dear Readers,

Due to the continuous growth of the CD laboratory there is also an increasing demand on experimental data. The activities in our fluid mechanics laboratory have therefore experienced a significant rise over the last years. In 2012 we extended our team by four part-time working students who made valuable contributions to our projects.

The quality of a numerical code inherently depends on the available data for validation and calibration. Basically all projects within the CD Lab and associated research activities contain experimental work packages to address this central issue.

Our experimental know-how is also a key for the knowledge transfer to real world applications. The cover page shows a perfect example how simple measurements techniques can unveil impressive details of fluid mechanics which most of us and our partners have never seen before.

Sincerely,



CONTENTS

ROCK 'N' ROLL

CFDEM	6
Resolved Particle Laden Flows	8
LIGGGHTS	10
Cohesive material	12
Die filling with cohesive powders	14
Resolved Coupling of LB and DEM	16
LIGGGHTS Radiation Model	18

VISITING SCIENTIST

Stefan Radl	20
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DUST 'N' DIRT

Eulerian Particle Model	22
Poor Man's LES	24
Cyclone Separation	26
Hybrid Particle Model	28
Modelling Bubble Columns	30

EXPERIMENTS

Bringing Experiments and Simulations together	32
Spout-Bed Regime Detection	34
Granular Material Properties	36
Raceway Formation	38
Cyclone Efficiency	39
Model Validation Test Rigs	40

INDUSTRIAL PARTNERS	41
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AWARDS AND SELECTED PUBLICATIONS	44
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ROCK 'N' ROLL | CFDEM

“*CFDEMcoupling has grown up*” – this could be the slogan of the last year’s work. While in former times most efforts were put into developing this multi-purpose CFD-DEM coupling, which we call *CFDEMcoupling*, this year’s focus was on improving usability and assuring the quality of the results. An intense study of the particulate flow in a spout fluidized bed was used to compare and validate our numerical predictions to those of other research groups. Further has the close cooperation with Stefan Radl helped to successfully “triple-check” our numerical implementation.

Following our goal of applicability to multi-physics problems a validation study on prediction of dust propagation at a transfer chute was conducted in cooperation with colleagues from Germany and Australia (Fig. 3). Application of *CFDEMcoupling* to model spray-wetting, to be presented at a conference, would be another multi-physics example.

Next steps were taken to test the application of *CFDEMcoupling*, to bigger test cases in terms of larger number of particles. Supported by a large series of experimental measurements of a bubbling bed, mainly conducted by Lukas von Berg, simulations of systems including several millions of particles were performed (Fig. 1, bubbling fluidized bed with 1.4 million particles). Image processing techniques are used to validate numerical results against experimental data (Fig. 2).

A great development allowing for simulation of even bigger systems was the implementation of a so called “coarse grained parcel” approach. This very promising approach will help to push the applicability of coupled CFD-DEM even further. In the frame of ongoing cooperation with Stefan Radl new model approaches will be developed and tested.

Applying smart models to improve the applicability of the models is very important, nevertheless a core asset of coupled CFD-DEM simulations is it’s affinity to “first principles”. Consequently it is a focus of recent and future work to further improve the numerical performance of our code to allow for direct simulation of large scale problems avoiding uncertainties of models.

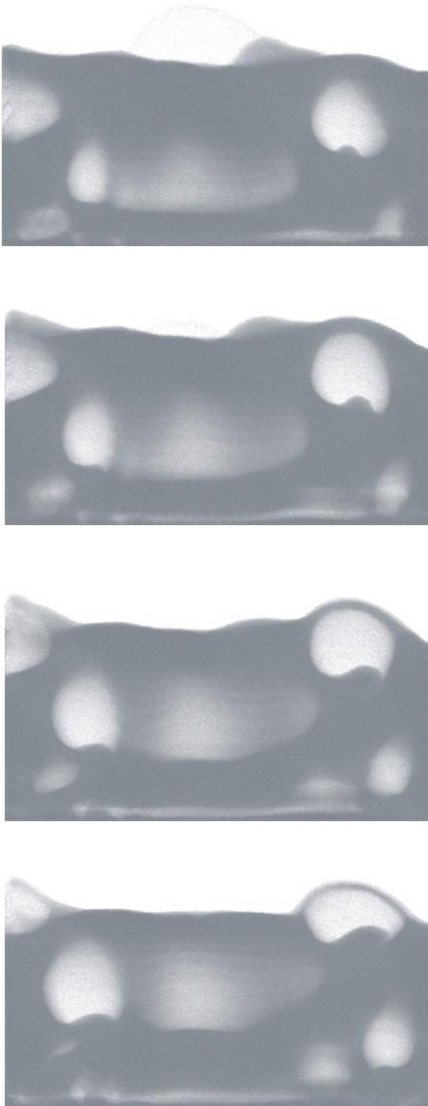


Fig. 1: CFD-DEM simulation of a bubbling fluidized bed.

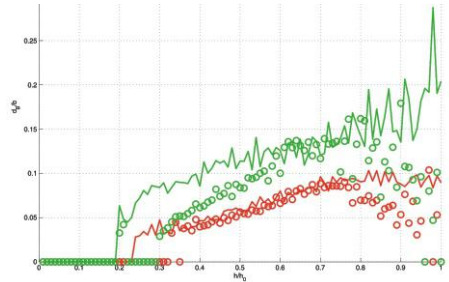


Fig. 2: Quantitative Comparison of measured and simulated bubble diameter over height.

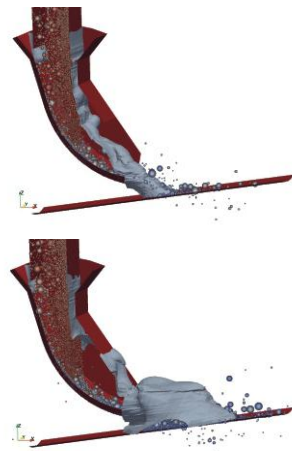
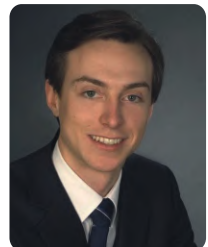


Fig. 3: CFD-DEM simulation dust propagation at a transfer chute.



ROCK 'N' ROLL | RESOLVED PARTICLE LADEN FLOWS

A parallel resolved CFD-DEM method within CFDEMcoupling

The toolbox CFDEMcoupling comprises - amongst others - a solver that allows the computation of the dynamics between immersed bodies and the surrounding fluid. The method used is generally known as fictitious domain method. As is customary for the solvers within CFDEMcoupling, the fluid phase is accounted for with an OpenFOAM®-based finite volume solver while the motion of the objects is calculated with LIGGGHTS. This particular method is a resolved method, meaning that a single body is represented by a number of mesh-cells. Some effort had to be put into representing the bodies accurately, especially the parallelization constituted an interesting challenge.

With the present version of the solver it is possible to tackle a wide range of problems: for purposes of validation we first calculated the drag force acting from the fluid onto a single fixed sphere or cylinder within a fluid flow (cf. Fig. 1.). Further investigations lead to a study of the settling behaviour of two spheres, released above each other in a cubic fluid domain. Fig. 2. shows the acceleration of the upper sphere as it reaches the wake of the lower one, just as predicted by literature. In a next step we added a model that allows the depiction of a rotational motion; Fig. 3. shows the streamlines developing around a rotating sphere in a laminar flow.

The phenomenon describing the accelerated sedimentation of blood cells within a tilted test tube is termed Boycott effect. It can be explained by the fact that the cells approach the wall and therefore increase the density of the suspension in the area (cf. Fig. 4.1). This leads to an overall circulating flow that also increases the settling velocity of the blood cells. Fig. 4.2. shows the flow behaviour of a vertical tube compared to the behaviour of the liquid in the tilted tube.

Prospects are the accurate representation of the blocking of tubes for example.

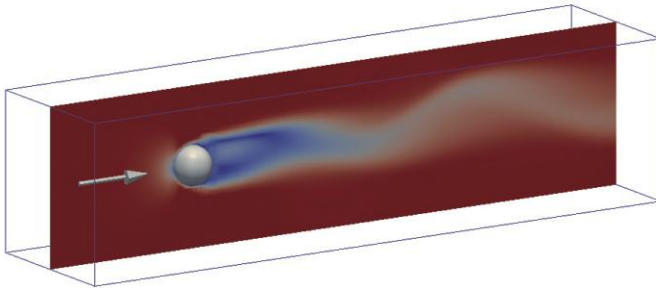


Fig. 1: Flow around a fixed sphere

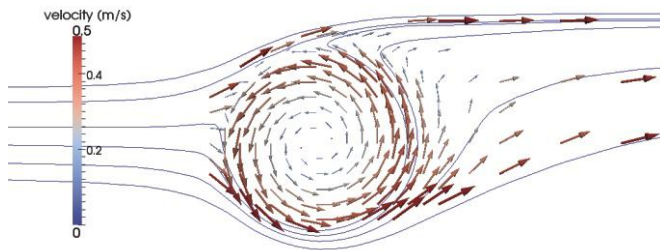


Fig. 3: Streamlines around a rotating sphere

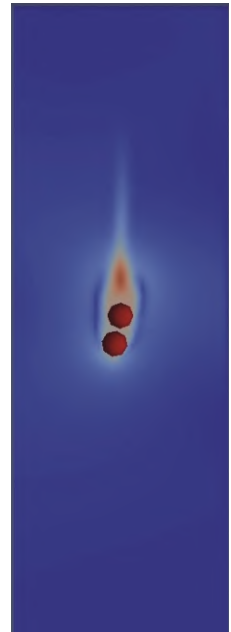


Fig. 2: Settling of two spheres

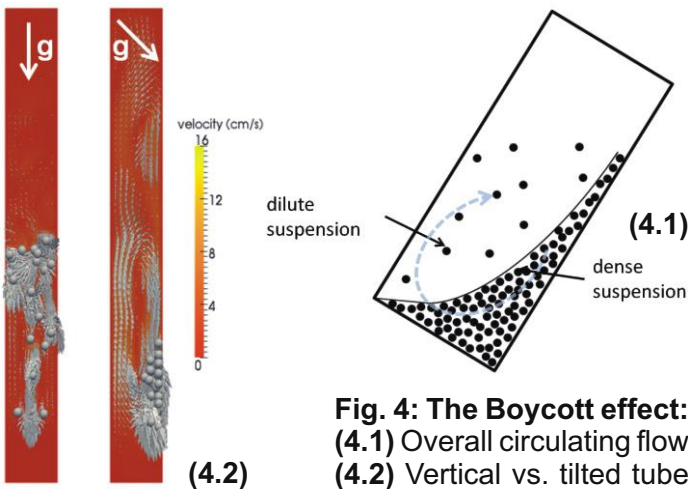


Fig. 4: The Boycott effect:
 (4.1) Overall circulating flow
 (4.2) Vertical vs. tilted tube



ROCK 'N' ROLL | LIGGGHTS

The **ability to solve real-world problems** and ensuring **usability in the industrial context** was the main focus of last year's work on LIGGGHTS. With the help of the whole group, comprising important contributions from Philippe Seil, Stefan Amberger, Andreas Aigner and myself, LIGGGHTS now offers **unrivalled performance compared to other commercial and open source DEM codes** for almost all applications of industrial relevance, being able to scale on big clusters. The readability of the LIGGGHTS scripting language was improved, and DCS Computing is now starting a project to **develop a graphical user interface (GUI)** for LIGGGHTS to ease usability in the industrial context. Just recently an external industrial benchmark of a rotating drum test showed that LIGGGHTS is well ahead of the two commercial market leaders in terms of speed with comparable simulation results. One big step for LIGGGHTS this year was the complete re-structuring of mesh implementation, which removed the last major bottle-neck (see Fig. 3). We'll continue this success path by allocating dedicated personal resources to performance optimization and software quality control.

Of course, as scientists we're aware that in addition to the code efficiency, ambitious **modelling efforts** are needed as well to ensure the applicability of our simulation models. Most importantly, stimulated by a collaboration project with Dr. Stefan Radl (Graz UT), we started to implement physically correct **coarse-graining methodologies** (see Fig. 1).

Further efforts resulting in new models and features comprise

- an MP-PIC method (well-know from a commercial CPFDF code)
- a wall servo to be able to numerically reproduce shear cell experiments and as a boundary condition for large-scale simulations
- an improved performance for particle insertion
- a deforming mesh feature (see Fig. 2)
- simple models for liquid bridges in particle-particle contacts

Also, we're working on a set of **material calibration experiments**, that will serve to extract a reliable set of material parameters for DEM simulations. Additionally, we'll continue with focusing on modeling approaches for non-sphericity and cohesion.

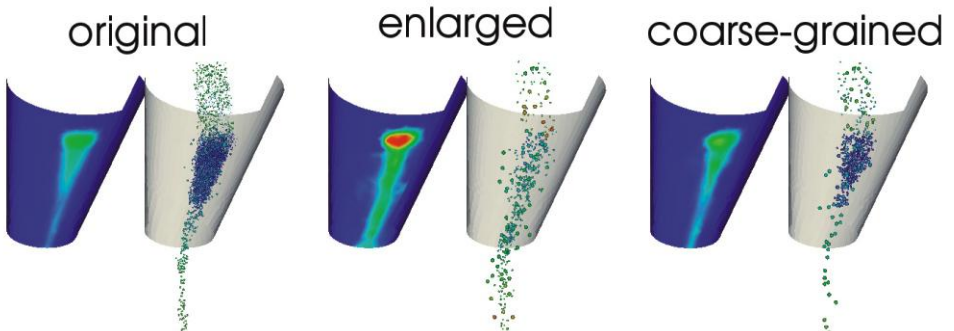


Fig. 1: Showing the difference between enlarged and correctly coarse-grained particles (same mass-flow rate for all 3 simulation) when simulating equipment wear.

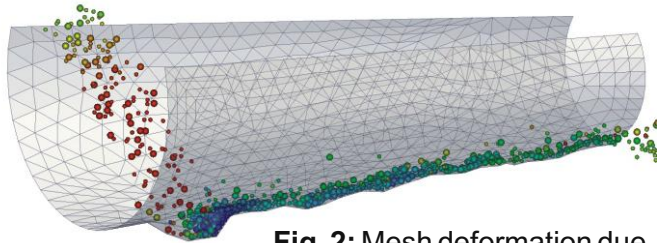


Fig. 2: Mesh deformation due to abrasive wear to chute.

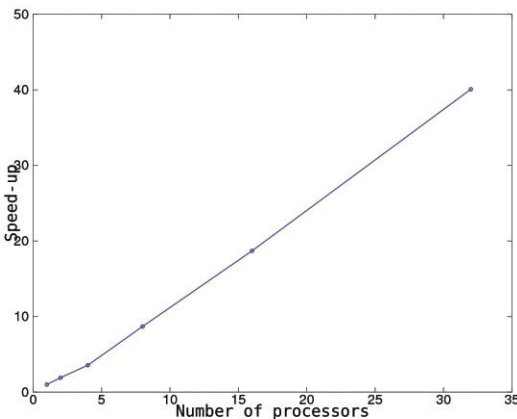


Fig. 3: Parallel scalability for mesh movement in LIGGGHTS 2



ROCK 'N' ROLL | COHESIVE MATERIAL

A wide range of industrial processes use granular media of microscopic scale, for instance coil powder in the blast furnace or the polypropylene powder after polymerisation.

Therefore, additional models are implemented in our simulation tool LIGGGHTS that take account of the increasing influence of cohesive forces due to decreasing particle radius.

In general these forces can be divided into two subgroups, namely contact and non-contact forces. The latter includes – among others – the van der Waals forces and are very small even for very fine powder considered in our projects. However, we expanded LIGGGHTS with a Hamaker constant model to study their influence and exclude them as a possible cause of investigated phenomenon.

On the contrary cohesive contact forces are dominant. Unfortunately, their dependency on the particle displacement is highly nonlinear and force measurements show up a hysteretic behaviour that is mainly caused by particle deformation. Simulation models, however, have to be as accurate as possible at acceptable computational costs. Whereas, we implemented a piece-wise linear, hysteretic, adhesive force-displacement model according to Luding (2008) into LIGGGHTS. (see Fig. 1)

All modelling efforts are worthless for our industrial partners without validating those by comparison of simulation results with analytic or experimental data available in literature or received by experiments. Thus we not only build up several test-rigs in our laboratory, but also we implemented new features into LIGGGHTS to be able to simulate these experiments.

Shear cells, for example, are used to characterize material properties. Therefore, a wall that exerts a defined stress on the material is indispensable. Recently we have added a force-controlled wall to our toolbox in order to simulate experiments done in our laboratory and FH Wels.

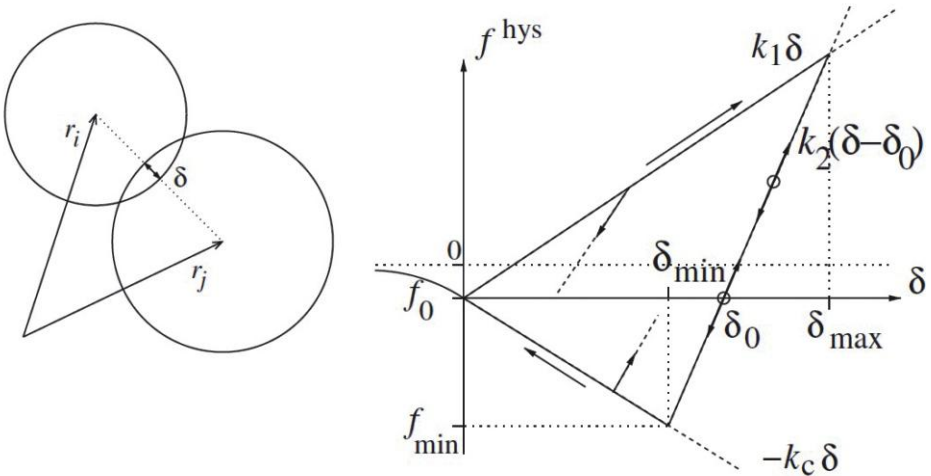


Fig. 1: **Left:** Two particle contact with overlap δ in normal direction. **Right:** Schematic graph of the piece-wise linear, hysteretic, adhesive force-displacement model in normal direction. The non-contact forces, e.g. Hamaker constant model, are indicated by f_0 and the line for negative δ . (cf. Luding, 2008)

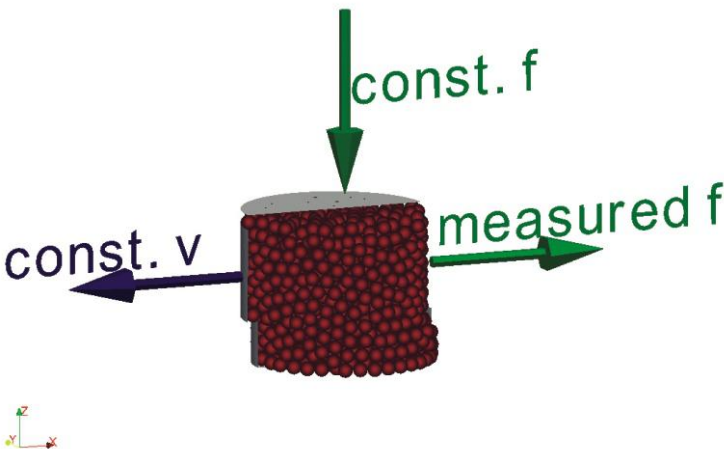


Fig. 2: Sketch of a simple shear cell, which was built up by a student.



ROCK 'N' ROLL | DIE FILLING WITH COHESIVE POWDERS

Powder compaction and sintering are important techniques for the mass production of geometrically complex parts. Powder is poured from a reservoir into the feeding shoe, which then passes the cavity thereby delivering powder into it. Uniaxial compaction of the powder creates a relatively brittle green body which is ejected from the cavity and sintered in a furnace. A consistent and uniform die filling process is always desirable. Heterogeneity during die filling can propagate through the subsequent processes and finally lead to serious product defects.

Powder modeling is a very challenging area inside DEM universe. Many different aspects like physics models and parameters, computational power and coarse graining require an extra attention when modeling in such small scale. Correctly understanding these factors is crucial for the success of powder dynamics modeling.

A feasibility study to understanding how current models of LIGGGHTS could reproduce the process was the first step of the project (Figure 1). Tests were done using current simplified JKR cohesion model and current contact model, with good results for low compression cases (Figure 2).

Further improvements in physical models are under development, like a liquid bridge model to correctly capture the cohesive effects in powders. An experimental apparatus was built to validate implemented models in LIGGGHTS (Figure 3). Also studies have been conducted to identify experiments that can correctly characterize the granular material (Figure 4).

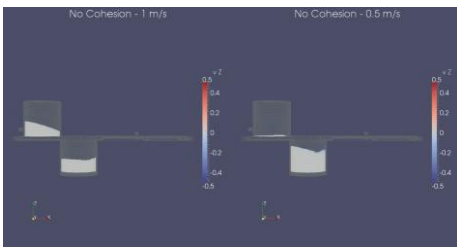


Fig. 1: Simplified die filling model to evaluation of different process parameters.

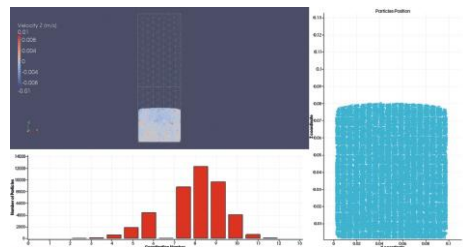


Fig. 2: Compressive stages and coordination number.

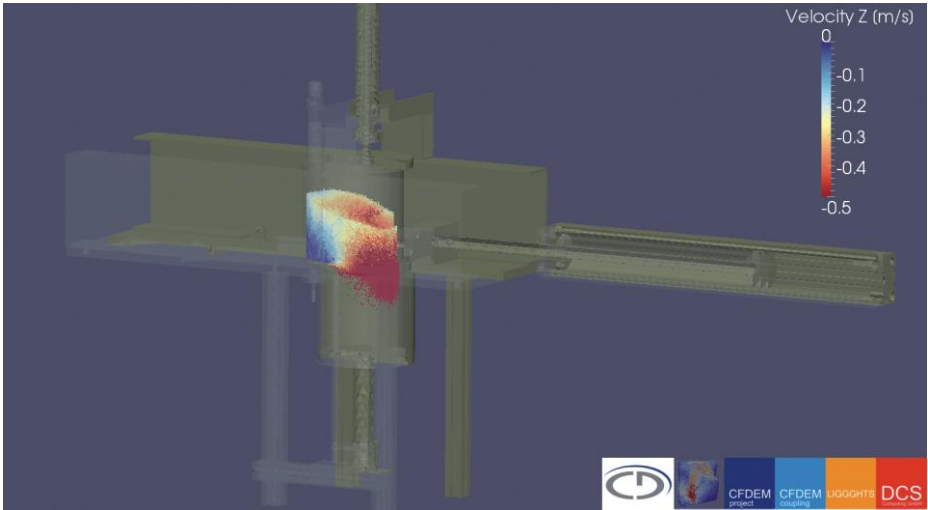


Fig. 3: Simulation of experimental apparatus built up in CD Lab.

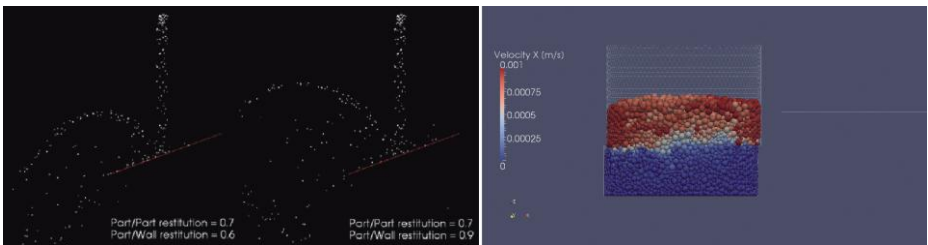


Fig. 4: Initial tests to calibrate coefficient of restitution (top) and internal friction and cohesion (bottom).



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ROCK 'N' ROLL |

RESOLVED COUPLING OF LB AND DEM

Lattice Boltzmann (LB) is a CFD method rooted in kinetic theory. Instead of solving the Navier-Stokes equations, a discretized version of the Boltzmann transport equation is solved directly. The fluid is represented by particle fractions (populations) that move in different directions. During the collision step, these fractions follow a tendency to local (within a grid cell) thermodynamic equilibrium. In the streaming step, the populations are redistributed according to their velocity. Macroscopic flow quantities such as velocity or pressure are deduced from the populations. One great advantage of LB is that, due to its origin in gas kinetics, imposing no-slip boundary conditions is very easy: The incoming particles on a solid boundary grid cell are reflected back to its origin.

Coupling to a particulate phase can be realized by immersed boundary methods that fully resolve the shape of a particle within the computational domain for the LB calculations. First, the solid fraction for each grid cell is computed (see figure 1). Then, the new particle populations are calculated as a superposition of bounce-back and collision, weighed by the solid fraction. In this step, it is also possible to account for moving surfaces. The forces on the particle can also be calculated in this step, making it possible to couple LB simulations to a DEM code and perform fully resolved simulations of granular flow.

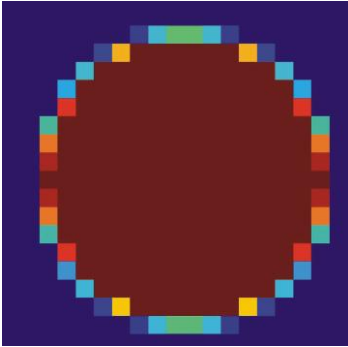


Fig. 1: Representation of a circular disk within the LB domain. Colors: solid fraction of a cell, blue = 0, red = 1



Fig. 3: Settling of two particles in a column of fluid

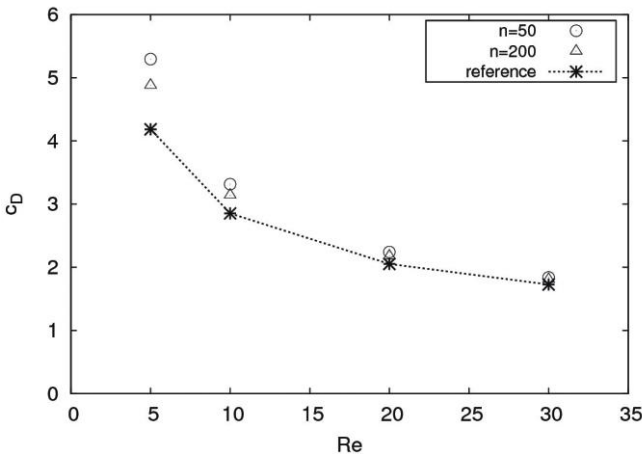


Fig. 2: Drag coefficient vs. Reynolds number for different resolutions, bold line: reference



ROCK 'N' ROLL | LIGGGHTS RADIATION MODEL

Radiation Model

Heat conduction in hot, medium to dense particle-flows is dominated by radiation, rather than conduction. Stefan Boltzmann's law is one model that describes the power radiated from a black body in terms of its temperature.

In order to enhance the capabilities and accuracy of LIGGGHTS for hot particle flows we developed, implemented and verified a model, based on Stefan Boltzmann's law (SB law) and the ray-tracing technique, that calculates the radiative heat-flux between particles themselves (particle-particle heat transfer) and between particles and the background (cooling). Fig. 1 shows a sketch of how ray-tracing is used in the model.

Verification included a comparison between the analytic solution of SB law for a single sphere and the results of a numeric simulation of the same setup (see Fig. 2 and Fig. 3), to verify the background-radiation behavior of the model, as well as a comparison between the analytic solution of the heat transfer between two parallel dishes and a simulation with a similar setup (see Fig. 4 and Fig. 5), to verify the heat-transfer behavior of the model. Deviations from the analytic solution for each of the setups were smaller than one percent.

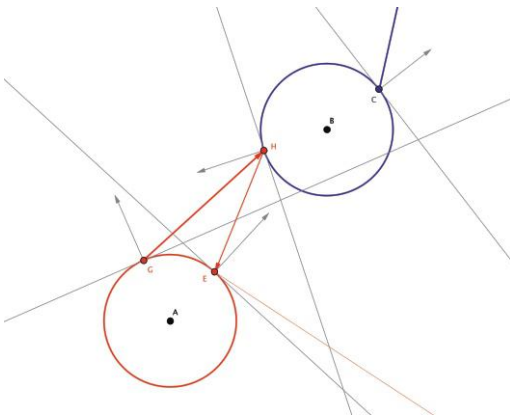


Fig. 1: In the model, ray-tracing is used to calculate the heat transfer, including reflection and background-radiation.

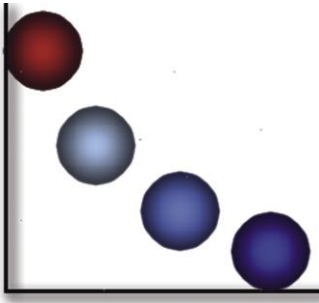


Fig. 2: Verification 1 – Cooling of a single sphere

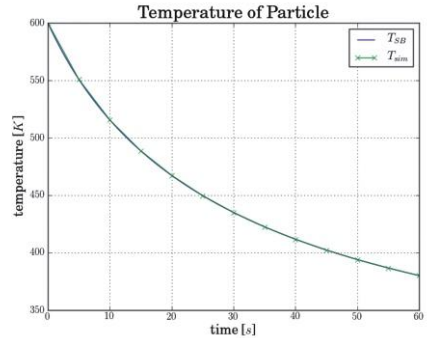


Fig. 3: Verification 1 – Result

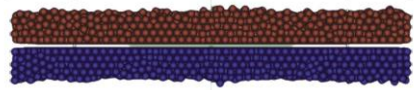
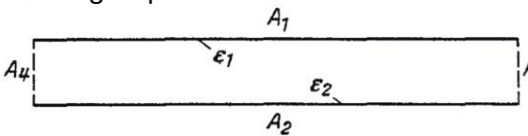


Fig. 4: Setup of Verification 2 – Heat transfer between two parallel dishes (left: see VDI Wärmeatlas, Vol. 7, 1994)

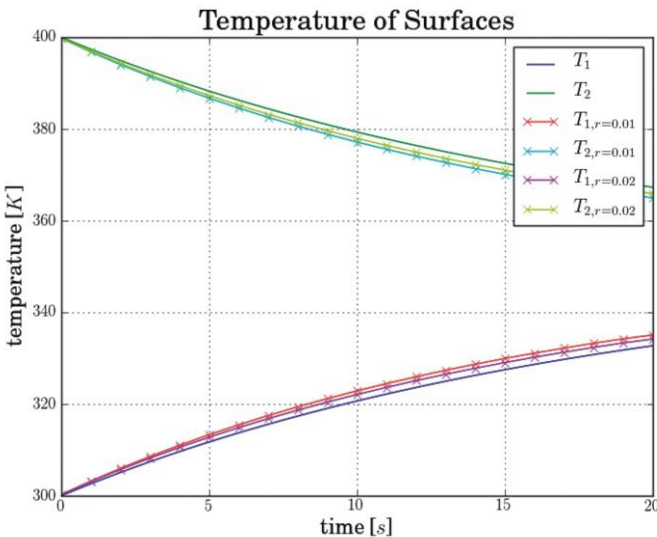


Fig. 5: Verification 2 – Result



Jumping over a Scale Gap with Parcels

In a parcel-based approach the particle population is represented by a relatively small number of computational entities, i.e., so-called parcels. Thus, one tries to “jump” from the particle level to a macroscopic description of the flow and still use a Lagrangian approach. While such an approach has been used in the spray community for decades, the application to relatively dense granular flows is still connected to major uncertainties (e.g., see O'Rourke and Snider, CES 80, 2012).

In a joint work of Stefan Radl (Graz University of Technology), Christoph Goniva and Christoph Kloss (JKU Linz), several parcel-based models were implemented into LIGGGHTS and CFDEM. Verification and validation simulations were run for relatively dilute granular flows (e.g., crossing of two granular jets, sedimentation of a gas-particle suspension) as well as dense granular flows near the close-packing limit (e.g., chute flow, hopper discharge). Selected results for the crossing of two granular jets are display in Figure 1, demonstrating that parcels can or cannot predict certain flow features depending on the model used. Guidelines were developed that now help industry to choose the right model formulation when using parcels.

In addition to parcel approaches, a new generation of drag models was implemented, which give more accurate predictions of the slip between gas and particles in moderately dense fluidized beds. Some key results for periodic domain simulations are shown in Figure 2, highlighting the performance of these advanced drag models.

This project showed that there is substantial more potential for cooperation between Graz and Linz: the group of Stefan Radl in Graz is focusing on the development of micro- and meso-scopic models for granular and gas-particle flow implementing these models into a joint, open-source platform such as LIGGGHTS or CFDEM is an extremely fruitful approach that has already opened new perspectives for industrial applications.

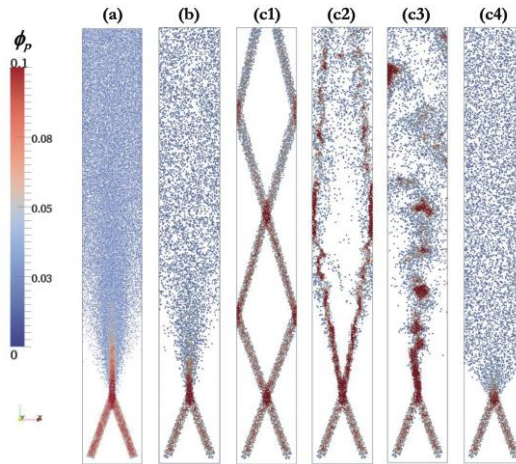


Fig. 1: Particle distribution (particles are colored according to their local particle volume fraction) for the granular jet crossing using (a) the DEM, (b) a parcel-based method with collision detection and relaxation model, (c1-c4) various flavors of a parcel-based method without collision detection.

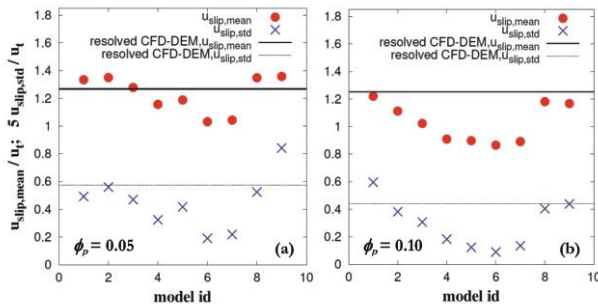


Fig. 2: Normalized domain-averaged slip velocity (mean, as well as standard deviation; lines indicate reference results from CFD-DEM simulations) obtained from parcel-based simulations with different model settings of sedimentation in a periodic domain (the most favorable models with ids 8 and 9 incorporate aspects of the kinetic theory of granular flows).



DUST 'N' DIRT | EULERIAN PARTICLE MODEL

Fluidized and moving beds are widely used in chemical and process industries. In the past decades two fluid models (TFM) have become a valuable design tool for modelling pilot plant scale gas-solid fluidized bed reactors. However, due to computational limitations a fully resolved simulation of industrial scale reactors is still unfeasible. It is, therefore, common to use coarse grids to reduce the demand on computational resources. Such a procedure inevitably neglects small (unresolved) scales, which leads to a considerable overestimation of the bed expansion in case of fine particles (figure 1b). It is generally agreed that the influence of these small scales on the drag force is a key parameter in the prediction of the bed expansion. It is further observed that in this case the simulation delivers a completely different behaviour of the fluidized bed (figure 1)

Therefore, we have developed a sub-grid drag model, which accounts for the unresolved small scales in fluidized bed reactors. The results show that applying the new sub-grid drag modification excellent agreement of predicted bed expansion and bed behaviour with the fully resolved simulation (figures 1&2) and with experiments. Furthermore, the computed bubble rise velocities using a coarse grid are in fairly good agreement with experiments (figure 3). Compared to the resolved simulation the computational demand is reduced by approximately two orders of magnitude using the coarse grid for equal time step sizes.

Additionally, we studied the influence of polymer particles on the rheology. It is observed that the inter-particle friction coefficient and small-scale non-sphericity of the grains have a significant influence on the discharge rate from hoppers, which has also been confirmed by experiments.

To conclude, these developments bring us a big step closer to the scale up of the numerical model to industrial scale fluidized bed reactors. Next steps will concentration on extending the current models by heat transfer and chemical reactions.

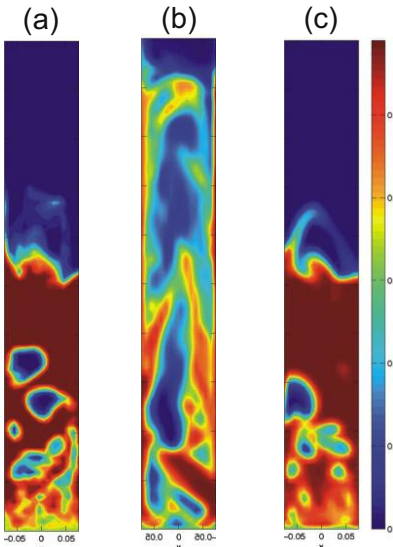


Fig. 1: Snapshot of the solids volume fraction (z in m). a) fully resolved, b) coarse grid using standard drag and c) coarse grid using new sub-grid drag modification.

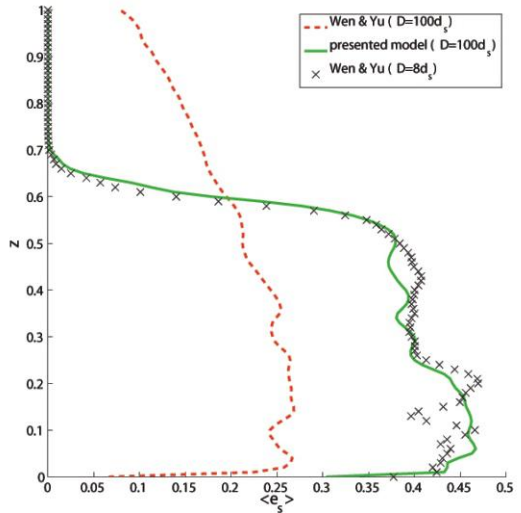


Fig. 2: Axial profile of the time averaged filtered solids volume fraction. X: fully resolved; ---: new sub-grid drag modification; - - -: standard drag.

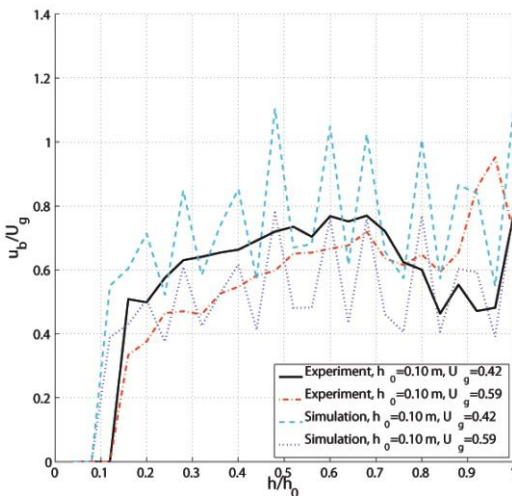


Fig. 3: Comparison of measured and computed bubble rise velocities.



DUST 'N' DIRT | POOR MAN'S LES

Thanks to an ambitious team of experienced senior scientists, who forward independent research and also supervision, I found some time for my own research. Developing new numerical models is a pleasing luxury beside all this administrative and organizing stuff that comes along with my position as head of the CD-Lab.

In gas-solid cyclones an interesting flow phenomenon can be observed in the top region. Once the rotating flow faces the stationary cover plate a Bödeward layer establishes which transports fluid towards the vortex finder. If this inward flow redirects towards the vortex finder entrance (see Fig.1) a short cut flow will establish. Obviously, such a flow configuration might impair the overall separation efficiency.

Actually, the occurrence of this phenomenon is triggered by turbulence. If the downward oriented short cut flow is dispersed by unsteady turbulent eddies the overall effect on separation efficiency might be negligible. Consequently, simulating this effect requires an unsteady scale resolving turbulence model like a Large Eddy Simulation (LES) model.

It is well known that the application of LES to engineering problems is limited by excess computational resources. This limitation of LES has been met by two measures. Firstly, LES is only applied in an interesting sub-region of the computational domain. In our case we can embed a LES just into the upper annulus part of the cyclone (see Fig.2). Secondly, we could realise LES not by conventional Finite Volume based CFD but by a lattice Boltzmann solver. Both measures increase computational efficiency by one to two orders of magnitude. Finally, in Fig. 3 a comparison with experimental data indicates that this turbulence model delivers accurate results.

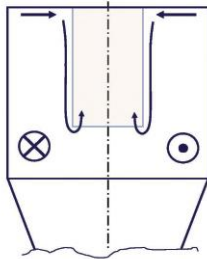


Fig.1: Sketch of short cut flow phenomenon

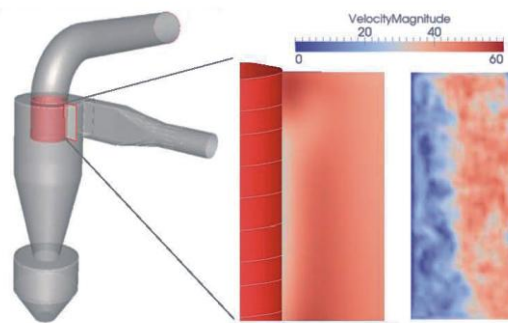


Fig. 2: Geometry of the cyclone, LES region and comparison between Reynolds Averaged Navier-Stokes (RANS) and embedded LES simulation

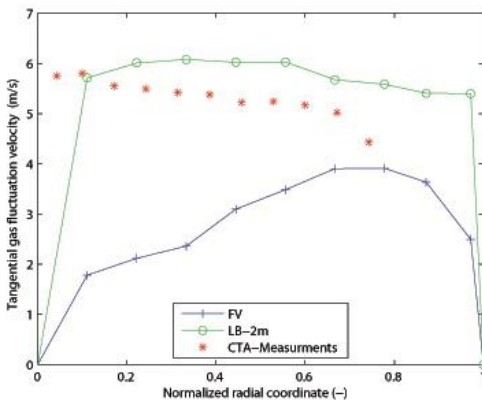


Fig.3: Comparison between (blue) RANS, (green) LES and (red) measurements



DUST 'N' DIRT | CYCLONE SEPARATION

Minimizing the pressure drop

The kinetic energy stored in the tangential component of the vortex motion is actually lost due to dissipation downstream. This is also the reason for decreasing pressure loss of the cyclone with increased mass loading and/or wall roughness: In this case the swirling motion is not so strong and the losses due to subsequent dissipation are smaller.

The attempts to regain the kinetic energy from the swirl and thus to minimize the pressure loss of the cyclone are almost as old as the cyclones themselves. In the majority of cases the pressure loss is decreased by installing diverse kinds of rectifying vanes or other built-in components inside the cyclone body or the vortex finder. Some improvements can also be made by changing the vortex finder geometry or position. However, there are certain types of cyclones which work under harsh conditions (high temperatures, danger of corrosion etc.), where such vanes or similar built-in components inside the cyclone body or the vortex finder should be avoided as far as possible. For this reason, a pressure recovery type diffuser on the top of the cyclone body is considered.

Furthermore, in cases of gas-particle flows with high humidity level there is a danger of settling and sticking down of particles on horizontal planes. For this reason the horizontal planes within the apparatus should be avoided as well. Therefore the second configuration has no horizontal planes. The radial diffuser on top of the cyclone body is arranged under the angle of 30° with respect to the horizontal. The two considered diffuser geometries are shown in Fig. 1 (see next page).

Both numerical simulations and experimental measurements are used to find the optimal dimensions of the diffuser. With the diffuser pictured on the next page up to 30% pressure recovery is possible. Also, the radial pressure distribution along the channel height is investigated (Fig. 2). This clearly shows that the position of the pressure measurement inside the channel is very important.

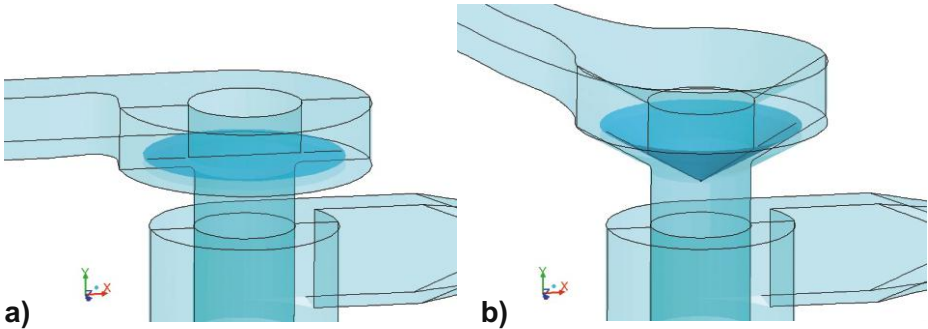


Fig. 1: Radial diffuser geometries, a) “horizontal”, b) “inclined”

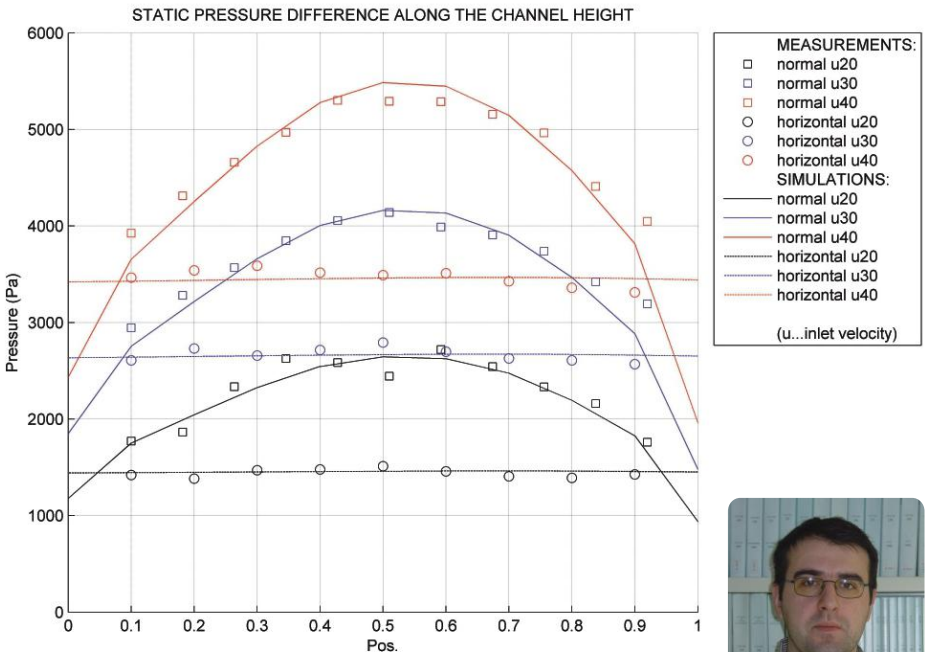


Fig. 2: Cyclone pressure loss: Comparison of normal and “horizontal” geometry



DUST 'N' DIRT | HYBRID PARTICLE MODEL

In dense laden gas-particle flows a mathematical representation of the individual particles (i.e. a Lagrangian particle tracking) is not possible due to an excess number of particles. In this case it is common use to smear out the individual particle properties and consider the multitude of particles as a continuous particle phase which can interpenetrate the gas phase.

While this Eulerian representation of a particle phase is well established for mono- or bi-disperse particle laden flows it is not applicable for general poly-disperse flows.

Within a co-operation with Polysius AG we tried to extend the applicability of Eulerian particle models to poly-disperse flows. This is achieved by introducing Lagrangian tracer particles which interact with the continuous particle phase. The resulting hybrid – Lagrangian and Eulerian – particle model is able to picture e.g. particle separation in a cyclone as shown in Fig. 1. This model combination has proven to deliver better results at significantly lower computational costs if compare to either pure Eulerian or pure Lagangian approaches.

In a separate research efforts this hybrid particle model has been extended in order to account for the effect of particle agglomeration. Especially, very small particles tend to permanently stick to larger particles during collision events. This influences the overall separation efficiency because those small particles will then be separated together with the larger host particles. In Fig.2 a sketch of this model extension is given and Fig. 3 depicts a first plausibility check.

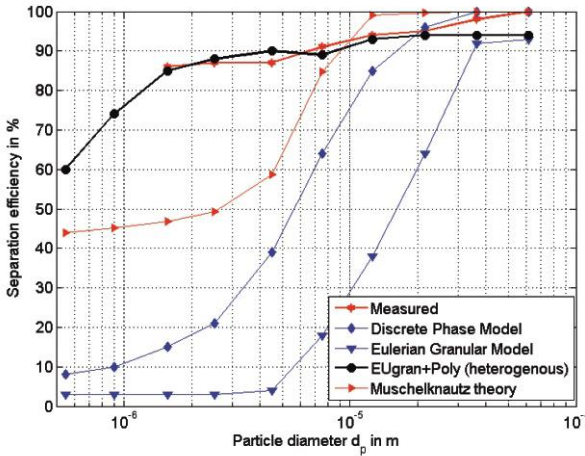


Fig. 1: Separation efficiency as result of several numerical models

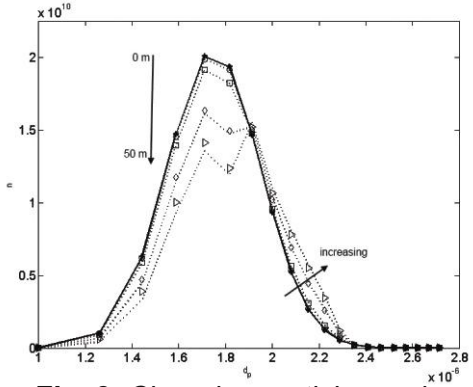
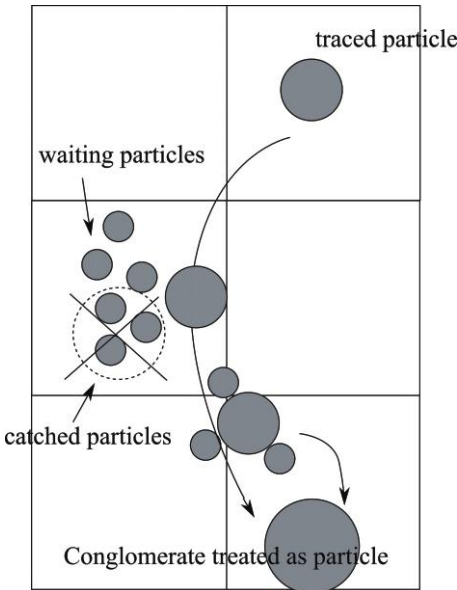


Fig. 3: Changing particle number density due to agglomeration.

Fig. 2: Sketch of the agglomeration model extension.



DUST 'N' DIRT | MODELLING 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.

In cooperation with SIEMENS AG counter-current flotation columns are investigated. As a fundament the study of bubble columns is necessary. These are modelled using analytic and numerical models and studied experimentally.

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.

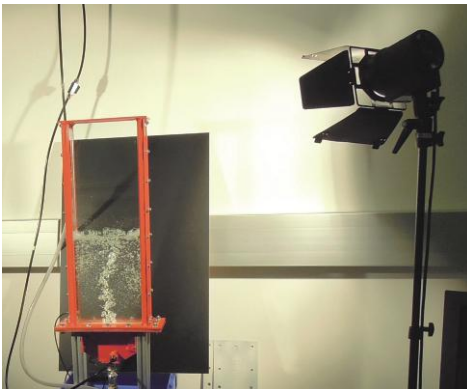


Fig. 1: Experimental setup in Operation



Fig. 2: Still image of high-speed video. The bubble column is aerated through a porous plate at the bottom.



A good qualitative accordance of simulation and experiment has already been accomplished. In a next step a quantitative investigation is to be conducted.

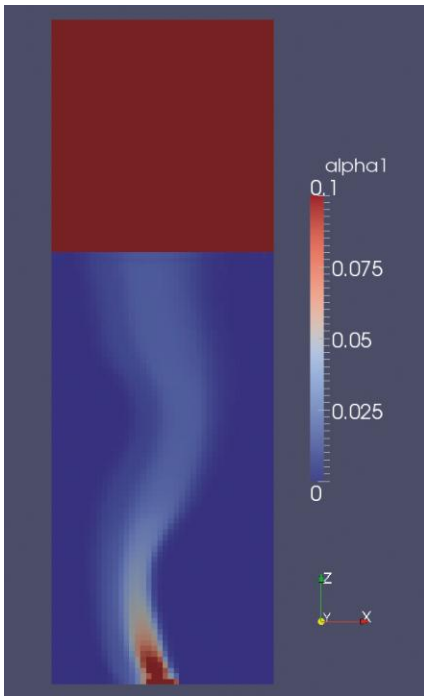


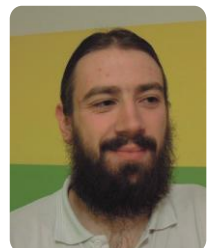
Fig. 3: simulation result



Fig. 4: experimental result

The cross-section and the water level are in both cases equal (width x depth x height = 20 x 5 x 39 cm).

Rising bubbles induce vortices inside the liquid. These vortices deflect the bubble plume and cause the formation of a meandering bubble plume.



Supervision: Schneiderbauer **Gerhard Holzinger** | gerhard.holzinger@jku.at

EXPERIMENTS | BRINGING EXPERIMENTS AND SIMULATIONS TOGETHER

Complex multiphase problems are also a challenge from the experimental point of view. Unlike numerical results where all physical values are available for the whole computational domain, experimental data is often limited to planar information (e.g. planar laser based imaging) or two-dimensional projections of the three-dimensional problem (global imaging). For these cases it is often impossible to extract quantitative data (like e.g. volume fraction of particles) and experimental analysis is limited to qualitative or pseudo-quantitative data.

The primary goal in comparing numerical with experimental results is therefore to bring the datasets on the same level of abstraction. This could mean to step down to qualitative analysis for the numerical results or to extract quantitative data from pure qualitative images by sophisticated image processing methods.

The figures on the right side demonstrate the data processing for fluidized bed experiments and simulations. In this case it is possible to obtain physical values like equivalent bubble diameters or bubble rise velocities. As a first step an object detection algorithm identifies all bubble objects (Fig. 2) fulfilling certain criteria. In a second step the objects are tracked in two consecutive images (Fig. 3). From the displacement vectors the bubble velocities can be calculated.

The example images show experimental data but the very same data processing can be applied to post-processing images from CFD or CFDEM simulations. This allows for direct data comparison (Fig. 4) and improvement of the numerical models.



Fig. 1: Fluidized bed test rig with background illumination

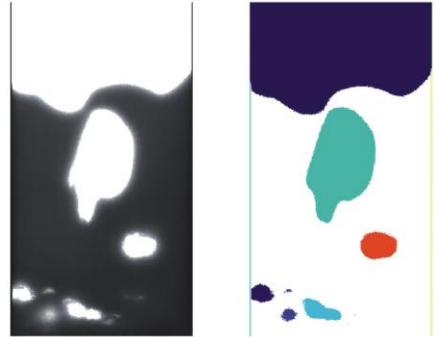


Fig. 2: Raw image from high-speed camera (left) and detected bubble objects (right)

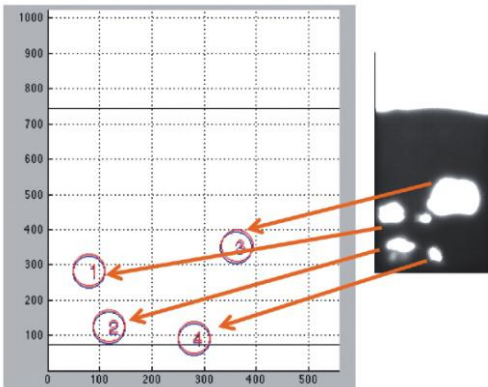


Fig. 3: Object tracking for velocity calculation

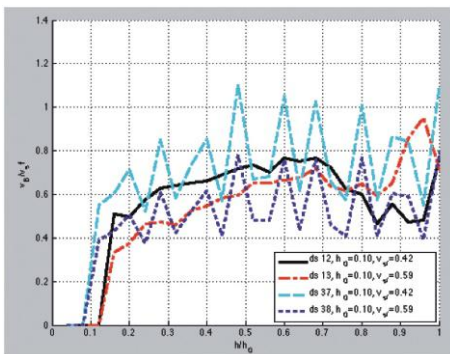


Fig. 4: Bubble rise velocities for experiments (black and red) and CFD (cyan and blue)



EXPERIMENTS |

SPOUT-BED REGIME DETECTION

Fluidized beds have a huge variety of applications in process industry. As the desired properties of the fluidized bed can strongly vary according to the process, it is crucial to have proper knowledge of the flow regimes within the fluidized bed. In typical large scale applications in industry, fluidized beds are operated with one or more spout sections without background fluidization. In such cases it is necessary to minimize dead zones between the spouts to avoid sticking of material in these areas. Spout operated beds also show some mixed regimes (like e.g. spouts within a bubbling bed). These mixed regimes might appear only within close borders of superficial velocity or bed height. Therefore, it is helpful to have regime maps or correlations to predict the bed behaviour for certain boundary conditions correctly.

After a general visual classification of the flow regime (Fig. 1), the recorded image sequences were processed in Matlab to identify the different bed zones. Calculating the mean images and pixel variance images allows identification of the dead zones and annular regions for the spout bed regimes (Fig. 3). In the bubbling zones a Lagrangian object tracking calculates equivalent bubble diameters and bubble rise velocities. In addition, a PIV (particle image velocimetry) cross correlation can calculate particle velocities. The basic idea for all processing steps is that they work equally on experimental images and post-processing images from CFD and CFD-DEM coupled simulations. This provides a good basis for data comparison and evaluation of simulation models.

From the pressure drop information the frequencies of spout collapsing or slugging can be extracted via FFT (Fast Fourier Transform). In the case of an internal jet with bubbling bed the bubble eruption frequency can be detected (Fig.2).

The observed values for minimum spout velocities and jet penetration length match quite well with correlations from literature.

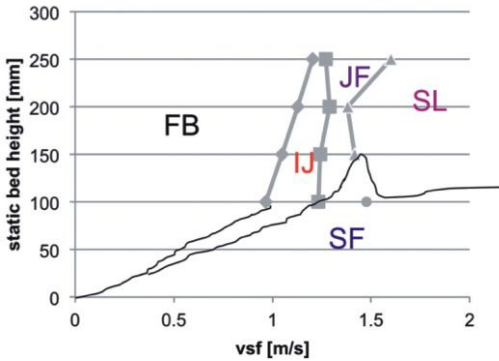


Fig. 1: Regime map for 2mm particles.

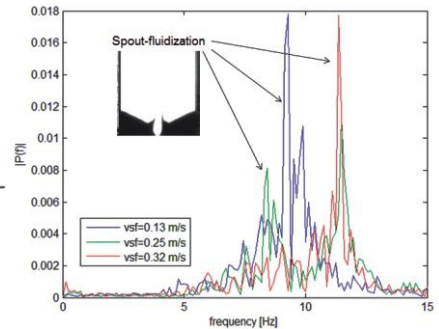


Fig. 2: Fourier transform of pressure signals.

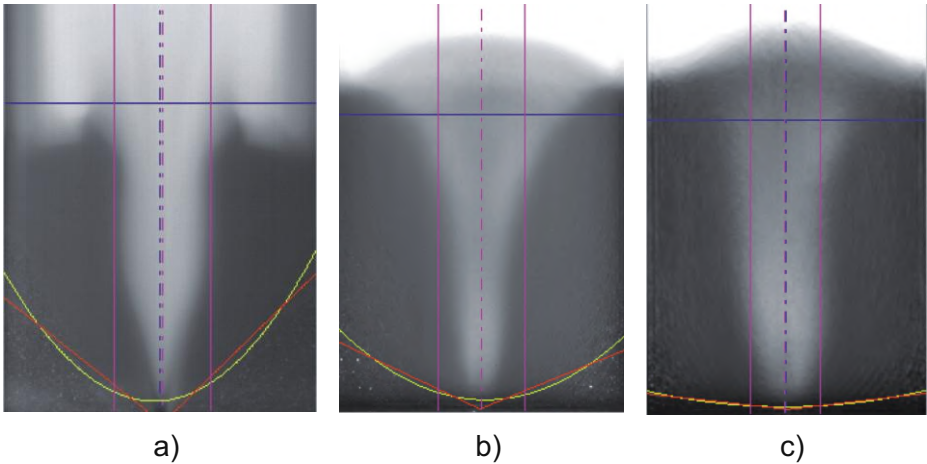


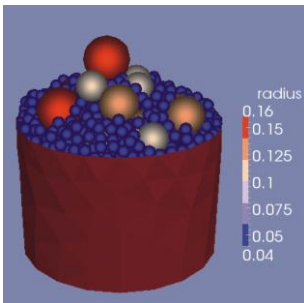
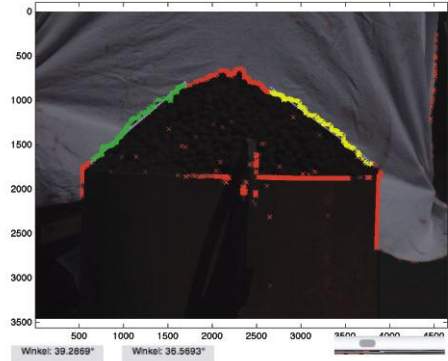
Fig. 3: Bed zones in spout-bed regime for a) 0.5mm, b) 2mm and c) 4mm particles. The blue line marks the static bed height, the magenta lines identify the spout regions and the yellow and red lines mark the dead zones via square and linear interpolation.



EXPERIMENTS | GRANULAR MATERIAL PROPERTIES

Angle of repose

A software for automatic calculation of the angle of repose has been implemented in Matlab. The software can be used in-house and also to do on-site tests at voestalpine with various materials, such as ore pellets, sinter and lump ore.

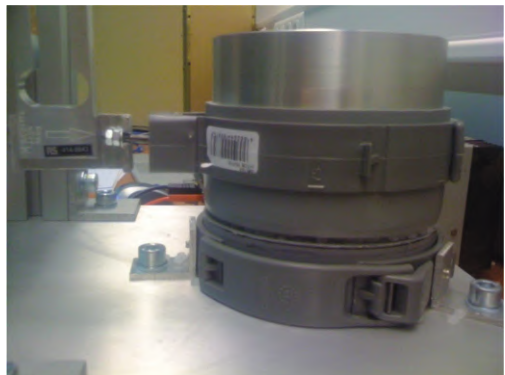


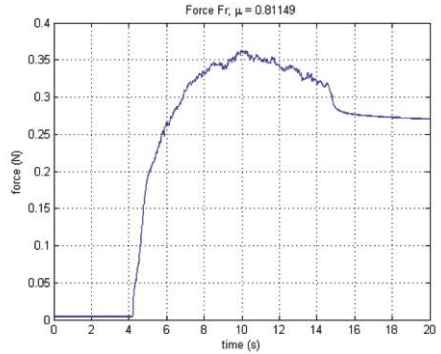
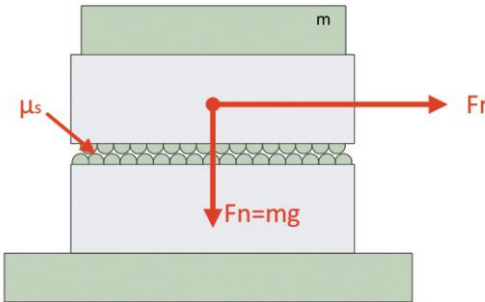
In addition simulations were done with LIGGGHTS to cross check the results of the experiments. The LIGGGHTS simulation was parameterized with the grain size distributions obtained from sieve analysis of the material.

Sliding friction

A device similar to a shear cell has been built to identify the coefficient of friction.

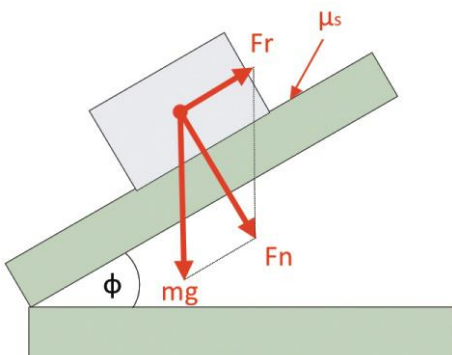
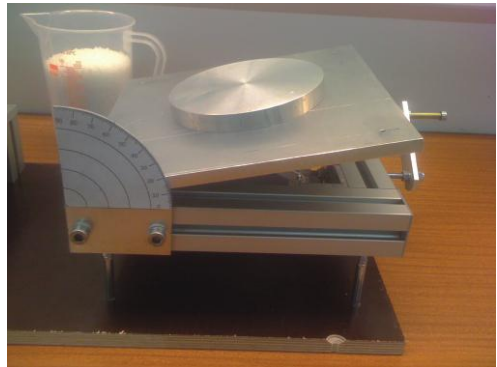
$$m_s = \frac{Fr}{Fn}$$





Rolling friction

To identify the rolling friction a thin layer of material is placed on an inclined surface. When the angle of inclination is increased, the particles will start to move at a certain level.



Florian Aigner | Michael Friedl



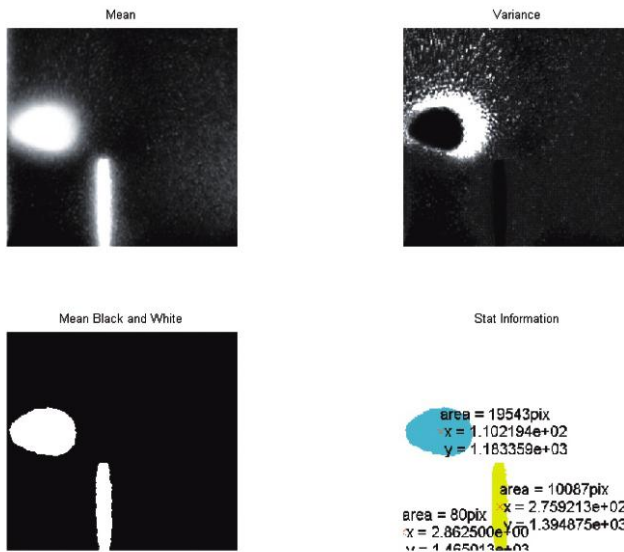
florian.aigner@jku.at | michael.friedl@jku.at

EXPERIMENTS | RACEWAY FORMATION



In a pseudo 2D test rig local fluidization can be investigated visually. Air is injected into a granular bed through a nozzle. As soon as the momentum of the air jet exceeds a certain level, the particles in the surrounding area start to move and circulating area similar to a blast furnace raceway. The behavior of the raceway is depended on air inlet velocity, bed height, nozzle diameter and particle shape and diameter. Aim of the experiment is to measure and analyze the formations and compare them with computer simulations.

Fig. 1: Video coverage and subsequent image analysis of raceway formation

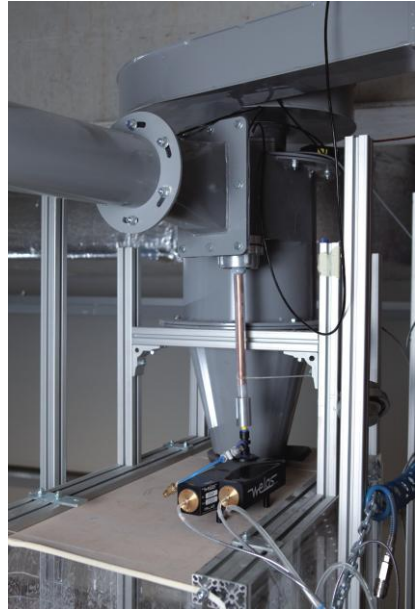


Nikolaus Dopplhammer

EXPERIMENTS | CYCLONE EFFICIENCY



CFD simulations with alternative cyclone heads have predicted possible reductions in pressure drop up to 30%. To validate this results detailed pressure measurements have been conducted with various cyclone heads. Experiments confirmed the CFD results.



By measuring the particle inlet and outlet spectra with a particle analyzer we could also demonstrate that the cyclone separation efficiency is not influenced by the type of cyclone head



Lukas Fiel | lukas.fiel@gmx.at

EXPERIMENTS | MODEL VALIDATION TEST RIGS

In accordance with the CD Labs three column concept, the created CFD models have to be validated with experimental data. Therefore it is necessary to think about adequate test bench principles, measurement- and analysis techniques and unify this into a precise, functional and adaptive facility.

For our studies we engineered multiple test benches, each fitted to the special requirements of the dedicated projects. Representative the two following projects should be named.

The so called SANDY project (see Fig. 3 on page 15) was developed in cooperation with Plansee and describes a semia.tomatic rig which is used to investigate liquid bridge building phenomena in powders. All aspects of structure work, measurement techniques, electronics design, automation algorithms and data processing was done in the CD Lab and guarantees great flexibility.

A just upcoming project in cooperation with LKR deals with high pressure die casting. Therefore design ideas for fast response and minimal invasive temperature measurement techniques was developed and again crosschecked with analytics and CFD studies. The great accordance of the experiment with the analytics and Fluent is shown in Fig 2 and indicates the succeeded principle.

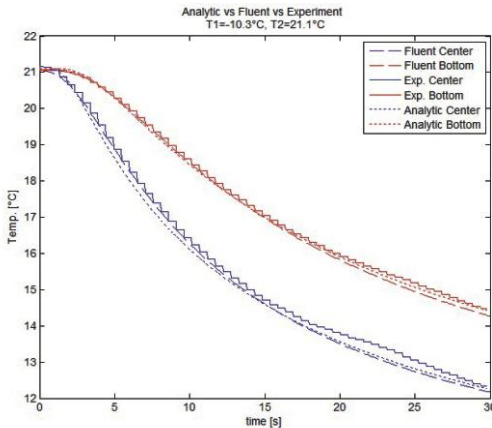
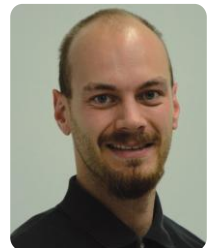


Fig. 1: Thermal wave propagation: Experiment, analytics and CFD



Supervision: Pirker, Puttinger

INDUSTRIAL PARTNERS

In a counter current reactor like the blast furnace the gas flow cannot be analyzed without considering the particle flow. There is a strong mechanical, thermal and chemical interaction between them. For this reason it is highly important for us as blast furnace operators to cooperate with specialized partners who support us with outstanding tools and knowledge to get deeper insight into our process. This partner we found in the team of the CD-Lab.

Christoph Feilmayr | voestalpine Stahl GmbH

Industrial plants such as COREX® and FINEX® are no place for experiments and yet continuous innovations are expected. Therefore we need the development und concurrent validation of fundamental models for the simulation of dense particulate flows. The simulation of particulate flows requires new techniques in experimental, analytical, mathematical and computer matters. For this purpose we rely on this CD-Lab as our scientific partner.

Franz Hauzenberger | Siemens VAI Metals Technologies GmbH

The competence and expertise of the CD Lab allows us to explore complex fluid dynamic processes, which are otherwise hidden due to the harsh conditions of iron- and steelmaking. For us as an industry partner it is crucial to validate the results of the simulations with laboratory scale tests to achieve useful knowledge, which can lead to an optimization of industrial plants and processes.

Hugo Stocker | voestalpine Stahl Donawitz GmbH

In cement plants and applications for the minerals industry a lot of fine particles like dust and powders are produced, transported and separated. As a turn-key supplier for this industry it is our aim to understand the physics behind the processes for improving our equipments and machineries furthermore. One focus in doing so lies in modern simulation techniques like CFD. Our goal is to be better than the commercially available state of the art. For us the cooperation with the CD-Lab on particulate flow modeling seems to be the key to the actual state of scientific research.

Ulrich Voss | ThyssenKrupp Polysius AG

Granular flows can be found throughout different production steps in the refractory industry. Examples are the feeding of the green mix into all different kinds of moulds or the flow of pellets when they are burnt in a shaft kiln. To get an deeper insight, especially for process steps with an limited accessibility modelling is an important tool. In that sense we found the CD Lab to be the right academic partner.

Gernot Hackl | RHI AG

Continuous development of our proprietary BORSTAR® technology demands in depth knowledge of multiphase hydrodynamics inside the polymerization reactors. Future plant sizes are beyond linear up-scalability, therefore CFD is seen as the most practicable way to achieve a reliable reactor design. The CD Lab on Particulate Flow Modelling is recognized in the worldwide scientific community and therefore the preferred partner to develop fundamental particulate flow models relevant for our own processes. The rigorous physical modeling and validation performed by this CD Lab flattens the path to further improvement and development.

Harald Herbst | Borealis AG

Since the CD-Lab resides at the utmost forefront in numerical and physical modeling of flow dynamics of particulate materials it allows a powder metallurgical company to study complex phenomena during the processing of such materials in a state where the processing steps physically are even not existing but stay in a conceptual phase. Mechanism-based understanding of the extraordinary flow behavior of refractory metal powders plays a crucial role in the design of such processing steps which is substantially being pushed forward by the CD-Lab within our collaboration.

In the actual year of cooperation the CD-Lab developed a novel experimental setup for physically simulating the filling behavior of highly cohesive refractory metal powders particularly including a new type of in-line powder conditioning and 3D measurement of a powder body in the filled state. This way, precise calibration of LIGGGHTS-parameters is expected the latter then being planned for application to real-scale powder filling problems.

Arno Plankensteiner | Plansee SE

AWARDS AND SELECTED PUBLICATIONS

“Edison Preis für Technology orientierte Ideen”: awarded to Christoph KLOSS and Christoph GONIVA for their CFD-DEM project (21.6.2012)

Siemens VAI – IEEE Student Paper Contest 2012 – second place: awarded to Klemens GRUBER for his Master Thesis “Sediment Transport in Open Channel Flows” supervised by Christoph GONIVA (25.6.2011)

SCHNEIDERBAUER S., AIGNER A. and PIRKER S. (2012), Comprehensive kinetic frictional model: Analysis of fluidized and moving bed regimes, *Chemical Engineering Science*, Vol. 80, pp. 279–92.

GONIVA C., KLOSS C., DEEN N., KUIPERS J.A.M. and PIRKER S. (2012), Influence of Rolling Friction Modelling on Single Spout Fluidized Bed Simulations, *Particuology*, Vol. 10, pp. 582–91.

SCHNEIDERBAUER S., SCHELLANDER D., LÖDERER A. and PIRKER S (2012), Non-equilibrium boundary conditions for collisional granular flows at frictional walls, *Int. J. Multiphase Flows*, Vol. 43, pp. 149–56.

KLOSS C., GONIVA C., HAGER A., AMBERGER S. and PIRKER S. (2012), Models, Algorithms and Validation for Open-Source DEM and CFD-DEM, *Progress in Computational Fluid Dynamics*, Vol. 12, pp. 140–52.

PUTTINGER S., HOLZINGER G. and PIRKER S. (2012) Investigation of highly laden particle jet dispersion by use of high-speed camera and parameter independent image analysis, *J. Powder Techn. Vol. 234*, pp.46-57.

PIRKER S., GONIVA C., KLOSS C., PUTTINGER S., HOUBEN J. and SCHNEIDERBAUER S. (accepted 2012) Revisiting the gas cyclone short-cut flow phenomenon by a hybrid – Lattice Boltzmann and Finite Volume – turbulence model, *J. Powder Techn.*

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