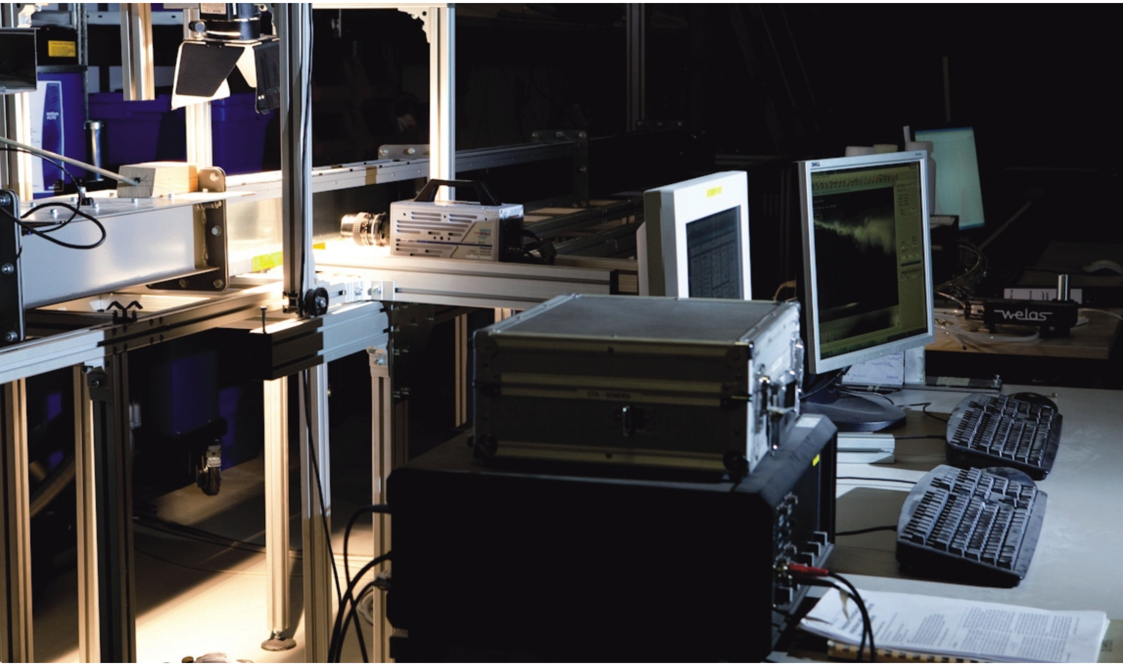

Christian-Doppler Laboratory
on Particulate Flow Modelling

Volume 2 | 2010

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Front cover: A snap-shot of our pneumatic test facility during a powder injection experiment © Heinisch & König

EDITORIAL 1

Dear Readers,

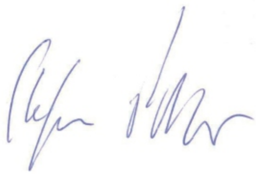
Within the first two years the Christian Doppler Laboratory on Particular Flow Modelling has been on a steep rise. New industrial partners trust in our research abilities and young ambitious co-workers join our forces. Recently, our efforts have been acknowledged by an euphoric scientific evaluation of Hans Kuipers from TU Eindhoven.

In order to handle the increasing work flow our research team has been organized into two major groups of five researchers each. Thereby, the first – Dust & Dirt – team deals with the modelling of powdery flows and the second – Rock 'n' Roll – group focuses grain based particle models.

While the activities in numerical modelling sometimes allow progress at high speed, experimental validation is nearly always associated with laborious testing and recurrent setbacks. Watching fascinated the international response to Christoph Kloss's numerical Liggghts code I still want to honour the value of experimental validation by placing a typical experimental snapshot on the front-cover of this brochure. Look at the dust on the keyboard!

With these introducing words I wish you a pleasant reading. I hope you enjoy it as much as I enjoy accompanying these research efforts !

Sincerely,



Stefan Pirker | stefan.pirker@jku.at

EDITORIAL 2

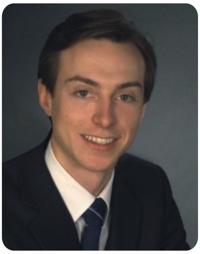
Dear Readers,

the last year was characterized by remarkable progress: The release of the open source DEM code LIGGGHTS and the CFD-DEM OpenFOAM®-LIGGGHTS coupling by our lab via www.cfdem.com attracted hundreds of researchers and engineers from all over the world, from Australia to Zimbabwe. The field of DEM and CFD-DEM particulate flow modelling is becoming an important and versatile tool for science and engineering and we want to continue contributing to spearhead this field. Moreover, we would also like to contribute to a paradigm shift in science: We think that it makes sense to share some of our work and involve a global community in model development, code testing and model validation. Our partners thereby profit from a better quality of our work. Critical code, models, plant data, and other customer data that is business-differentiating for our partners will instead (of course!) always be kept in-house.

We are aware that the next steps must maintain a good balance between fundamental progress and making these methods feasible for large-scale industrial use, comprising experimental validation, code quality assurance, parallelization, and material characterization. Together with our motivated co-workers, we are very confident that we are on a sustainable way for the future.

Sincerely,

Christoph Kloss | Christoph Goniva



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DUST & DIRT

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DUST & DIRT | HYBRID MODEL

General

The Hybrid Particle Model in cooperation with Polysius AG a numerical model for simulating particle transport and separation systems should be validated and extended. Based on this basis hybrid model – called EUgran+ – extensions should consider e.g. particle agglomeration effects.

The Hybrid Model

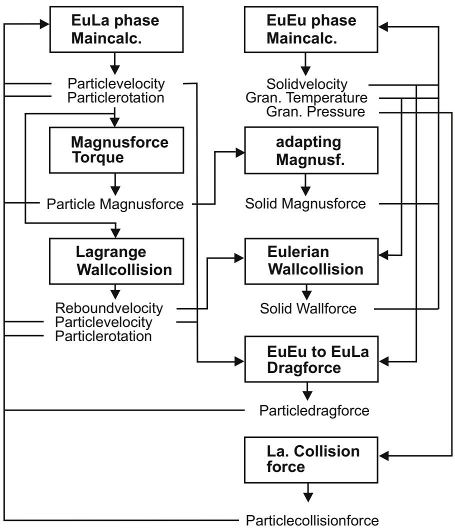
EUgran+ is a new approach in modelling particle conveying simulations with regions of high and low mass loading regions. In a domain with low loading, Lagrangian trajectories are not inflected by the Eulerian granular phase, because particle diffusion is controlled by kinetic transport rather than by particle collisions. In regions with high loading – higher expectation of particle-particle collisions – the Lagrangian trajectories are forced to follow the Eulerian particle phase. In the Lagrangian part for example, particle rotation and wall collision can be modelled. In the Eulerian phase, particle collisions and additional drag force, for example from particle strands, can be modelled. Therefore forces which describe the interaction between the two granular phases are used to generate a coupling between them. The coupling combines both models and creates our new modelling approach as hybrid model Eugran+.

Fields of Application

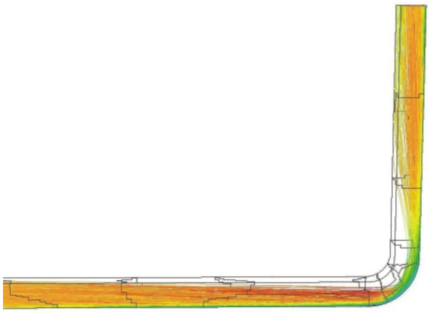
The hybrid model can be used for every simulation containing particle movement based on a flow. The results are in domains with low loading are near to simulations only using Lagrangian particle movement, the results for high loaded regions are dominated by Eulerian granular particle movement.

Conclusion

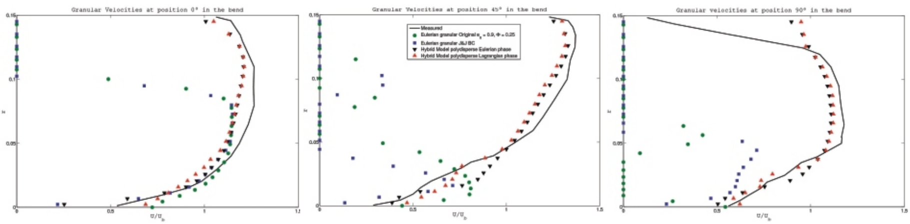
The hybrid model significantly reduces the computational effort, compared to a Lagrangian simulation with equivalent results. The hybrid model seems to be a good alternative for particle conveying simulations, because it uses both worlds. The world of Lagrangian and Eulerian particle transport.



Flow sheet of the hybrid particle model



Simulation of particle flow in a 90° duct bend



Comparison of granular velocity using different numerical particulate models at different positions in a 90° bend

David Schellander | david.schellander@jku.at

DUST & DIRT | CYCLONE SEPARATION

In a collaborate research effort with Siemens VAI Metals Technologies GmbH (SVAI), voestalpine Stahl GmbH (VAS) and voestalpine Donawitz GmbH (VASD) the handling of dust within metallurgical processes should be investigated.

This includes Pulverised Coal Injection (PCI) and particle movement inside the lance and the blowpipe of a blast furnace as well as particle separation in cyclones or the transportation of particles towards dust burners.

Minimizing pressure drop in a cyclone separator is of special interest. The pressure loss of a cyclone separator is divided into three main sources:

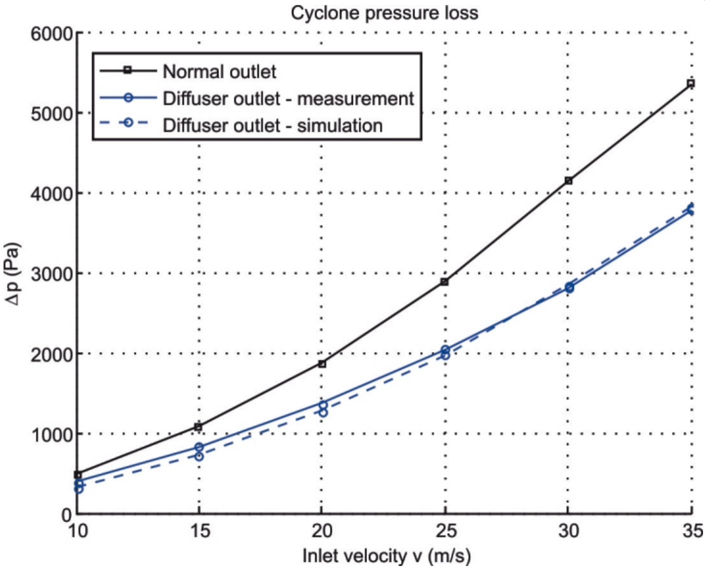
- Cyclone inlet
- Cyclone body
- Vortex finder

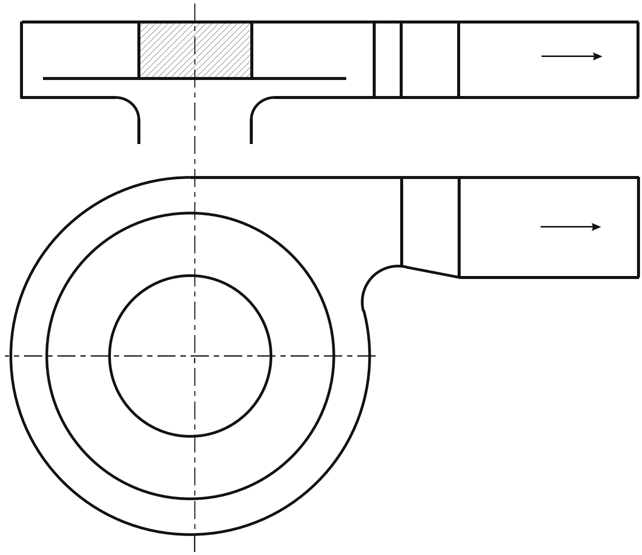
The gas swirl inside the cyclone body is very useful for the particle separation, but as this swirl exits the cyclone through the vortex finder, the rotational energy which is stored within is actually lost. This is the main source of the pressure loss of a cyclone separator.

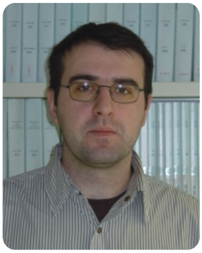
In order to minimize the cyclone pressure loss, a pressure recovery type diffuser is used on top of the cyclone body (see next page). This diffuser converts the rotational energy of the exiting gas back into static pressure.

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.

In addition to the pressure loss minimizing, efforts are also made on improving the analytical prediction tools for cyclone separators. As the pipe configuration and the transport regime prior to the cyclone are also very important for the separation efficiency, the new analytical tool should be able to account for the concentration profile of particles along the cyclone inlet.







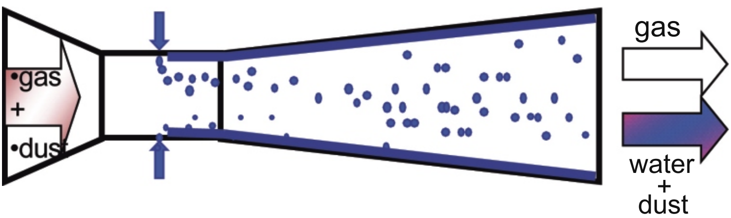
Damir Kahrimanovic | damir.k@jku.at

DUST & DIRT | WET SCRUBBING

In cooperation with voestalpine Stahl GmbH a numerical model for the wet scrubbing process has been developed during the last three years. The outcome is a hybrid Eulerian-Lagrangian model approach realised in the framework of an open source CFD toolbox.

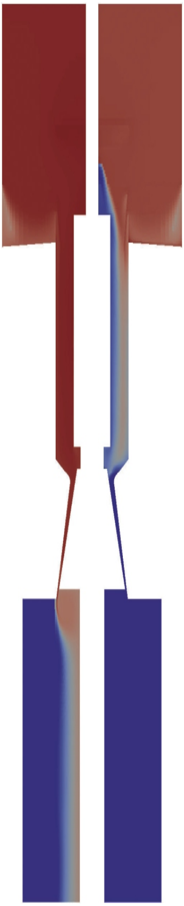
From a physical point of view the scrubbing process comprises a whole set of phenomena starting from droplet breakup and coalescence to the behaviour of the wall film and the dust capturing mechanism itself. Thus a modular approach comprising sub-models, each dedicated to one of the phases - gas, droplets, wall-film and dust – and physical phenomena respectively is chosen. Representative droplets are traced in a Lagrangian frame of reference, while the fine dust particles are treated as additional passive Eulerian phases. These passive dust phases are allowed to drift with respect to the gas phase due to gravitational and centrifugal forces. Droplet breakup, a key phenomenon in this process, is considered by a droplet breakup model. Furthermore, dust capturing is triggered by impaction, interception and diffusion mechanism.

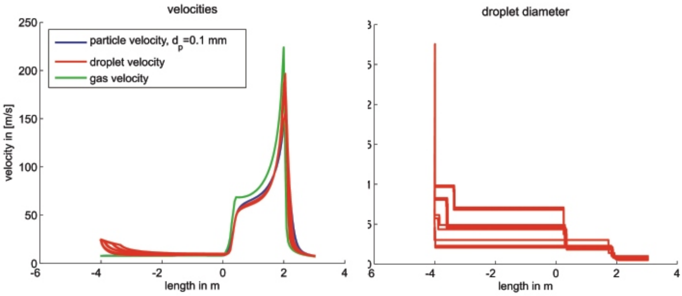
The validity of this model approach could be shown by comparison with profound measurement data available in literature and "in-house" experiments. Setting up the model step by step and validating each of the sub-models led to very encouraging results. This progress enables us to gain deeper insight into the scrubbing process and consequently improve scrubbing devices as well as operating conditions.



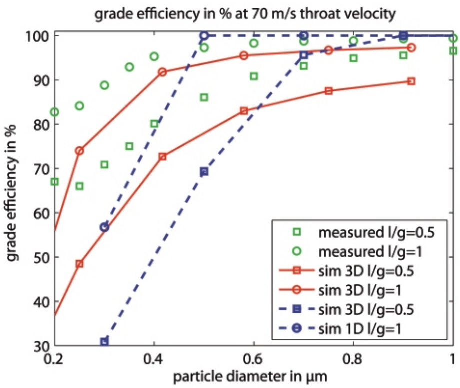
Venturi wet scrubber

Future work on this topic will cover further testing of the derived model as well as the application to industrial scale wet scrubbers





Velocities in an industrial wet scrubber **(left)**, droplet breakup cascade **(right)**.



CFD-Simulation of industrial plant (left), grade efficiency curves (above).

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DUST & DIRT | EROSION

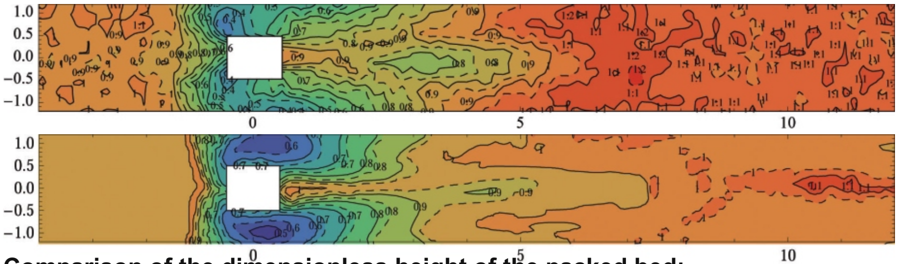
The topic of environmental particle transport has attracted many researchers. For example the drift of sand forms the famous Barchan dunes, the drift of snow leads to the formation of snow cornices and additional snow deposits at leeward mountainsides, the spreading of contaminants respectively air pollutants threatens human health in dense populated areas and finally, the sediment transport in storage lakes influences non-negligibly the efficiency of hydroelectric power plants.

Supported by a DOC-fellowship of the Austrian Academy of Sciences a general and robust numerical model for erosion and sedimentation of sand, snow and river sediments has been developed. On the one hand, this model has been validated by experiments investigating the local erosion of glass beads in the vicinity of a massive obstacle in a wind tunnel. On the other hand, it has been transferred to snow drift in alpine areas and successfully tested by measured snow distributions obtained by terrestrial laser scanning, which is appreciated by a publication in the high reputed Journal of Glaciology.

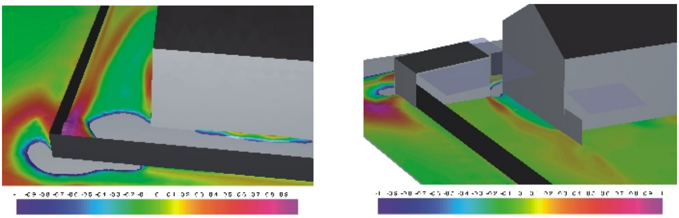
The current research in the CD-Lab focuses on the additional model transfer to river bed erosion to get a deeper insight to the processes affecting the efficiency of hydroelectric power plants. To this end, the local erosion in the vicinity of an obstacle in an open channel flow is investigated by an “in-house” experiment and by numerical simulations. For the latter task a more sophisticated turbulence model (LES) is applied to improve the prediction of the transient behavior of the flow in the low Reynolds number regions downwind of obstacles (i.e. recirculation region). First results are very encouraging (see figure LES simulation).

Future work on this topic will cover further testing of these models in the case of river bed erosion as well as the application to large scale environmental storage lakes.

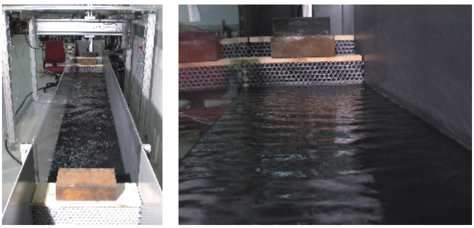
River bed erosion outside and sedimentation inside sharp turns (Schlögener Schlinge, Upper Austria)



Comparison of the dimensionless height of the packed bed:
a) LES Simulation, **b)** Measurement



Snow drift in the vicinity of a one family home. The robust erosion and sedimentation model allows the simulation of "geometry collisions" of the snow cover and the garden fence (left figure)



River bed erosion Experiment

Simon Schneiderbauer | simon.schneiderbauer@jku.at

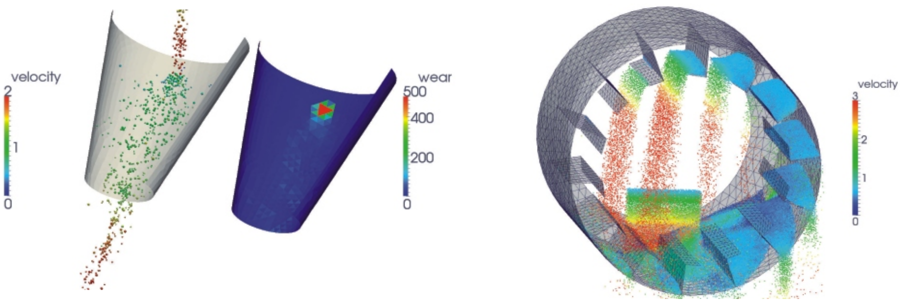
ROCK ´N´ ROLL | LIGGGHTS

LIGGGHTS is a Discrete Element Particle Simulation Code. The abbreviation stands for ‘LAMMPS Improved for General Granular and Granular Heat Transfer Simulations’, and is based on the popular molecular dynamics code **LAMMPS** by **Sandia National Labs USA**, adding ~25.000 lines of code to the LAMMPS codebase (250,000 lines).

Professional administration of such a large code is quite a lot of work but we are sure that this is a good investment as we now have a **flexible, no-cost, parallel (cluster-ready) and very fast DEM code** at hand, that we can customize as it would never be possible with a commercial tool. This is especially in the field of CFD-DEM coupling.

Apart from the experimental validation performed in-house, LIGGGHTS has been **tested and validated** against the market-leading **commercial code** by a joint effort of the CD-Lab, **P&G USA, BASF, Mecalysis Pty**, and **Intrame Madrid with a set of 12 test-cases**. The results are very encouraging, as they show good agreement with the commercial code combined with considerably faster calculation time (for most cases, a speed-up of factor of 4-8 could be achieved).

After the rapid development regarding LIGGGHTS in 2010, a phase of consolidation is intended for 2011, comprising the following topics:



■ **Simulation of chute wear** (left) and **a rotary dryer containing 600,000 particles** (right) **with LIGGGHTS**

■ **Model validation:** Dedicated experimental validation of numerical models will be a key topic.

■ **Quality assurance - Test harness:** This effort is motivated by our perception that not only wrong numerical models, but also software bugs, typos and sloppy programming contribute to error-proneness of a simulation approach. This effort will be led by Stefan Amberger and stands for is an automated quality assurance tool for the LIGGGHTS code to ensure the integrity of the software and the numerical models.

■ **Large-Scale Industrial Application:** Efficient parallelization and coarse-graining will be key topics to improve applicability.

■ **Material identification:** Another important topic is the determination of material parameters for the numerical models. It is desired to develop a series of experiments together with a procedure to quickly and reliably assess these parameters.

■ **Non-Spherical Particles:**
Non-sphericity of particles often plays an important role. It is thus desired to implement and validate models that can accurately picture the physical phenomena that arise out of the non-sphericity.

Stefan Amberger | Christoph Kloss

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ROCK ´N´ ROLL | SOLIDS CHARGING

- In this research module the charging of coal and direct reduced iron (DRI) into a melting gasifyer (MG) of a COREX plant is investigated together with Siemens VAI Metals Technologies GmbH (SVAI).

- The goal of the project is to develop a comprehensive model to describe (a) the physics of the granular media involved and (b) the interaction of the granular media with the fluid phase, which is the gas injected into the MG.

- Coal and DRI are charged into the melter gasifier, with variable chutes exerting influence on the direction of the particles. After a free-fall, the particles impact onto a granular bed, where they are subject to (a) inter-particle forces (b) forces exerted by the wall and (c) forces exerted by the fluid flow through the packed bed.

- A granular charging facility was especially designed to conduct dedicated validation experiments. With the help of measurements and scaling considerations appropriate validations of the developed numerical models are going hand in hand with simulations.

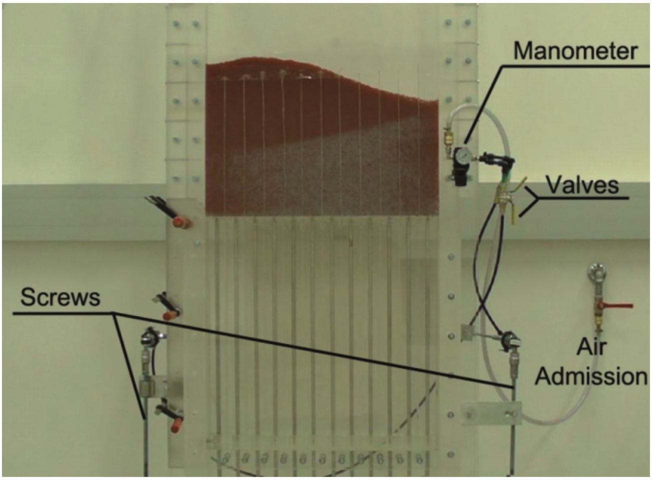
- Because this physics is complex with different physical regimes in each stage of the charging/operation process and the scale of the industrial plants is large, a synthesis of the models best fit for the very problem seems to be the best trade-off between capturing the physics and computability.

- This is achieved by a coupling CFD-DEM approach. Optionally, it could be extended by a continuum model for granular flow.

Particle Charging Experiments

- A flexible experimental facility was designed to validate numerical models for particle charging, bed build-up, segregation. For metallurgical applications, melting can be mimicked by lowering some of the stamps that serve as horizontal wall. The facility can also serve to indentify particle parameters for numerical models.

- Dedicated experiments for granular flow and coupled fluid-granular flow comprising coarse particles can be performed with this facility and can be used for validation of the numerical models



- Particle charging facility

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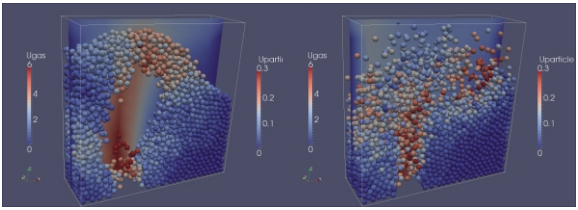
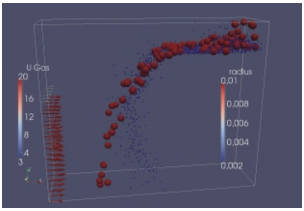
ROCK ´N´ ROLL | CFDEM

Many processes in industry or nature can be described as particlulate flow. It is therefore good to have a strong and reliable DEM code at hand. Yet, neglecting the flow of interstitial fluid, as it is done in “classical” (“dry”) DEM, can lead to erroneous results. This is when the CFD-DEM method comes into play. It is a synthesis of computational fluid dynamics (CFD) and discrete element method (DEM). In order to create an efficient routine, which couples two methods, it is necessary to have full access to the code. Consequently a realisation is only possible within an open source environment.

Our group has successfully created a CFD-DEM coupling routine based on the CFD toolbox OpenFOAM® and the DEM toolbox LIGGGHTS. In the spirit of open source software we provide this code to a dynamically growing group of users via a dedicated web portal (www.cfdem.com). We understand this coupling more as a link between particle-based methods and Eulerian methods than a pure routine for coupling particulate and fluid flow. Following this idea we created a very versatile and modular tool which allows the user to simply add and modify physical effects and models. The range of possible applications is therefore tremendous ranging from fluidised bed, blast furnace, sedimentation and erosion, fluid-structure-interaction, floatation process to particle conveying.

The flexibility on physical side is accompanied by the need of modular and diverse numerical methods. Especially the variety of possible size ratios of geometry to particulate phase is a challenging task which we want to handle by the following topics:





Partly fluidised bed (left) and **surge conveyor** (right) with OpenFOAM® and LIGGGHTS coupling.

- **Model validation:** Dedicated experimental validation of numerical models will be a key topic.

- **Large-Scale Industrial Application:** Efficient parallelization will be key topic to improve applicability. Furthermore a smart coupling, reducing the amount of data to be transferred between DEM and CFD, is crucial for large scale applications.

- **Parameter Identification:** Another important topic is the determination of model parameters for the numerical models. The particulate phase (DEM) is represented by some model in the fluid phase (CFD). It is desired to develop a series of experiments together with a procedure to quickly and reliably assess these models parameters.

- **Particle Size Range:** The expansion of CFD-DEM coupling to different size ranges is planned by the use of volume averaged methods (classic approach) and immersed boundary method.

- **Non-Spherical Particles:** Non-sphericity of particles often plays an important role. It is thus desired to implement and validate models that can accurately picture the fluid –particle interaction for non-spherical particles.

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EXPERIMENTS | POWDER INJECTION

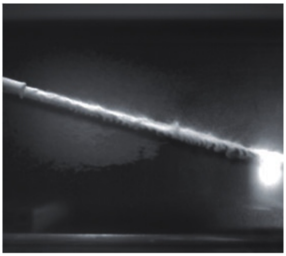
In a collaborate research effort with voestalpine Donawitz GmbH (VASD) the injection of pulverized coal into a blast furnace should be investigated. It is believed that the dispersion behaviour directly behind the injection lance determines the combustion efficiency. To get to a better understanding of the injection process a lab-scale experiment under cold conditions was designed to investigate fluid flow and particle dispersion directly downstream the injection lance.

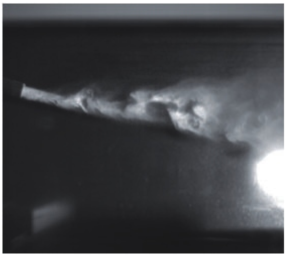
In our pneumatic test facility ceramic powder is injected by a lance into a main gas flow. While the main gas velocity can be adjusted from 0..40m/s the mass flow ratio between the powder and the gas in the injection lance which is controlled by the pressure in the powder storage hopper can reach values up to 100 in steady state. The particle distribution behind the lance is investigated by use of a high-speed camera and subsequent image processing.

In evaluating these experimental results the gigabytes of image data have to be reduced to some significant quantities. Therefore, at a distance from the lance tip the vertical luminosity distribution is extracted and approximated by a Gaussian curve fit. The time dependent evolution of the mean and the variance of this curve fit characterizes the unsteady dispersion behaviour very well. Furthermore, by a Fourier analysis of these monitors characteristic frequencies of e.g. eruptive dispersion events can be identified.

In a second investigation effort the same flow situation is pictured by numerical simulations. Thereby, a hybrid Eulerian-Lagrangian particle model is applied. While the bulk particle flow inside the jet is modeled by a kinetic theory based Eulerian particle model further physical effects like particle rotation and poly-dispersity are introduced by additional Lagrangian tracer particles. While classical Reynolds averaged turbulence models fail in predicting the unsteady dispersion behaviour the results of scale resolving (large eddy) models agree better with the experiments.

Bird eye view of our modular pneumatic test facility





Powder dispersion behaviour at low **(top)** and high **(bottom)** conveying line mass loading

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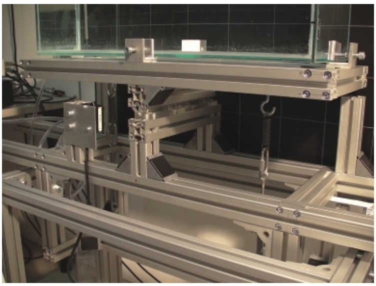
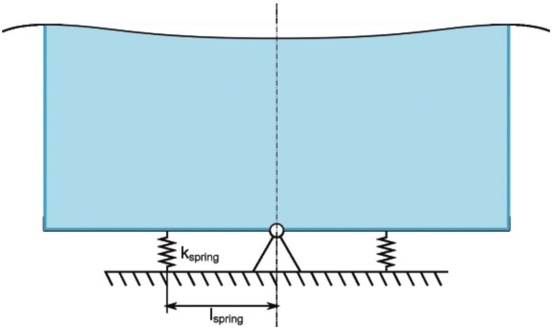
EXPERIMENTS | SLOSHING TANK

In modern steel mills vessels with a capacity up to several hundred tonnes of liquid iron are used to produce stainless steel and other high grade alloys. During this procedure a high amount of gas is injected into the metal bath. If the converter vessel starts to oscillate, tremendous forces will act on gear and support bearings. To reduce wear and maintenance costs we are investigating together with our industrial partners the coupling between the liquid iron bath, the gas jet and the mechanical system of the vessel's suspension.

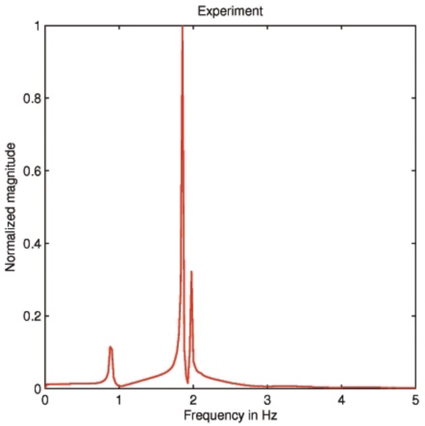
According to our research strategy the first step is the explanation of the physical key phenomenon – the fluid-structure coupling. As a main part a cold-water experiment was build up consisting of a rectangular tank mounted at a see-saw. In order to control the mechanical oscillation frequency the position of springs mounted below the tank can be varied. Other influencing variables determined by doing experiments are the fill level inside the tank and volume flow rate of the injected gas.

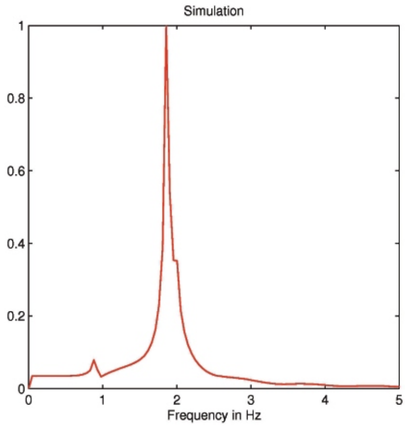
So as to understand the fluid behaviour for itself in a better way the see-saw function was disabled primarily. The comparison of these experimental results with analytic solutions and simulation data revealed good match.

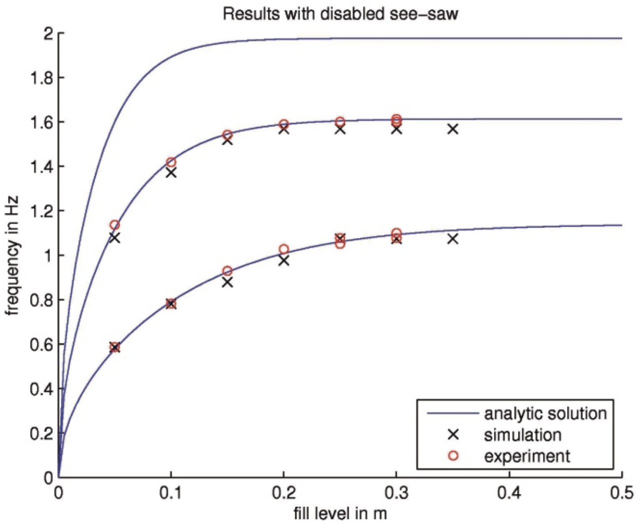




In following experiments oscillation pattern – a beat – that are similar to the measured data from real steel plants can be reproduced. To obtain these results the mechanical frequency has to approach the wave frequency, which can be calculated previously. In this way it is also possible to excite harmonics of the fundamental oscillation.







Andreas Aigner | andreas.aigner@jku.at

INDUSTRIAL PARTNERS

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.

Georg Aichinger | 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 Donawitz GmbH & Co KG

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 bet the key to the actual state of scientific research.

Ulrich Voss | Polysius AG

Since the CD-Lab always tries to combine numerical simulations with accompanying dedicated experiments, we have confidence in the thus obtained results. With respect to particulate flows I have the feeling that this CD-Lab is 'one step ahead' of other groups.

Thomas Bürgler | Voestalpine Stahl GmbH

SCIENTIFIC EVALUATION

After two years of operation each CD-Lab has to stand an international evaluation by a distinguished expert in the particular field of research. In our case Prof. Hans Kuipers from TU Einhoven has been invited by the CDG to have a close look on our research activities. In the following some remarks of his evaluation report are cited.

[…]

The performed research is highly innovative and of a very high scientific level. The CD laboratory is working in the field of computational modelling of particulate flows using sophisticated hybrid models. In addition, where possible, experimental validation is undertaken with sophisticated non-invasive monitoring methods. The balance between the computational and experimental work is in very good shape.

The strong point of the research program is given by the fact that the basic research is inspired by a large body of industrial applications. I praise the very good balance between application-oriented research activities and basic research.

The CD-Laboratory is fully working according to its schedule. It is in fact amazing to observe that under the scientific and inspiring leadership of Prof. Stefan Pirker the laboratory has become very much visible in this highly competitive area within only a few years. This is really an outstanding achievement.

The aims for the future funding period are ambitious (but realistic) and clearly explained by the scientific director of the laboratory.

[…]

Prof. Hans Kuipers | TU-Eindhoven **|** The Nederlands

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Imprint:

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