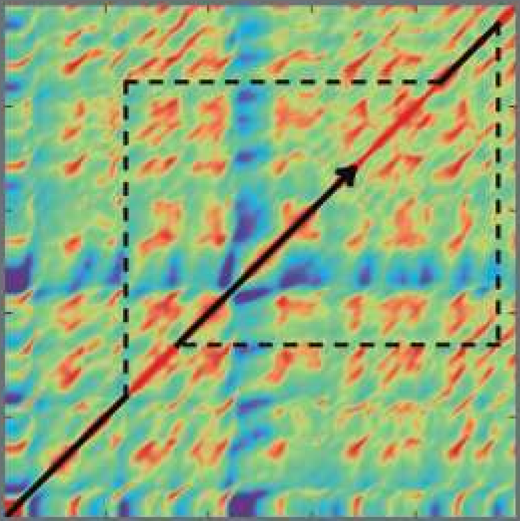

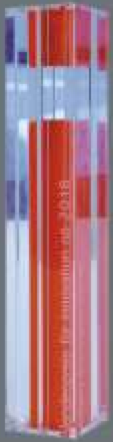

JKU | Department of Particulate Flow Modelling

Annual Report | 2016

JKU DEPARTMENT OF PARTICULATE FLOW MODELLING

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Front cover: Plot of the recurrence norm of a bubbling fluidized bed with arrows denoting a possible flow sequence generated by recurrence CFD; the blue pattern strips indicate a rare event (in this case a very large bubble); for this new method we received the governmental innovation award (right) © Th. Lichtenegger & S. Pirker

EDITORIAL

Dear Readers,

It's a very rewarding experience: at some point you have an idea which does not give you any peace until after months of tedious efforts you can realize it. In our case this led to the development of recurrence CFD – a new simulation technique which speeds up conventional CFD simulations of typical industrial processes by orders of magnitude.

Innovative ideas are the essential fuel for the scientific development of our research group. We want to transform our curiosity into multi-scale and scale-bridging simulation methods. In order to facilitate this, we reorganized ourselves into working groups on Micro-, Meso- and Macro-modelling which are backed up by an Experimental group.

For the future we are well prepared: While our JKU Department focuses on fundamental research of new simulation methods, we closely collaborate with an industrial competence center for applied research, thus realizing a smooth knowledge transfer. Beyond that, we are actively extending our collaborations on European level and, finally, Simon Schneiderbauer was awarded a new CD-Lab on Multi-scale Simulation of Multiphase Flows (see next page) – what a great perspective!

With these introducing words I wish you a pleasant reading!

Sincerely,

Stefan Pirker | stefan.pirker@jku.at

EDITORIAL | NEW CD-LAB

Dear Readers,

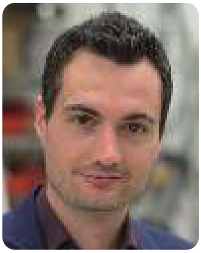
Last February the Christian Doppler Laboratory for “Multi-scale modeling of multiphase flows” officially started. This laboratory stands for new challenges in field of multiphase processes with special attention on multi-scale aspects.

For example, in this first research year we significantly contributed to the research on gas-solid turbulence. Such multiphase turbulence models are urgently required for the numerical simulation of large scale industrial processes. Furthermore, we developed novel and efficient models for the numerical simulation of liquid-liquid emulsions in stirred tank reactors. Finally, we are heading for an efficient numerical tool for the numerical assessment of industrial scale iron ore reduction.

The latter research topic supports the K1MET activities by accompanying basic research activities and novel multi-scale modeling strategies. These involve especially the above mentioned gas-solid turbulence modelling activities, which are expected to generalized coarse grained models required for the analysis of those industrial scale processes.

I am looking forward to a prosperous future of this CD-Laboratory!

Sincerely,



Simon Schneiderbauer | simon.schneiderbauer@jku.at

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EDITORIAL | MICRO

Dear Readers,

At the beginning of 2016, we revisited our ongoing research activities involved with **hybrid** and **embedded** modelling approaches. Since in both cases, an in-depth understanding of the multiphase fluid dynamics in the microscale level is of crucial importance, our research is heading toward the physics of flow in the microscale and appropriate modelling methods. This can be done through the (i) fully microscale simulation, (ii) co-simulation (embedded) and (iii) sub-grid scale modelling (hybrid). Recently, we decided to extend our ongoing research on multiscale modelling of liquid atomization, towards interfacial flows (two-phase flow with a distinct interface) with a variety of applications from microfluidics to metallurgical and process engineering.

Following this research strategy, we joined the **MicroNeedle** project, an FFG research project in life science, to model the capillary-driven interfacial flow as well as the wetting behavior in micro-channels with application in transdermal drug delivery.

Together with **K1-MET**, we proceed with modelling turbulent interfacial flow in the continuous casting mold and the unsteady flow/vortex interaction with the liquid-liquid interface which leads to slag entrainment. This will establish a proper framework for our hybrid and/or embedded modelling approaches.

We are also investigating a new hybrid simulation methodology through a master thesis in applied mathematics to improve our classical dynamic grid VOF model by scale-bridging using a kind of Lagrangian interface tracking .

Let’s keep walking on the “interfaces”!

Sincerely,

Mahdi Saeedipour

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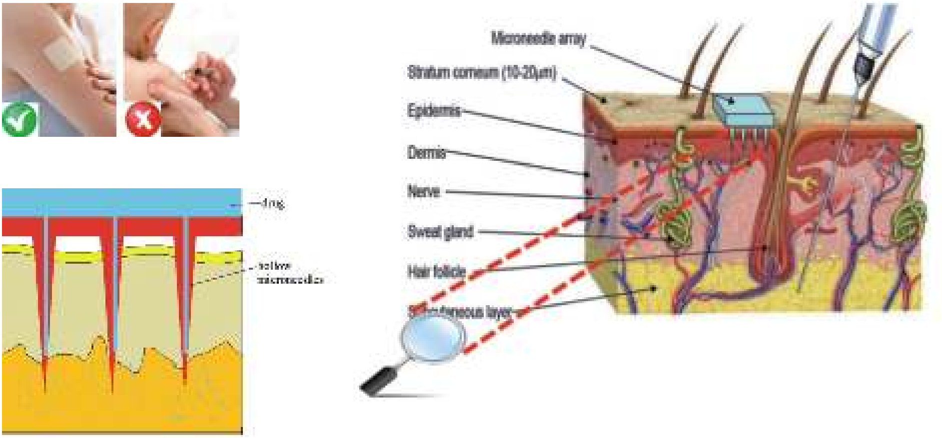

Fig.1: MicroNeedle vs. conventional vaccination syringe (right). Schematic of liquid flow inside the hollow microneedles for the drug delivery (left). Figures are brought from Prausnitz (2004) and Iliescu et al. (2014).

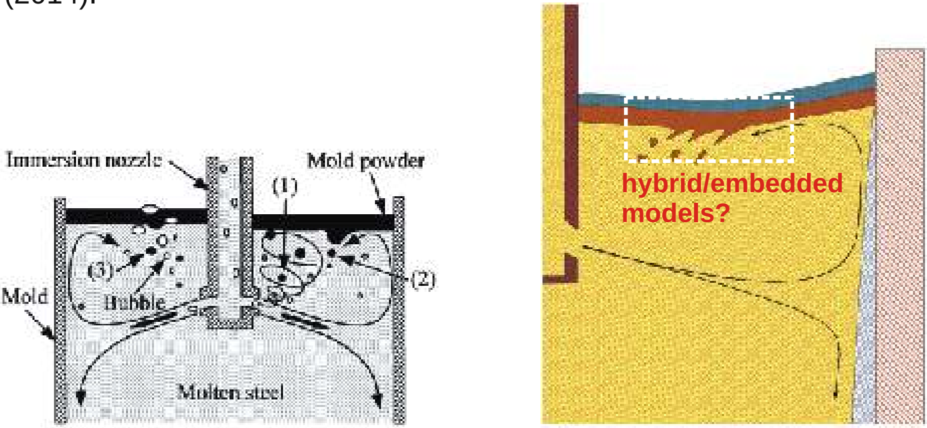

Fig.2: Schematic of two-phase flow in the continuous casting mold (left). The metal-slag interface instability – the region of interest for modelling (right). Figures are brought from Iguchi et al. (2000) and Hibbeler & Thomas (2013).

MICRO | LIQUID FLOW IN SMALL CHANNELS

Why do we consider micro-fluidic flow as part of our research focus? Because although everything seems to happen on small scale at first glance, picturing the propagation of a liquid surface in a small channel is truly a multi-scale challenge!

Micro-fluidic flows seem to obey by their own physics, which sometimes contradict to one's expectations. At small channel endings, liquid seems to stick in the channel (liquid pinning) and given a hydrophilic surface, liquid start creeping upward against gravitation.

In small capillaries liquid flow is dominantly controlled by surface tension and wall adhesion. Both physical effects can be related to the local surface curvature. From a computational perspective this requires a finely resolved representation of the liquid surface and here we have a multi-scale challenge.

In a first step we addressed these microscopic flows by conventional Volume of Fluid (VoF) methods with an artificial surface compression scheme. At the propagating liquid surface we additionally applied dynamic multi-level grid refinement in order to concentrate computational resources accordingly.

Based on these model settings, we could show the accelerating effect of surface roughness on the propagation of the liquid surface (Fig. 1,2). At the moment first validation experiments are performed at the JKU Institute of Biomedical Mechatronics.

While dynamic grid refinement enables us to perform small scale micro-fluidic simulations, we are still far away from simulating e.g. a set of interconnected channels. To achieve this, we propose a (once again) hybrid modelling approach between multi-level grid refinement and Lagrangian surface tracers which are then used to describe sub-grid surface curvature on coarser grid levels (Fig. 3).

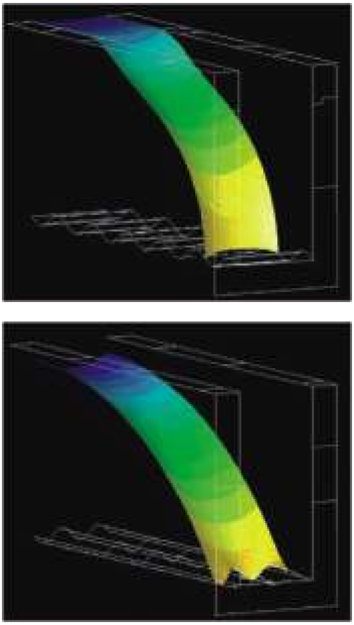

Fig.1: Propagation of liquid in a hydrophilic micro channel with (top) normal and (bottom) streamline oriented roughness structures

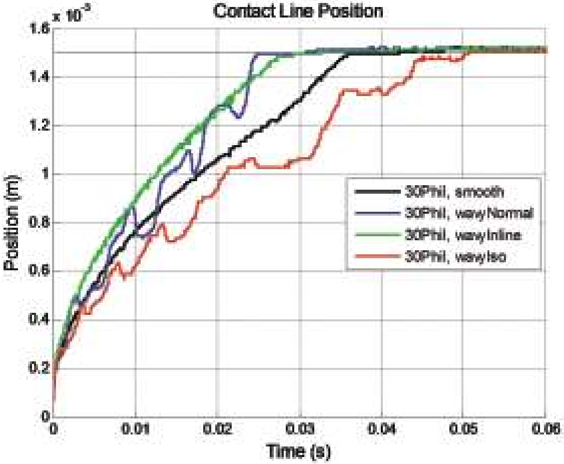

Fig.2: Propagation of contact line with time for different configurations of smooth and rough micro-channels

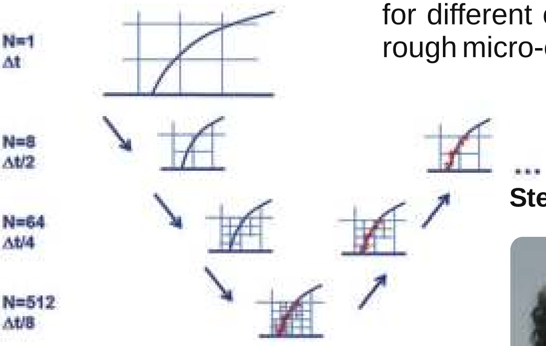

Fig.3: Concept of hybrid surface capturing

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MICRO |
SUSPENSIONS IN SQUARE CHANNELS

Flow of suspensions in microchannels received increasing attention over the last years. The discovery of Segré and Silberberg [1] that a sphere in laminar pipe flow laterally migrates towards an off-center equilibrium position at ~0.62R_{pipe} distance to the pipe axis was found to be highly interesting from an academic point of view, but applications only emerged during the last two decades. Nowadays, the effect of lateral migration is mainly used to filter fluids and sort particles by size, shape, or density (for an overview of applications, the reader is referred to Di Carlo [2]). Devices employing the Segré-Silberberg effect usually use square or rectangular channels due to ease of fabrication. In square channels, up to eight equilibrium positions exist, depending on the channel Reynolds number (see figure 1): four at the channel faces, and four at the corners. Miura et al. [3] found through experiments that below Re_{ch} = 260 only the face positions are stable, while at Re_{ch} > 260 the corners become stable too. However, these experiments examined the behaviour in the limit of a single particle, neglecting particle-particle interactions in denser suspensions.

Using our software *LBDEMcoupling*, we performed simulations of particulate suspension flow with D_{ch}/d_p ~ 10 in a periodic, pressure-driven square channel for several channel Reynolds numbers. and varied the solid fraction in the range f_s = 0.01% - 3%. Doing so, two new effects were found.

At Re_{ch} = 310, both face and corner positions are stable in the dilute limit. When particles are added, however, these additional particles will not go to corner and face positions equally, but almost exclusively migrate towards the corner positions (figure 2). The reason is that particles push each other to the side when they pass each other, and the corner positions are geometrically more confined.

At Re_{ch} = 60, all particles were found to migrate to the face positions. When increasing the solid fraction, a secondary equilibrium position ~0.5d_p closer to the channel center was found (see figures 3a, 3b). Again, the origin of this new pattern is particle-particle interactions, but the exact mechanism is subject to further studies.

With characterization of these two new effects, we broaden the knowledge on suspension flow in channels and hope to lay a foundation for new applications.

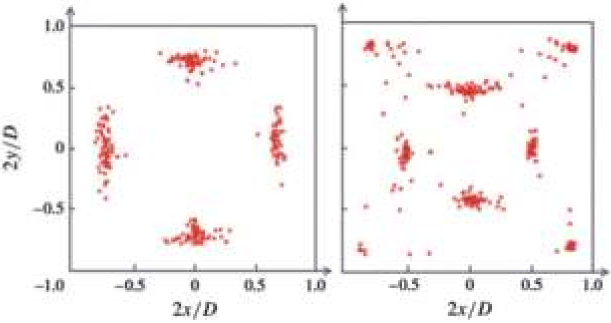
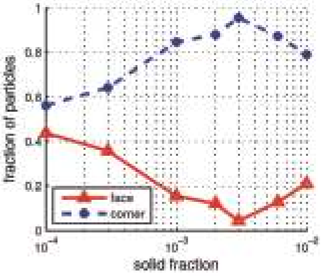


Fig.1 (left): Equilibrium positions at $Re_{ch}=144$ (left) and $Re_{ch}=968$ (right). Face equilibrium positions are always stable, while corner equilibrium positions are only occupied for $Re_{ch}>260$. Source: Miura et al. [3]

Fig. 2 (right): Fraction of particles found at the face (red) and corner (blue) equilibrium positions over solid fraction. At f_s = 0.3%, almost all particles migrate towards the corner. For higher f_s, focusing breaks down.



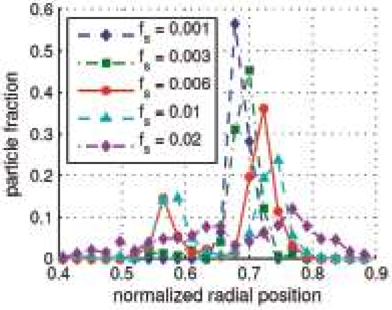
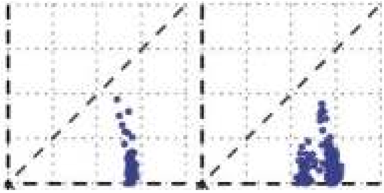


Fig. 3a (below): particle positions for f_s = 0.3%, 0.6% (left, right). A secondary equilibrium position appears at the higher solid fraction.

Fig.3b (above): Particle distribution over radial distance for different f_s. The evolution of a second peak closer to the axis can be clearly seen.



[1] Segre, G., & Silberberg, A. (1962). *Journal of Fluid Mechanics*, *14*(01), 136-157.
[2] Di Carlo, D. (2009). *Lab on a Chip*, *9*(21), 3038-3046.
[3] Miura, K., Itano, T., & Sugihara-Seki, M. (2014). *Journal of Fluid Mechanics*, *749*, 320-330.

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MICRO | NUMERICAL SIMULATION OF SLAG ENTRAINMENT IN CONTINUOUS CASTING PROCESS

Slag entrainment can alter the quality of the final product of continuous casting significantly if the entrained droplets become trapped in the molten metal. Therefore it has received much attention in the steel industry over the past three decades, resulting in several proposed mechanism. (Hibbeler 2013)

The identified mechanisms for slag entrainment vary from fluid mechanics to process and metallurgical engineering aspects. But from a purely fluid-dynamic viewpoint, the fluctuations of the meniscus at the top of the mold as well as the shear-layer instability at the molten metal-slag interface, known as Kelvin-Helmholtz instability, are identified as the cause of slag entrainment. Further to this, the vortex formation around the submerged entry nozzle (SEN) due to the asymmetric flow interacts with the slag layer and pulls slag down to the liquid metal in the form of small droplets. These mechanisms are associated with the unsteady flow situation near the interface in particular due to the turbulent nature of the flow field in the casting mold.

Numerical modelling is a challenging task due to different physical scales involved in the real process. As the first step we employed a classical large eddy simulation - volume of fluid (LES-VOF) approach to investigate the flow behavior upon injection into the mold and the unsteady flow/vortex interaction with the meniscus interface. Different geometries with various inflow conditions were considered for the numerical simulation.

The preliminary simulation results are compared to a water/oil benchmark experiment using PIV and a promising agreement is revealed. However, the small scale fluctuations of the liquid-liquid interface, which are important in oil droplet entrainment, are not captured by the current model. Therefore a sub-grid scale (SGS) modelling should be considered to improve the LES-VOF approach.

Future steps will focus on improving the simulations results and heading towards the multiscale modelling approach.

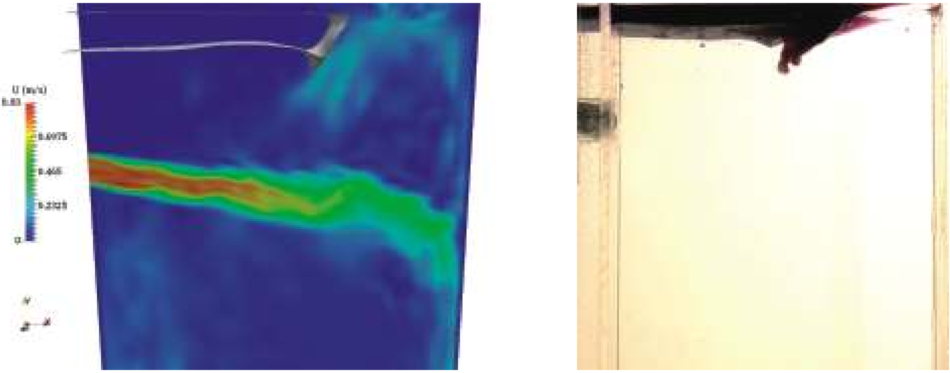

Fig.1: Qualitative comparison of oil-water interface dynamics from simulation (left) and experiments (right) for the flow rate of 0.26 (lit/s) and inlet configuration of θ = -10°. The iso-surface of 0.5 are visualised.

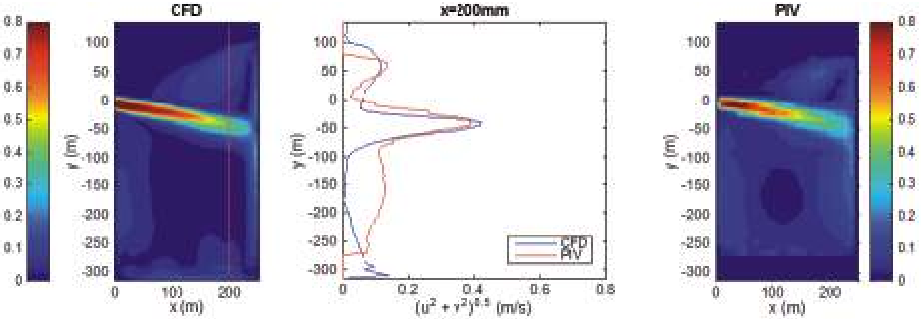

Fig.2: Comparison of CFD simulation results (left) with PIV measurement (right) for the flow rate of 0.26 (lit/s) and inlet configuration of θ = -10°. The averaged velocity at the x=200 mm from the inlet is also plotted in the middle sub-figure.

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EDITORIAL | MESO

Dear Readers,

During the course of 2016, we recognized that all the (former) Rock‘n‘Roll groups‘ activities have one common property: we aim to connect detailed microscopic descriptions of particulate systems with macroscopic flows of industrial-scale. Our research focus lies on the bridge between those worlds, the **mesoscopic** domain.

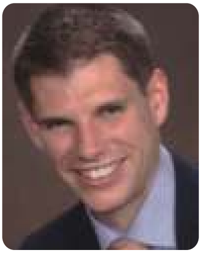
The spectrum of scales reflects in the variety of techniques we employ to increase our understanding of the mesoscopic world. Well-conceived physical models are at the heart of our projects. They need to contain the relevant mechanisms but at the same time allow for a feasible numerical description. Algorithmic developments give us the opportunity to apply our models to systems of increasing size and complexity. However, it is experimental validation that has the final word whether our models and their numerical treatment agree with nature or if we have to return to the start.

Two new PhD students joined our group this year: **Alija Vila** from Bosnia and Herzegovina investigates the interaction of cohesive powders with gas flow in various regimes both theoretically and experimentally. **Mustafa Efe Kinaci** from Turkey devotes his energy to the implementation of particle-chemistry models in our code base and their subsequent up-scaling to large system sizes.

Just like with all our team members, I am enjoying to see their passion for research creating new knowledge from which science in general and our industrial partners in particular will benefit.

Sincerely,

Thomas Lichtenegger



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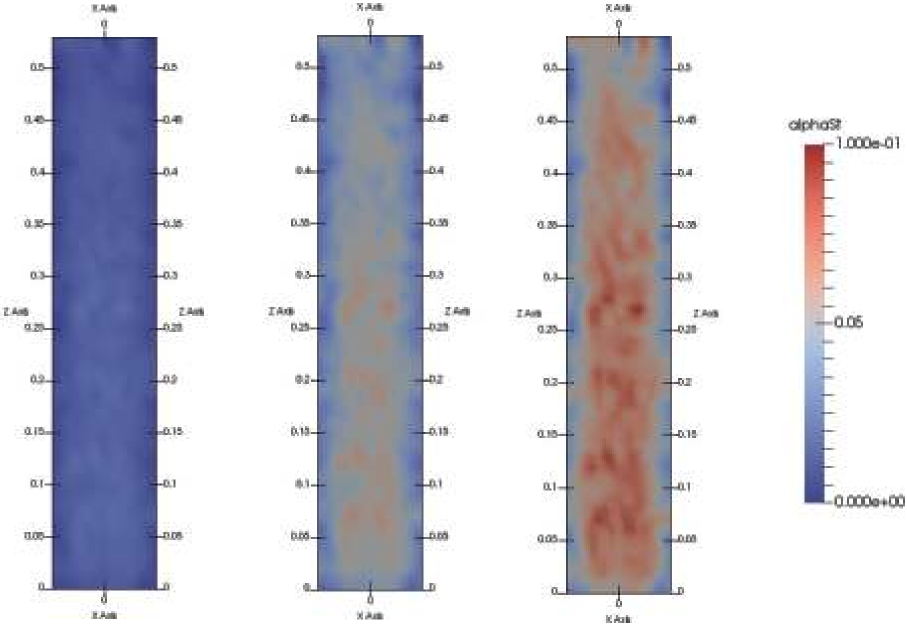

Fig.1: Fines deposition in a packed bed column. With increasing process time (from left to right), fines get trapped inside the particle bed while near-wall regions remain relatively open.

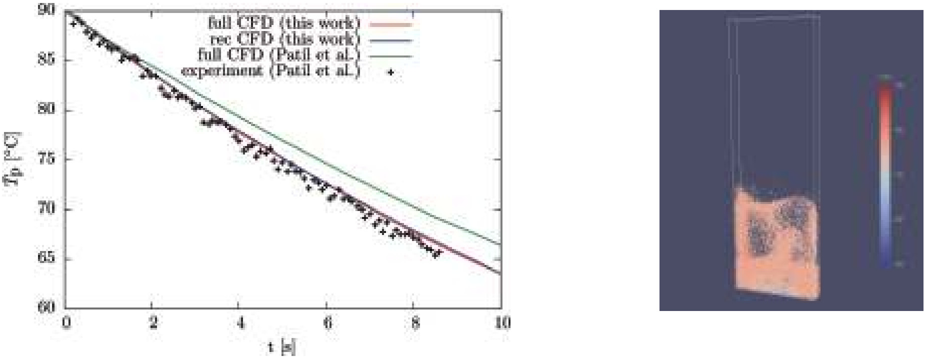

Fig.2: Heat transfer in a fluidized bed. The average particle temperature is simulated with a conventional CFD-DEM approach and the novel recurrence CFD technique. Results are in excellent agreement with experiments by Patil et al. (Chem. Eng. J. 277, 2015).

MESO | TOWARDS LARGE-SCALE DEM SIMULATIONS

Tracking the state of each individual particle is a fundamental concept of the discrete element method (DEM). As a consequence, the number of particles involved in a simulation determines the computational demands of the method. This in turn means that simulations of industrial-scale systems consisting of millions of particles require a substantial amount of computational resources, making DEM simulations time-consuming and expensive.

Coarse grain (cg) models can help to reduce the computational costs by replacing a group of particles by a representative coarse particle. However, for effects that intrinsically depend on particle size, they fail to correctly predict the behavior of the system.

We have developed a method to combine the best of both worlds. We start out with a coarse grain simulation of the large system. Wherever a higher level of detail is required we embed a sub-region with an atomistic representation of the particles.

We can expect a speedup that is proportional to the reduced number of particles. We demonstrate this using the setup shown in Fig. 1, which mimics one of the experiments conducted in our laboratory. We measure the discharge rate of a rectangular bin, which depends on the particle diameter. The bin has inner dimensions of 40 mm x 40 mm x 1500 mm. The outflow orifice at the bottom right is 40 mm x 10 mm. The original particles have a diameter of 2 mm.

We conducted a reference size simulation consisting of 120.000 particles resulting in an initial bed height of about 500 mm. Then we repeated the simulation using a coarse grain model with a coarse grain ratio of 2, i.e., 15.000 particles with a diameter of 4 mm. As can be seen from Table 1, the coarse grain simulation is indeed much faster than the reference simulation. However, Fig. 2 shows that the predicted mass flow rates differ significantly.

To remedy this deficiency, we embedded a fully resolved sub-region at the bottom of the bin (red rectangle in Fig. 1d), containing about 15.000 additional particles of original size. With this combination we were able to correctly predict the discharge rate (Fig. 2) and still achieve a significant speedup compared to the reference simulation (Table 1).

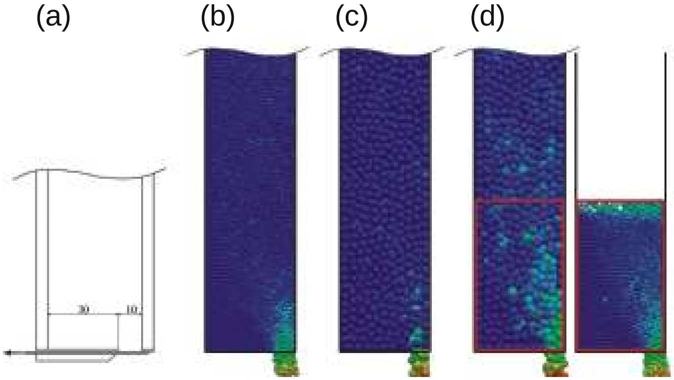

Fig.1: (a) setup with the outflow orifice at the bottom right of the bin, (b) reference simulation, (c) cg simulation, (d) coupled cg and resolved simulation.

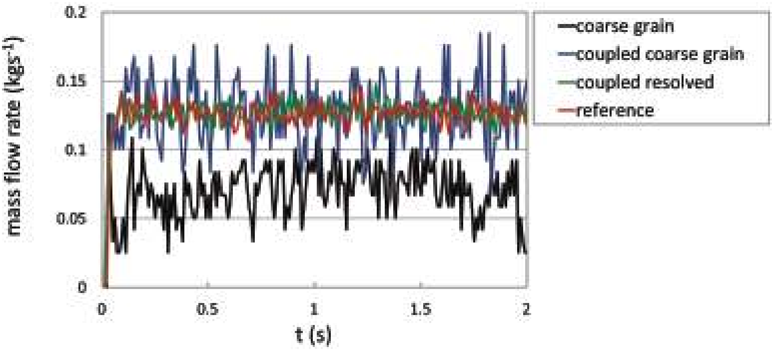

Fig.2: The rate of discharge in kgs^{-1} of 2 mm particles using the default model, the cg model and the coupled model.

Simulation	$\langle \dot{m} \rangle$	$\sigma(\dot{m})$	speedup
reference	0.127	0.007	1x
coarse grain	0.072	0.018	12.8x
coupled resolved	0.128	0.006	5.6x
coupled coarse grain	0.128	0.023	

Table 1: Average discharge rates with standard deviations in kgs^{-1} and relative speedup.

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MESO | MODELLING OF CHEMICAL REACTIONS IN METALLURGICAL PROCESSES

Developing ways for the direct reduction of iron ores has attracted much research interest in the last three decades, since it can be considered as a core process in steel industry. One of the most advantageous direct reduction processes are fluidized bed reactors. These are used not only to reduce the iron ore rapidly and efficiently but they are also used in several other branches of process industry (polymer production, carbon capture, fluid catalytic cracking, biomass reactors).

Since access to the reactor is limited due to the harsh conditions inside, carrying out measurements to investigate the processes is complicated. In order to improve our understanding of these reactors, simulation tools such as the CFD-DEM method are utilized. Within the CFD-DEM framework, the gas phase equations of motion as well as gas chemical reactions are taking place on the CFD side, whereas the particle chemical reactions and particle dynamics take place on the DEM side.

The two most common types of representation models for the chemical reactions between gas and particle are the Shrinking Particle Model (SPM) and the Unreacted Shrinking Core Model (USCM) (see Fig-1a,b). With the help of the SPM model, the CFD-DEM framework has been extended to cover the communication between the gas and the particle phases. It has been established in such a way that only the required data is communicated between the phases with an adaptable communication interval. Thus, a successful application can be carried out with an efficient implementation. This framework has been verified by running some preliminary cases and comparing the species mass balances (see Fig. 2).

The main reaction for the direct reduction of the iron with coal-based or gaseous reactant can be expressed in three reaction steps (see Fig.3). Therefore, the USCM is a fitting model for the investigation of this process. As a next step, the DEM is going to be extended to cover the model for iron-ore reduction, thereby allowing numerical simulations with realistic particle chemistry.

References:
[1] E.Donskoi and D. L. S. McElwain. Esitmation and modeling of parameters for direct reduction in iron ore /coal composites: Part I. Physical parameters. *Metallurgical and Materials Transactions B,* 34:93 – 102, 2010.
[2] Octave Levenspiel. *Chemical Reaction Engineering*. 1999.

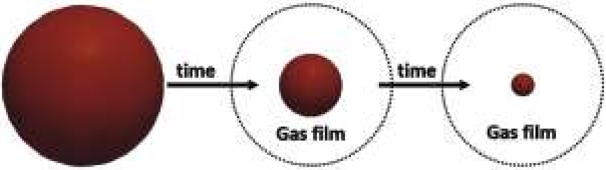


Fig.1a: In SPM, the fluid reacts with the particle there is no formation of an ash layer.

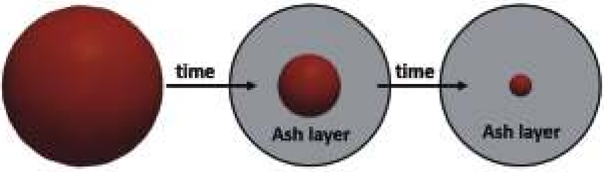
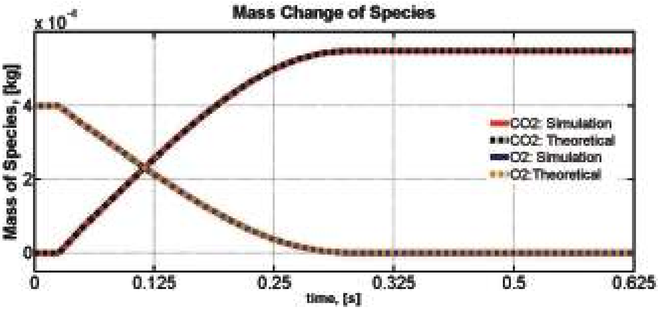


Fig.1b: In USCM, the reacting fluid diffuses through an ash layer which is formed as the particle reacts.

Fig.2: Simulation case in order to verify the communication framework. The results for the mass change over time for reacting species O_2 and product Co_2.



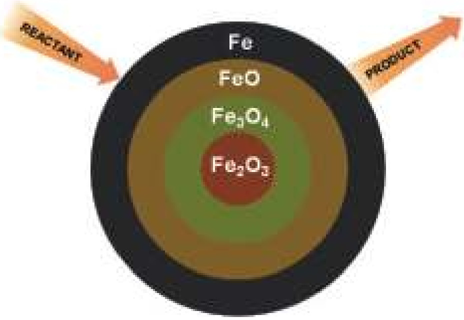
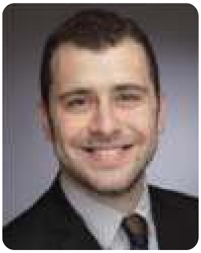


Fig.3: 3-Layer Unreacted Shrinking Core Model used in the modelling of iron-ore reduction.



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MESO | MODELING OF BLAST FURNACE TAPPING

The blast furnace hearth is a complex area containing hot liquid iron, a liquid slag layer, hot air and a dense, porous structure of solid coke particles (often referred to as the deadman). The shape of the deadman depends on the weight and distribution of the burden column above and the counteracting buoyancy forces from the liquids in the hearth, as illustrated in Figure 1. Depending on the state of the operation, the weight of the burden and the amount of liquids in the hearth vary, which influences the shape of the deadman. This transient behavior of the deadman leads to different flow patterns in the hearth during tapping, which in turn causes non-uniform wear on the refractory lining.

In order to understand how the flow pattern looks like during different times in an operational cycle, a multiphase CFD (Computational Fluid Dynamics) - DEM (Discrete Element Method) coupled model was developed. To handle the multiple continuous phases, a VOF (Volume of Fluid) method is used on the CFD side. As an example, Figure 2 shows the volume flow rate for a water-oil-air system that has been drained through a particle bed.

To demonstrate some of the model's capabilities, two examples of free surface flows are shown in Figures 3 and 4. Figure 3 illustrates the evolution of a collapsing water pillar with particles inside. The wave propagation in the tank can be observed as well as how the particles are dragged along the water. Figure 4 shows a block of particles being dropped into a container of water. The red line represents the theoretical new water level due to particle displacement, which is used to ensure volume conservation.

The model is currently undergoing validation against lab experiments and once a successful validation is achieved, it will be scaled up and applied to blast furnace simulations.

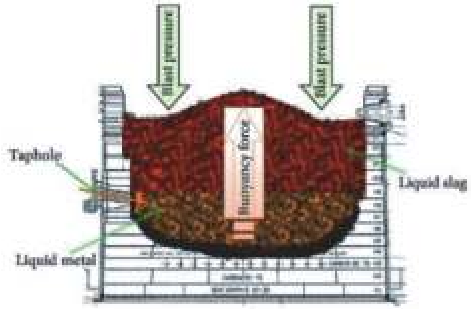

Fig.1: Illustration of a blast furnace hearth.

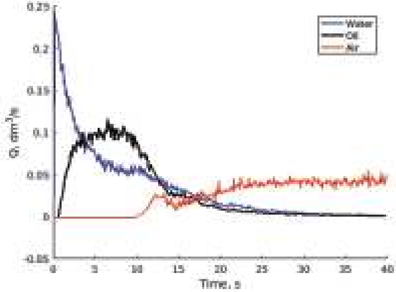

Fig.2: Volume flow rate of stratified fluids drained through a particle bed.

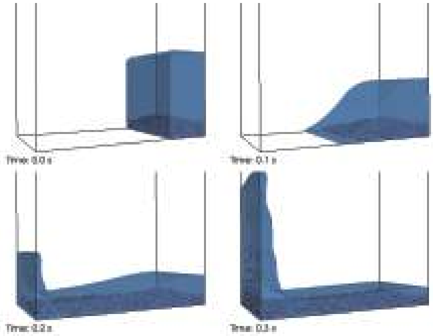

Fig.3: Simulation of a collapsing water pillar with particles.

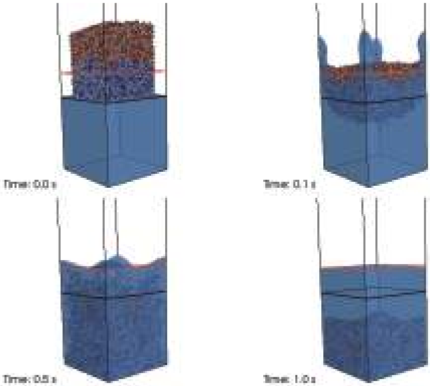

Fig.4: Simulation of a block of particles dropped into water.

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MESO | BRIDGING SPATIAL AND TEMPORAL SCALES IN PARTICLE SIMULATIONS

The successful description of particulate systems requires sound underlying models and fast algorithms to handle the former efficiently. The art of physical modeling almost always involves capturing too complicated phenomena in simpler, more feasible ways.

Granular materials with broad particle size distributions, in extreme cases ranging from macroscopic grains to sub-micron dust, pose a real challenge. Keeping track of each single constituent is clearly out of question due to their huge numbers. However, fines can play a critical role, e.g. when they get trapped between larger particles and clog the pores of dense beds.

Two main questions need to be answered in this regard. How can one describe the transport, deposition and release of fines in a simple yet accurate way? What is their effect on the surrounding large particles and fluid flow, especially when they accumulate?

Based on a force balance criterion, the local mean velocity of a fines-concentration field is obtained. Kinematic considerations are then used to determine the amounts of deposited/released material which in turn influences the bed's local morphology and its resistance to fluid flow. Figure 1 shows the pressure drop over a particle column with and without fines and compares simulation results with measurements.

Besides strongly separated spatial scales, distinct temporal scales call for special treatment, too. The dynamics of fluidized beds, for example, is governed by short-term collisions while heat transfer between particulate and gas phase takes much longer. Employing our new approach recurrence CFD, one can easily extrapolate their motion using results from conventional CFD-DEM simulations. Figure 2 demonstrates that the correct average particle distribution is recovered.

Heat transfer may then be studied on the extrapolated fields, which represents a strong decoupling of fast from slow degrees of freedom. Speed-up factors of about 300 are achieved at minor accuracy impairments. It is shown in Fig. 3 that while the particle temperature distribution turns out to be a bit too sharp in comparison to CFD-DEM calculations, the average values agree very well.

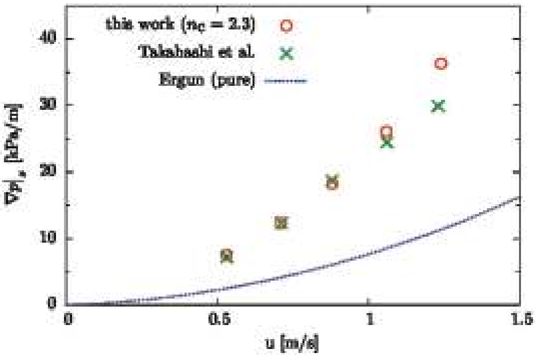


Fig.1: Pressure drop of gas flowing through a packed bed with fines transport and deposition. Simulation results (red circles) agree very well with measurements by Takahashi et al. ISIJ 51 (2011) (green crosses). The blue line represents the Ergun pressure drop without fines.

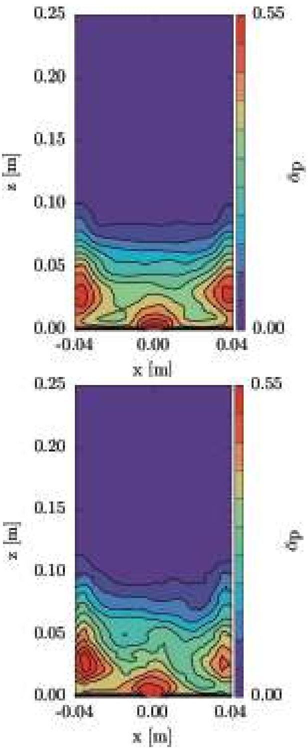


Fig.2: Averaged particle distribution in a fluidized bed. Recurrence-CFD results (bottom) compare very well with those from CFD-DEM (top).

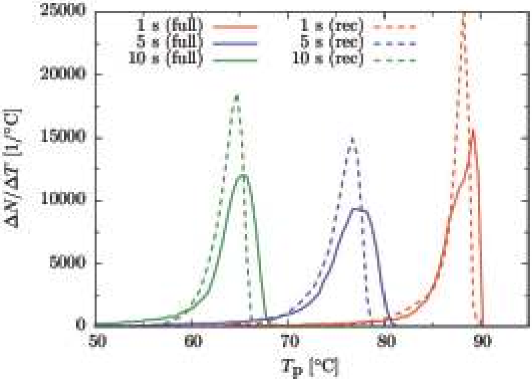
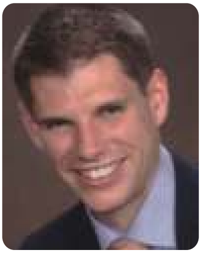


Fig.3: Particle temperature distributions in a fluidized bed after 1 s, 5 s and 10 s process time. Recurrence-CFD results are narrower than those from conventional CFD-DEM, but the average values agree.



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MESO | COMPARISON OF DRAG LAWS FOR SPHERICAL PARTICLES

Different closures for the drag laws were proposed from theoretical, experimental and numerical studies. Theoretical relations are typically limited to low particle volume fractions and low Re. Some of the earliest available empirical correlations, based on experimental data were those by Ergun (1952) for dense systems (> 0.8) and Wen and Yu (1966) for dilute systems. With the increase of computational power, direct numerical simulation (DNS) had become a powerful tool for obtaining accurate drag correlations. Several researchers used the Lattice Boltzmann method (LBM) to study the drag force over a wide range of Re and (Ladd, 1994; Hill et al., 2001; Beetstra et al., 2007). Immersed Boundary Method (IBM) can also be applied for arrays of randomly arranged mono-disperse spheres (Uhlmann, 2005; Tenneti et al., 2011; Tang, 2015).

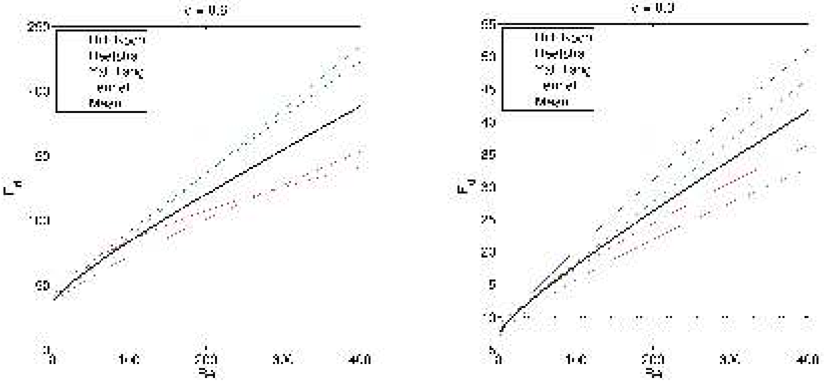

Fig.1: Comparison of drag law correlations based on numerical simulations

Hill-Koch and Beetstra correlations are in reasonable agreements with Tang correlation for Re up to 100. However, for higher Re, the results are significantly different, regardless of . New correlation obtained by Tang is in agreement with reports by Tenneti et al. where authors concluded that Hill-Koch correlation is valid for Re < 100. Additionally, for dense systems the differences between LBM and IBM correlations are more noticeable. That could be caused by grid effects and constant resolution for a wide range of ϕ, making it under resolved for increased values of particle volume fraction ϕ.

MESO | MODEL CONCEPT

Fluidization of cohesive particles is characterized by non-homogenities in the bed, such as channels, cracks or phenomena of slugging and clusters of particles moving as solid plugs. Starting point in deriving the drag law that would describe the formation of channels could be a fluid flow in porous media. Simplifying the channels as vertical parallel tubes is very rough estimation, and there are other factors that could have a strong influence on the flow and channeling phenomena. Tortuosity of the channels is an important factor, as actual length of the passage is greater than the layer thickness.

It is necessary to impose a size distribution and establish the parameters that have influence on the channel properties and distributions, and to what extent, so a correlation can be derived as a function of the properties (such as fluid velocity and viscosity, solid volume fraction etc.).

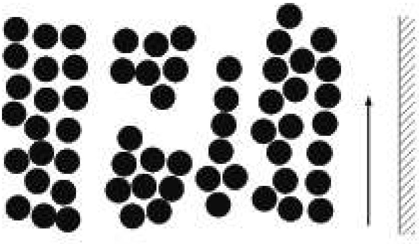

Fig.2: Channeling occurs and fluid flows through preferred paths, often resulting in poor fluidization properties

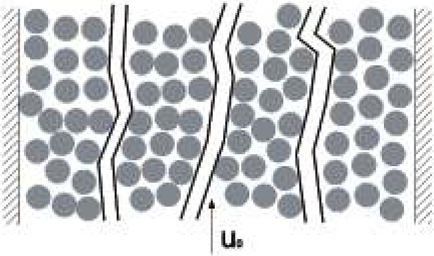

Fig.3: Flow is affected by the level of tortuosity

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EDITORIAL | MACRO

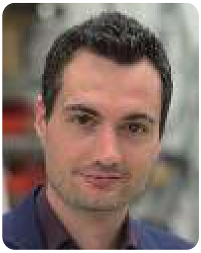
Dear Readers,

During the last years the research activities of the formerly called Dust’n’Dirt group focused on macroscale problems. In particular, we aimed to analyze industrial scale processes by a ”coarse grained” model, where the micro-scale behavior is accounted by proper sub-grid models. This concept is, however, not restricted to a certain numerical method, which makes it more representative to reference those activities by the spatial scale, which is particularly the macro-scale.

Currently, our research efforts are dedicated to macro-scale problems, which includes, for example, the numerical simulation of iron ore reduction in fluidized beds (Figure 1), the development of a novel gas-solid turbulence model (Figure 2, In contrast to single phase flow, turbulence in multiphase systems is considerably triggered by interfacial work) and the numerical analysis of the formation of liquid-liquid emulsions in stirred tank reactors (Figure 3). The reduction of iron ore and the emulsion problem are attacked by employing a hybrid modelling approach, which combines the a large-scale turbulent multiphase model with additional tracer particles accounting for chemical reactions as well as droplet breakup/coalescence.

Finally I want to thank my team members for their encouragement and their excellent work.

Sincerely,



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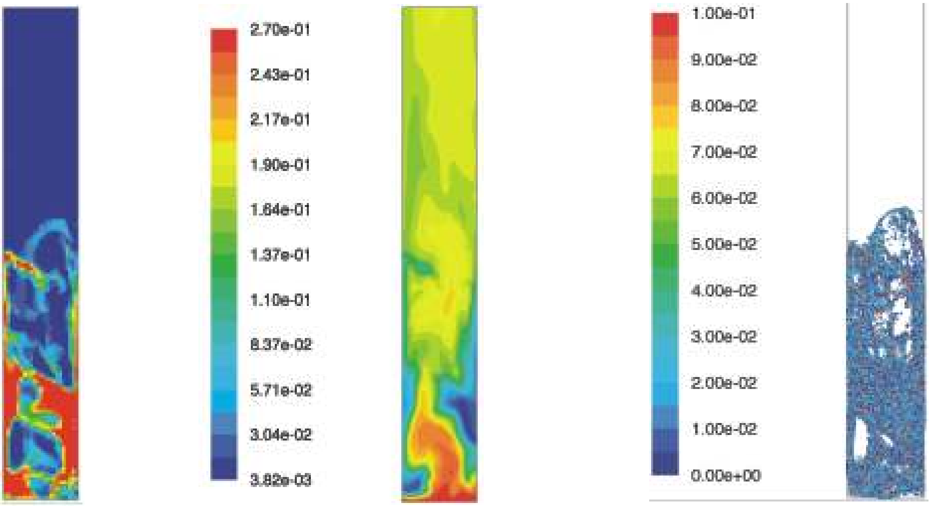

Fig.1: Direct reduction of iron ore in a fluidized bed; left: particle volume fraction: middle: mass fraction of CO, which is consumed in dense regions due to reduction; right: fractional reduction of individual parcels.

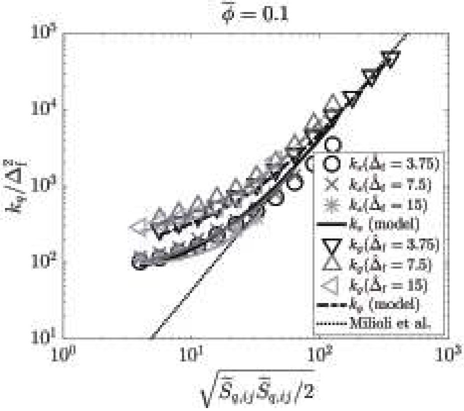

Fig.2: Turbulent kinetic energies (TKE) of both, gas and solid phase, as a function of local shear rate. In regions of low shear the TKEs are determined by interfacial work due to gas-solid drag.

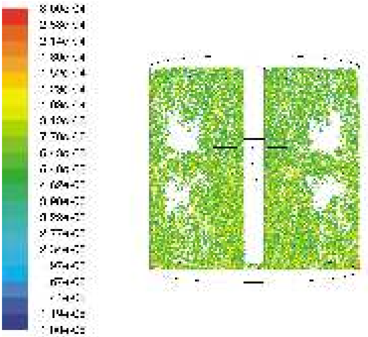

Fig. 3: Final droplet size distribution in a liquid-liquid stirred tank. The DSD unveils a sharp log-normal behavior, but some large droplet remain ”unmixed” in dead zones.

MACRO | MODELLING OF EMULSION IN STIRRED TANK REACTOR

Liquid-liquid (Emulsion) systems are widely used in the several industries such as food, pharmaceutical, cosmetic, chemical and petroleum. Liquid-liquid systems are mainly created in Stirred tank reactors. Drop size distribution (DSD) plays a key role as it strongly affects the overall mass and heat transfer in this system.

Taylor-Couette flow experiment:
The well-defined pattern of the Taylor-Couette flow enables the possibility to investigate DSD as a function of the local fluid dynamic properties, such as shear rate (a=U/h).This is in contrast to more complex devices such as stirred tank reactors. Experiments were performed in a Cylindrical Taylor-Couette flow device (Fig.1). Several oils were examined and from high speed camera images (Fig.2), we extracted data regarding to DSD (Fig.3) employing image processing. Furthermore, we found a simple correlation for the Sauter mean diameter D32 which reads,

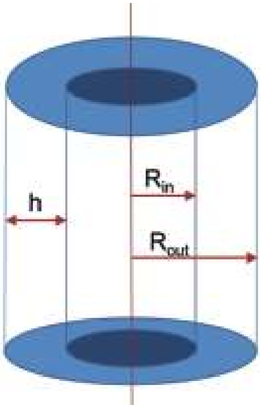

Fig.1: Schematic view of Taylor-Couette flow device

$$\frac{D_{32}}{h} = 0.64\,We^{-\frac{1}{6}}\,Re^{-\frac{1}{4}}\left(\frac{\mu_d}{\mu_c}\right)^{0.32}\left(\frac{\rho_d}{\rho_c}\right)^{-0.6} \qquad (1)$$

μ_d :Viscosity of dispersed phase
μ_c :Viscosity of continues phase
ρ_d :Density of dispersed phase
ρ_c :Density of continues phase
γ :Interfacial tension

$$Re = \frac{\rho_c a h^2}{\mu_c}$$

$$We = \frac{\rho_c a^2 h^3}{\gamma}$$

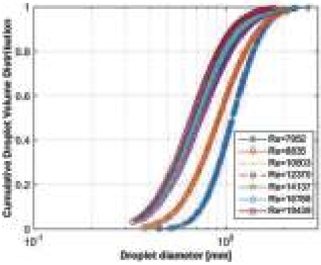

Fig.3: Cumulative Drop volume distribution- Raps oil-in-water

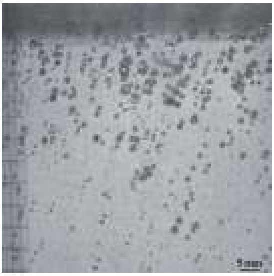

Fig.2: Raps oil –in-water, Re=8836

CFD Simulation:

A novel breakup model has been developed, which is based on the correlation for the local droplet size distribution. From the experiment, it was observed that the standard deviation of the DSD is a linear function of sauter mean diameter. Therefore, droplet breakup is modelled as a random process following the local DSD. To verify the presented approach we selected a numerical setup presented by Roudsari et al. (2012) which is based on the experimental data of Boxall et al. (2010). Hybrid Eulerian-Lagrangian scheme along with the K-e turbulence model was used to simulate the emulsion in the stirred tank reactor. Rotation of the impeller was modelled by sliding mesh method.

Initial droplets with diameter of 0.3 mm were injected at t=0. Simulation were performed for 300 rpm and 600 rpm. Simulation stopped when the final drop size distribution did not change any more. Fig.5 shows the cumulative drop size distribution for 600 rpm. As it can be seen in the figure, the simulated results and the experimental data are in a good agreement.

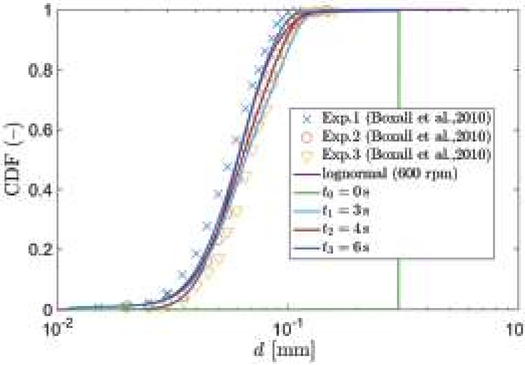

Fig.5: Cumulative drop size distribution, simulation results vs experimental data by Boxall et al. (2010)- 600 RPM

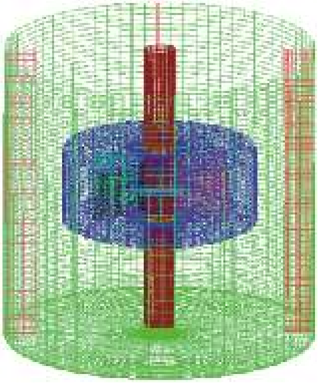

Fig.4: Stirred tank reactor mesh the same as Roudsari et al (2012)

Boxall et al., Ind. Eng. Chem. Res. **49**, 1412 (2010)
Roudsari et al., Comput. Chem. Eng. **45**, 124 (2012

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MACRO | RECURRENCE CFD

Well, what should I say – recurrence CFD (**rCFD**) developed really good in the last year. Beyond the innovation award and associated press and television releases, we have made major steps on the scientific side. While **rCFD** has reached some maturity, two years after the idea was born, it still fascinates us by opening the door towards simulation possibilities we haven't imagined before.

In our group we further develop **rCFD** by two main directions of research. While Thomas Lichtenegger works on the theoretical framework and focuses on model accuracy (see page 20f), I try to figure out new algorithms which might accelerate **rCFD** simulations even more.

In the last year we have applied **rCFD** to scale resolving single- and multiphase flows occurring in metallurgical processes. In both cases we were interested in the species transport of dissolved hydrogen. By means of classical CFD simulations such predictions are very expensive because high spatial and temporal resolutions are needed. By means of **rCFD** simulations, we can picture these long term processes very efficiently. Actually, we obtained nearly identical results with only less than 1% of the original computational costs!

So at this point we arrived at scale resolved simulations of industrial processes which are only one order of magnitude slower than the process itself. This achievement earned us the governmental innovation award – but is this the end of the story?

Not at all – here the story just becomes really interesting: By switching from a Eulerian to a Lagrangian description of flow statistics, **rCFD** can be accelerated dramatically. As a result, we can now run scale resolved simulations an order of magnitude **faster** than real-time! So we opened the door towards online simulations and we won't close it again in near future …

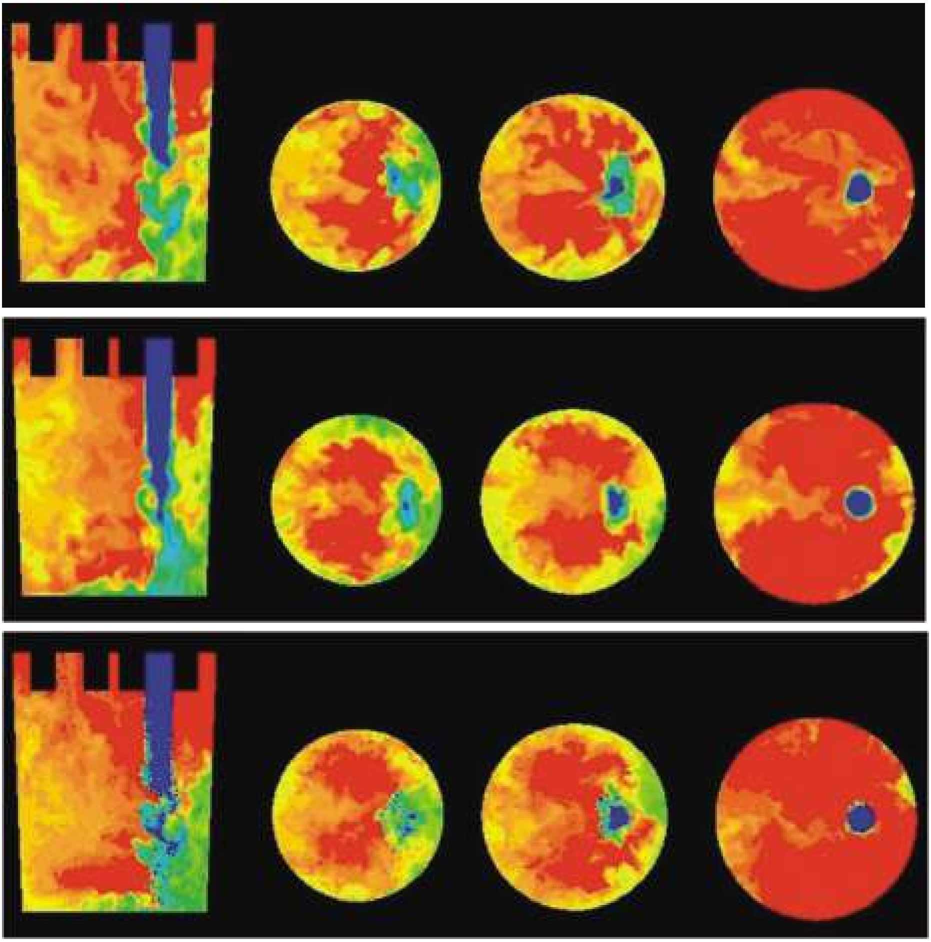

Fig.1: Hydrogen concentration in a steel ladle as result of (top) full CFD, (middle) Eulerian **rCFD** and (bottom) our new Lagrangian **rCFD**; simulation times for 60 sec of process time account to 26 h, 17 min and 1.6 sec respectively.

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EDITORIAL | EXPERIMENTS

Dear Readers,

During the last year a lot of former colleagues have finished their PhDs and the next generation is now in charge to bring new life and new experiments to the laboratory.

For the future there will be two main fields of research concering measurement techniques and data analysis:

On the one hand we will continue to setup dedicated **lab scale experiments** to capture certain effects in multiphase flows. Examples are the K1-Met activities in Project 4.4 to model slag entrainment or the experiments in Project 4.3 to investigate particle trajectories and voidage formation in moving bed reactors (Fig.1).

On the other hand I established a long term project together with voestalpine (Project 2.1) where we try to use available plant data to squeeze out more information about the process which can then be used to optimize process control. In addition to this **on-plant activities** we were granted a FFG/Bridge funding together with the Institute of Electrical Measurement and Measurement Signal Processing at Graz Technical University to develop a field applicable sensor for tomographic mass flow measurements of granular materials (Fig.2).

Sincerely,

Stefan Puttinger | stefan.puttinger@jku.at

Fig.1: Modelling slag entrainment in a lab scale experiment using water and colored oil.

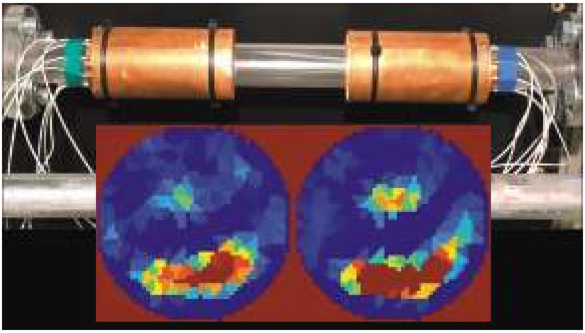


Fig.2: Two plane ECT sensor for pneumatic conveying and the online reconstruction of the particle distribution.

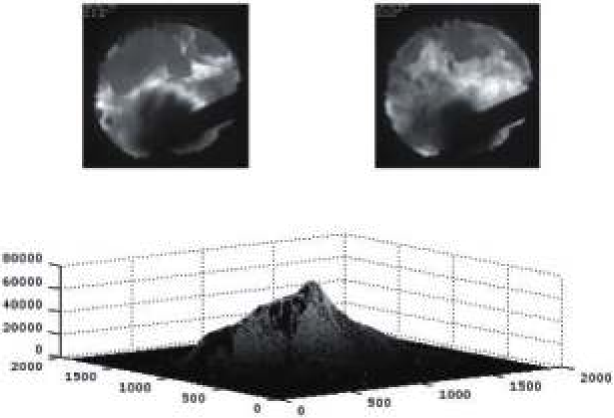


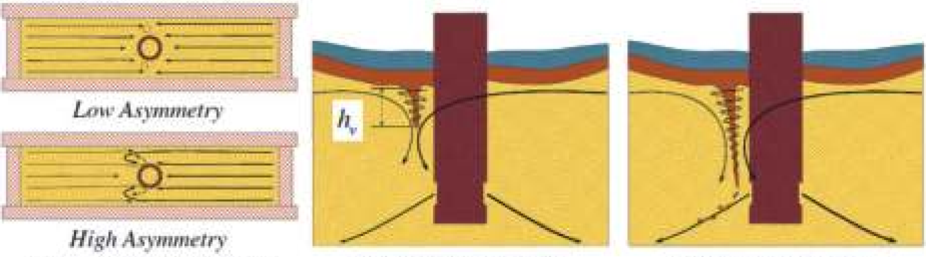
Fig.3: Example of image correlation for raceway blockage detection.

EXPERIMENTS | SLAG ENTRAINMENT

Slag entrainment is based on various effects of the fluid mechanics in multiphase flows. To support the development of CFD model development we built two downscaled benchmark experiments in the lab to obtain qualitative and quantitative validation data. Water plus Paraffinum liquidum were used to model the combination of liquid steel and the slag layer in both cases.

Experiment 1 produces a so-called bathtub vortex in a cylindrical vessel with tangential inlet. The swirl flow in the vessel will then form a vortex in the center which is deforming the interface (Fig.1). Such vortices are formed due to asymmetries in the mold flow in continous casting (Fig.2).

Fig.1: Bathtub vortex experiment for the cases of water/air (left) and water/oil/air (right). The reduced density ratio due to the presence of an oil (slag) layer, highly increases the interface deformation and oil entrainment.



(a) Vortexing from asymmetric flow (b) Subcritical vortex formation (c) Entrainment by deep vortex

Fig.2: Slag entrainment mechanism in mold flow due to vortex formation

Source: L.C. Hibbeler, B.G. Thomas, Mold slag entrainment mechanisms in continuous casting molds, Iron Steel Technol. 10 (2013) 121–136.

Experiment 2 is a rectangular tank in a 1:3 scale of a continous casting mould. The inlet from the submerged entry nozzle (SEN) is realized via an inlet pipe in the center (symmetry) plane and can be adjusted to various inlet angles. The outlet is realized as a homogenous sink flow at the bottom.

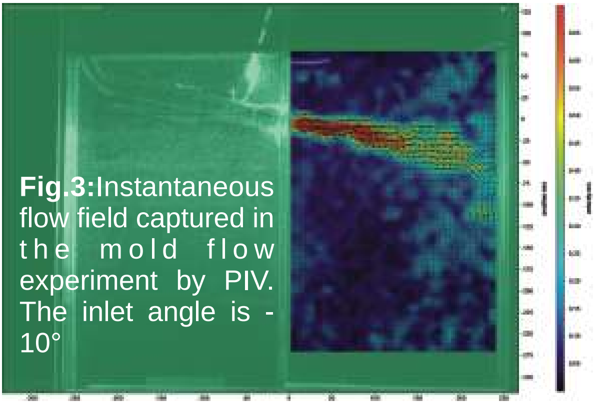
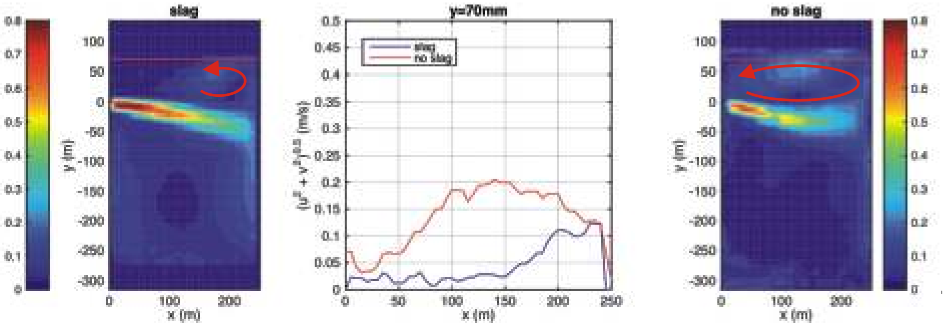


Fig.3: Instantaneous flow field captured in the mold flow experiment by PIV. The inlet angle is -10°



Stefan Puttinger | Nikolaus Doppelhammer

Fig.4: The comparison of the cases with and without slag (oil) layer shows the influence of the slag layer on vortex formation and velocity profiles close to the surface

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EXPERIMENTS |
RACEWAY BLOCKAGE DETECTION

To achieve minimal coke rates in blast furnace operation it is crucial to obtain optimal burning of additional fuels like e.g. pulverized coal (PC). However, there are operating conditions, where an optimal burning is not possible and it is beneficial to shut down the PC supply on one or more injection lances. The frequent case of raceway blockages can lead to reduced wind throughput on the effected tuyere. If PC is injected in that tuyere the unburned coal might lead to locally reduced permeability of the burden. Thus it is necessary to have reliable information of the current raceway condition to be able to shut down PCI lances if beneficial and to do so with short latency.

In this project the goal is to find an optimized approach for processing pressure senor data representing the hot blast flow rates in the tuyeres. This sensor signals will then be combined with visual information of tuyere cameras to improve raceway blockage detection.

To test various algorithms for signal processing and image processing, I implemented a modular software test bench in Matlab/Octave which can be used for parameter testing and automatic processing of multiple datasets.

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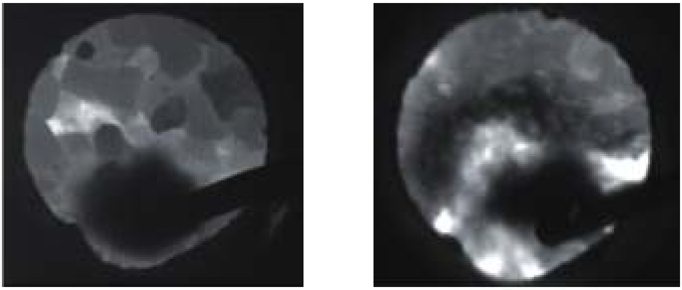
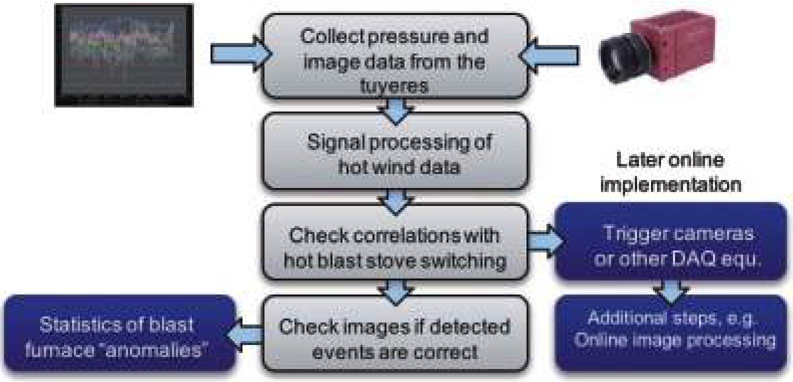


Fig.1: Raceway in normal operation (left), and blocked by a big chunk of coke (right).



Collect pressure and image data from the tuyeres

Signal processing of hot wind data

Check correlations with hot blast stove switching

Check images if detected events are correct

Statistics of blast furnace "anomalies"

Later online implementation

Trigger cameras or other DAQ equ.

Additional steps, e.g. Online image processing

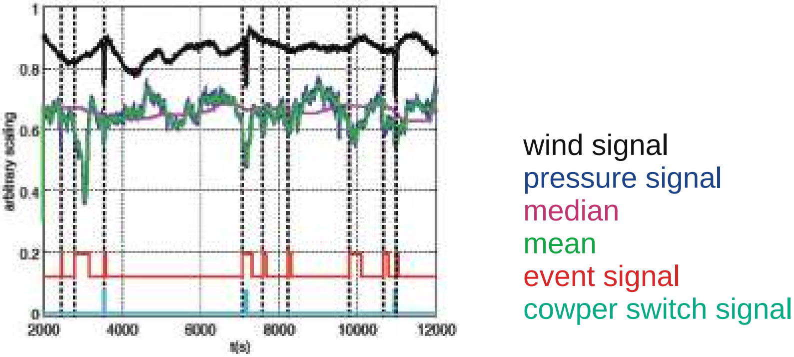


Fig.3: Example of signal processing results and blockage detection

EXPERIMENTS | PARTICLE MOVEMENT IN A REDUCTION SHAFT

Moving bed reactors might have some additional installations in the particle bed to introduce a process gas. In the case of COREX reduction shaft a gas mixture is injected via two pipes located in the shaft with a certain distance. An experimental mockup can be seen in Fig.1 .

While the bed of particles in the duct is bridging can happen near those pipes due to the occurence of force chains in the granular material. Therefore the particle flow is locally prohibited and the efficiency of the reduction process decreases. The experiment was designed to simulate, observe and measure this phenomenon with non-spherical particle flows.

The moving particles are filmed with a camera and then processes with the well known method of Particle Image Velocimetry (PIV) to obtain the velocity field of the particle layer next to the wall (Fig. 2) .

Figure 3 shows the time dependend velocity profiles at y=6cm (right below the two obstacles). The unsteady behaviour is clearly to the occasional formation of bridges and the collapse of them after some time.

This kind of experiments can provide valuable validation data for the model tuning in CFD-DEM simulations and the dynamic coarse graining activities of Daniel Queteschiner.

Fig.1: Photograph of the experimental setup

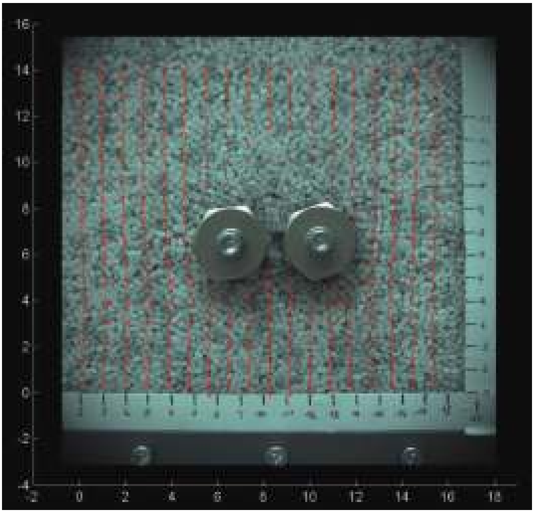


Fig.2: Particle velocities after processing with PIV software.

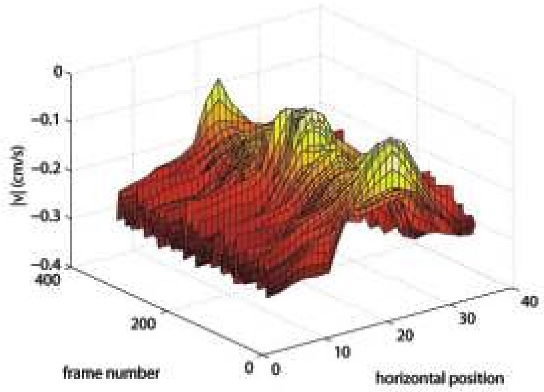
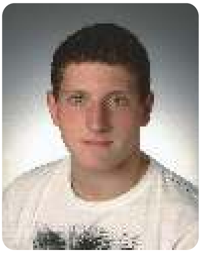


Fig.3: Velocity profiles of moving bed below the two cylindrical obstacles over time. One can see the unsteady behaviour due to bridge collapsing.



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SCIENTIFIC FRIENDS | ELECTRICAL CAPACITANCE TOMOGRAPHY

With the beginning of 2016 the first ECT (Electrical Capacitance Tomography) system resulting from our collaboration with the Institute of Electrical Measurement and Measurement Signal Processing (EMT) at Graz Technology University was ready to use and handed over to PFM for measurements in our laboratory.

The tomographic reconstruction is able to run online (with real time visualization) and allows insight in transport pipes of granular material of fluidized bed experiments.

Figure 1 illustrates the reconstruction of a hopper discharge experiment in our laboratory. The slices show the particle distribution inside the pipe for certain instants of time. The particle is disturbed with a pressure pulse which also increases the discharge rate from the hopper. Both details can be clearly resolved by the reconstruction of the ECT data.

Figure 2 shows the comparison of the mass flow rates estimated by the ECT system in comparison with load cell signals from a collecting bin below the hopper discharge experiment. Considering the fact, that the calibration of the system is solely done on an empty and a completely filled pipe, the matching is nearly perfect and the overshoot effects resulting from the numerical implementation are minor issuses which can be optimized.

The cooperation with EMT will be prolonged in the frame of a FFG / Bridge project to develop a field applicable sensor for ECT measurements of the pneumatic conveying of pulverized coal at voestalpine.

Particulate Flow Modelling

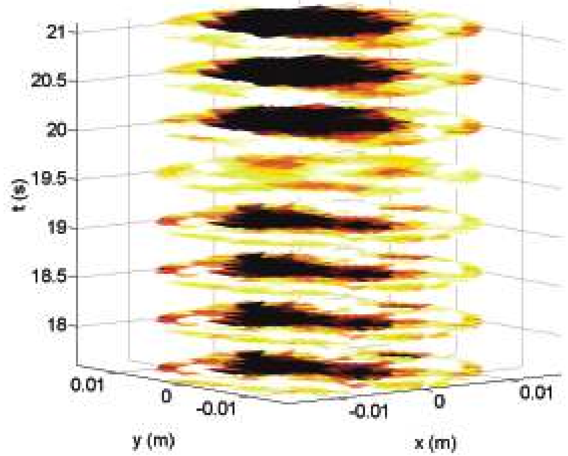


Fig.1: Slices of tomographic reconstruction of the particle mass flow in the pipe. One can see the air pulse at t=19.5s disturbing the flow and the increased mass flow rate afterwards.

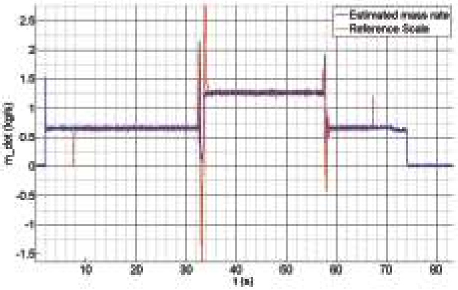
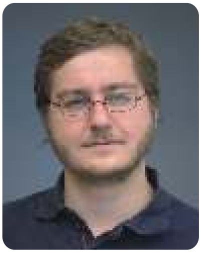


Fig. 2: Histogram of the load cell signal in comparison with the calculated mass flow rate of the ECT. Beside some overshoot effects the matching is very good.



Markus Neumayer **|** Matthias Flatscher **|** Thomas Bretterklieber

SCIENTIFIC FRIENDS | TUNDISH FLOTATION

Non-metallic inclusions (NMIs) in steel are primarily caused by entrained slag and the oxides formed by de-oxidation agents, e.g. aluminium, which is oxidized by dissolved oxygen within liquid steel.

As slag and de-oxidation products are lighter than steel, given enough time, NMIs float out of the melt. However, the retention time of the melt within the tundish sets a natural size-limit for the removal of NMIs. Very small NMIs would need an unfeasible amount of time to float-out due to their small terminal rise velocity.

Besides natural float-out there are other mechanisms of inclusion removal. The NMI's tendency to agglomerate and stick to the refractory can be exploited by enhancing turbulence or refractory contact. Another method to remove NMIs is argon flotation. When NMIs come into contact with an argon bubble, they adhere to the bubble and are essentially removed from the melt, once the bubble rises to the steel-slag interface.

The special properties of the argon-steel system leads to rather large gas bubbles. Thus, models developed for mineral flotation (based on air-water systems) can not be readily employed for inclusion flotation. In literature on modelling of inclusion removal by argon bubbles, however, models can be found that were specifically developed for argon-steel systems.

A population balance model (PBM) has been implemented to cover agglomeration of the NMIs. This model is extended with a model for argon bubble flotation. Agglomeration is considered in our model, since it alters the NMI's size-distribution and the NMI's size has a strong impact on its interaction with argon bubbles.

A two-phase Eulerian flow solver has been extended with our implemented inclusion flotation model. Thus, we are able to simulate the argon-steel flow and the evolution of the inclusion population within the tundish in an integrated manner. For this, the open-source CFD framework of OpenFOAM has been used, as it offers the most freedom. For testing purposes a zero-dimensional solver was implemented, which applies the flotation model to one computational cell without the need of changing the utilized flotation model.

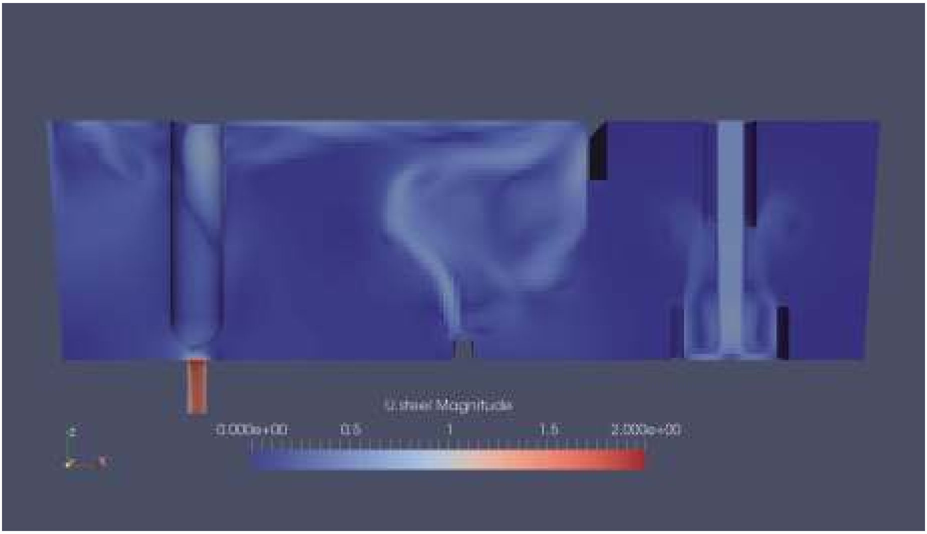


Fig.1: Liquid steel velocity within a single-strand tundish equipped with turbulence inhibitor, argon purging and weir. The weir shields the inlet region from the recirculation induced by the rising argon.

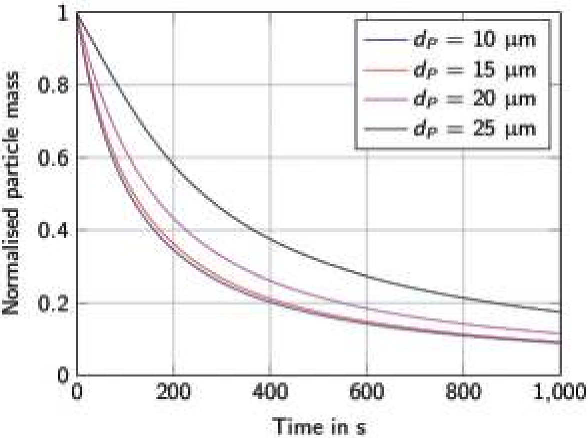


Fig.2: Evolution of normalized particle masses of five size-classes under pure agglomeration in a zero-dimensional test case.

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SEMINAR |
PROPER ORTHOGONAL DECOMPOSITION

“Once you stop learning, you start dying.” While this quotation that is attributed to Albert Einstein sounds quite drastic, we believe it to be especially true with regard to scientific life. Researchers who do not steadily increase their knowledge will stop being innovative.

Therefore, each winter term we hold a seminar where we devote some of our time to get to know a new topic we are interested in. This year’s subject is a computational technique called “proper orthogonal decomposition” to solve partial differential equations like the Navier-Stokes equations for fluid flow.

The physical reasoning behind this method is the observation that many flows contain coherent structures. These are “organized spatial features which repeatedly appear […] and undergo a characteristic temporal life cycle”[1], e.g. eddies in turbulent flow or bubbles in fluidized beds.

In a first step, we investigate how one can identify such structures from a series of flow fields, either obtained from classical CFD simulations or experiments. We ask ourselves “What are the most similar states to a given flow *on average*?”

It turns out that already a few of these states, also called eigenmodes of the flow, suffice to approximately describe it. The full fields are assumed to be superpositions of their modes with time-dependent coefficients, i.e. they are decomposed into an orthogonal basis. The complexity of the Navier-Stokes equations solved on N computational cells is reduced to determining the appropriate coefficients, usually orders of magnitude fewer than cells.

To conclude, we broaden our repertoire with a technique that allows us to analyse flows from a different perspective and to simplify certain calculations.

1 Berkooz et al., Ann. Rev. Fluid Mech. 25 (1993)

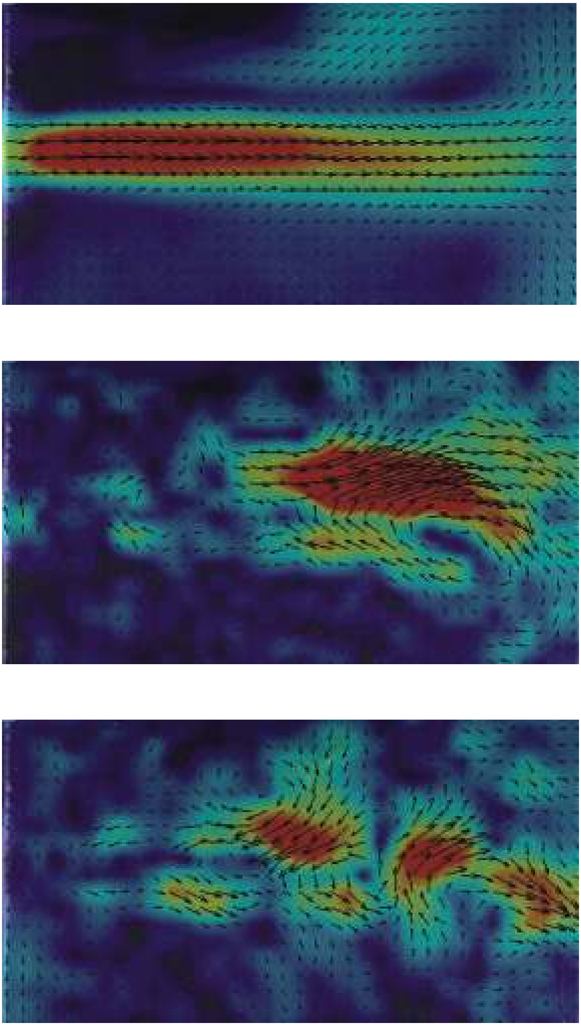

Fig.1: The average velocity field and the first two eigenmodes (top to bottom) of a jet hitting a wall.

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SELECTED PUBLICATION

Benvenuti L., Kloss C., Pirker S. Identification of DEM simulation parameters by Artificial Neural Networks and bulk experiments, in: Powder Technology, Volume 291, Page(s) 456-465, 2016.

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AWARDS

Stefan Pirker: Landespreis für Innovation 2016, Muster basierte Simulation von Partikel basierten Prozessen und Strömungen
Reza Farzad: Best Presentation Award, Experimental Fluid Mechanics Conference, Mariánské Lázne, Czech Republic.

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