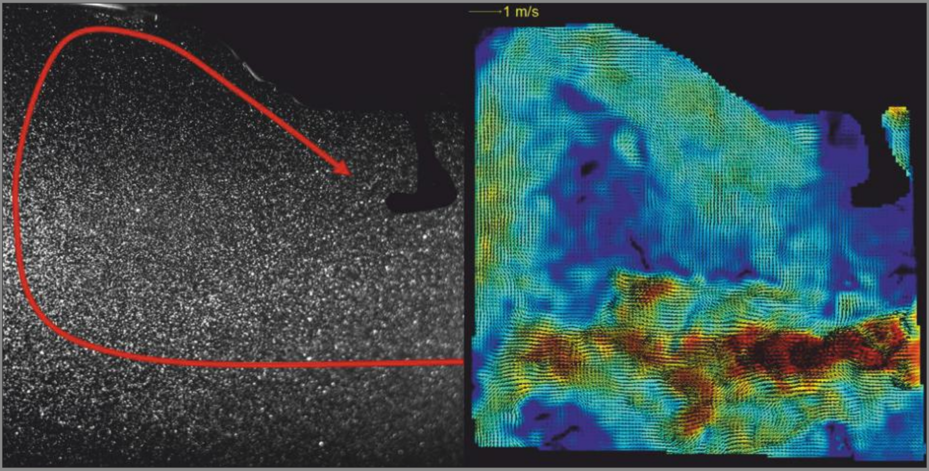

JKU | Department of Particulate Flow Modelling

Annual Report | 2018

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Front cover: Entrainment of a lighter liquid phase into the main flow caused by shear forces due to recirculating flow patterns. The Images were captured via time resolved PIV and resulted in a series of vector fields with 1ms time resolution and 0.5mm spatial resolution, respectively. This high resolution data is perfectly suited for validating LES results. © S. Puttinger

EDITORIAL

Dear Readers,

In the course of the years, PFM has become a mature research group experiencing continual success.

One major key for success are our senior researchers, who follow their own research ideas and independently supervise their own students. At the same time we have not one single research island, which is not interlinked to other seniors. This balance between individual fruition and interactive synergies forms an environment for joyful (and successful) research.

Another major key for success are our junior researchers - a colorful bunch of smart individuals from ten different countries. Despite their different (cultural) origins, they form a coherent group of mutually supportive PhD candidates and postdocs. They are sticking their heads together and find solutions based on their individual strengths.

A third major key for success are our industrial colleagues. They support us in doing real research - excavating the physical core of their processes, instead of expecting quick solutions. They motivate us to look beyond existing knowledge, fueling new ideas and scientific developments.

Many thanks for that!

With these introducing words I wish you a pleasant reading!

Sincerely,

Stefan Pirker | stefan.pirker@jku.at

EDITORIAL

Dear Readers,

Following the successful two year's evaluation at the end of 2017 the Christian Doppler Laboratory for "Multi-scale modeling of multiphase flows" went into an expansion phase. First, the RHI Feuerfest GmbH joined the Laboratory funding one additional researcher. In this project, we investigate the efficient numerical simulation of the transport and mixing of cohesive particles, which additional exhibit a wide particle size distribution. Second, the voestalpine Stahl Gmbh will considerably increase its share, which enables the closer investigation of the stability of liquid steel-slag interfaces.

One fundament of the successful development of numerical tool for industry are the sound theoretical fundaments. The focus of the CD-Laboratory on the physical and mathematical understanding of the industrial processes led to several high impact publication, which considerably increased the international visibility of the laboratory. One highlight of the last year was the invited professorship at the Institut de Mécanique des Fluides de Toulouse (Prof. Fede and Prof. Simonin), which is one of the leading groups in particle flow modeling.

Finally, I want to thank my team for their great work and their engagement and I am looking forward to a prosperous future of this CD-Laboratory.

Sincerely,

Simon Schneiderbauer | simon.schneiderbauer@jku.at

CONTENTS

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EDITORIAL | MICRO

Dear Readers,

Within the last year, our research activities in modelling small-scale phenomena in multiphase flows have been further developed. In close collaboration with our scientific friends and industrial partners, new computational methodologies are developed for turbulent interfacial flows as well as laminar biological flows.

Our recent progress in subgrid modelling of two-phase large eddy simulation has been validated with highly accurate time-resolved PIV experiment showing very good agreement. It reflects the capabilities of our improved approximate deconvolution-based two-phase LES model (called ADM-VOF) to account for small-scale effects of the interfacial dynamics and surface tension force in turbulent two-phase flows. Such method provides a wider perspective for connecting the physics of interfacial turbulence to process control aspects of metallurgical industry.

Furthermore, our PhD student Achuth B. Nair has been doing research on mathematical modelling of complex blood flow in microfluidic devices in which the dynamics of red blood cells is captured by a reduced-order modelling approach. In this approach, a deformable biological cell is represented as a clump of spherical particles inter-connected by means of mathematical bonds. Such cost-efficient technique is essential in the investigation of blood flow behavior in different conditions.

Let’s have a look at how we model micro-scale physics.

Sincerely,

Mahdi Saeedipour

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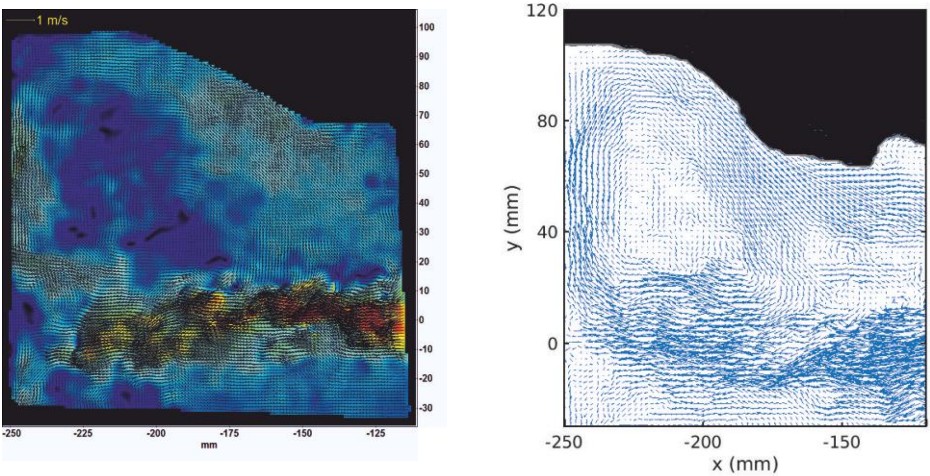

Fig.1: Snapshots of turbulent fields near the oil-water interface obtained by time-resolved PIV experiment (left) and large eddy simulation (right). These snapshots are used for statistical analysis of turbulence-interface interactions in liquid-liquid flows. This is an important step in investigation of fluid dynamics and metallurgical phenomena across the fluid interfaces.

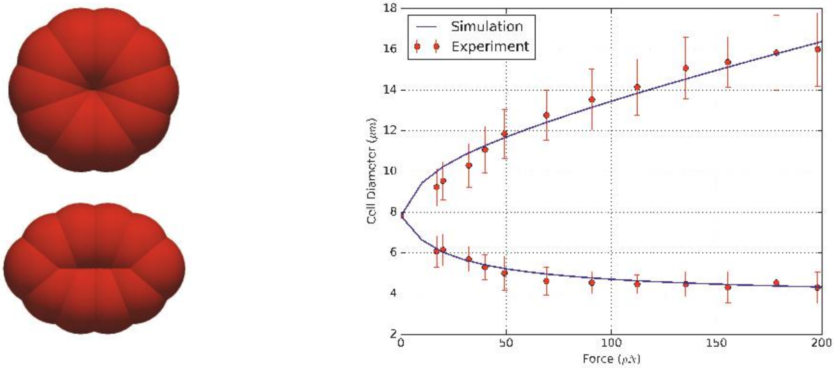

Fig.2: The reduced order modelling representation of a red blood cell before and after deformation (left). Force-displacement curve for deformable red blood cell in comparison with experiments from the literature. This curve reflects the accuracy of such cost-efficient method in predicting the dynamics of biological cells in blood flow.

MICRO | REDUCED-ORDER MODELLING OF RED BLOOD CELLS

Blood is an important physiological fluid which transports oxygen and other vital components to the various parts of the body. It consists of biological cells and can be considered to be analogous to a fluid with suspended particles. During in-vitro experiments it was found that the apparent viscosity of blood reduced with the channel diameter (Fahraeus-Lindqvist effect). It was observed that the flow consisted of an erythrocyte-populated core and a cell-free layer (CFL). This was attributed to the radial migration of erythrocytes towards the centre of the channel as a result of their deformability. Thus, it is important to model the cell behaviour when considering the rheology of whole blood.

A reduced-order modelling approach was adopted in which the geometric complexity and mechanical behaviour of biological cells were simplified. A biological cell was modelled using an arrangement of spheres and the sphere centres were connected using mechanical bonds. The bonds behave similar to cantilever beams and can rotate and translate with the spheres. The deformability of the biological cells was controlled by the bond parameters and with proper calibration of the model parameters can be found from physical units. An example of a healthy erythrocyte is shown in Fig 1. The surface area and volume of an erythrocyte are 132.76 132.76μ^2 and 93.89μ^3, which are close to the physical values for an erythrocyte.

The calibration of the bond parameters is performed by means of force-displacement curves and the plot for a healthy erythrocyte is shown in Fig 2. Additionally, in Fig 3, the force-displacement curves for the different stages of Malaria infection is shown and it is an example of the feasibility of the model for different cell types. Thus, with proper calibration of physical units to model parameters, various cell types can be mimicked using the deformable particle model.

The coupling of the deformable particle model with the CFD solver paves the way to simulation of whole blood. The various phenomena such as the Fahraeus-Lindqvist effect, CFL formation and the behaviour in flows through can be studied to verify the feasibility of the method for the applications in microfluidics.

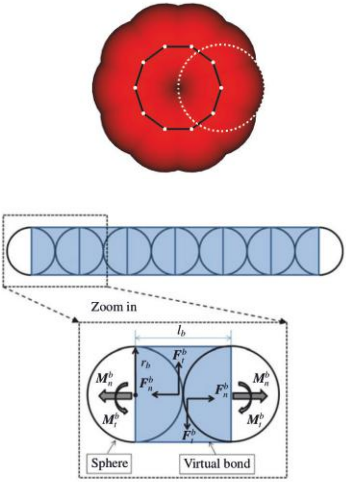

Fig.1: Reduced-order representation of an erythrocyte (top). Schematics of the bond model (bottom).

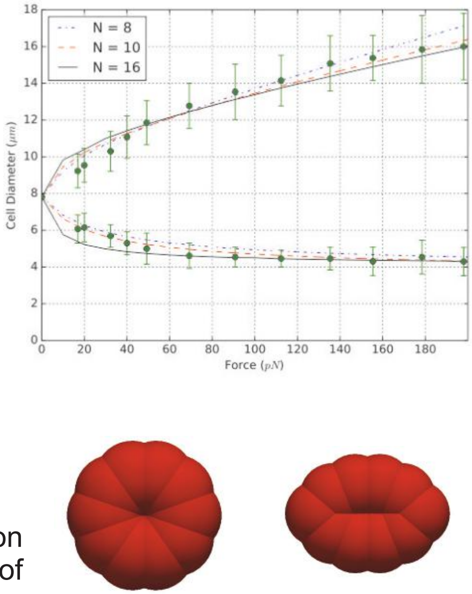

Fig.2: Force-displacement curves for different cell resolutions (top). The relaxed and deformed state of an erythrocyte for F = 100 pN (bottom).

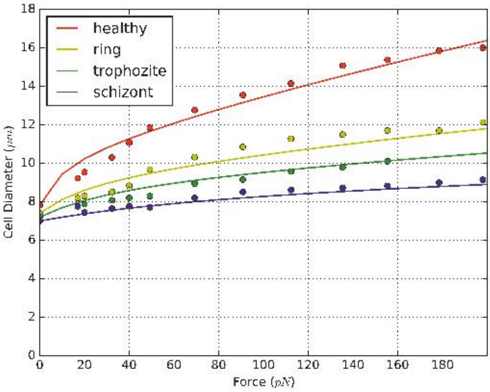

Fig.3: Force-displacement curves for various stages of Malaria infection.

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MICRO | SUBGRID SCALE MODELLING OF TWO-PHASE FLOW LARGE EDDY SIMULATION

Large Eddy Simulation (LES) is currently widespread in turbulence modelling research. Although LES has reached a mature level in modelling single-phase turbulent flows even in industrial scales, the challenges with LES of turbulent interfacial flows still remain. Introducing spatial filtering to the one-fluid equations of the interfacial flows results in appearing various subgrid terms that should be accounted via subgrid scale (SGS) closure models. Here, the major shortcoming comes from the lack of general conclusion on the SGS closure modelling, where the small-scale physics of the flow as well as the small-scale interfacial topological changes must be accounted.

In our recent study [1], a new large eddy simulation formulation is developed where all the subgrid scale (SGS) terms appearing in the filtered governing equations are closed by a volume of fluid-based Approximate Deconvolution Model (ADM-VOF). In this structural turbulence modelling approach, the SGS terms of stress tensor and surface tension in the Navier-Stokes equations, as well as the interface dynamics in the VOF transport equation, are mathematically reconstructed from the resolved scales. We have implemented the ADM-VOF method in the frame of C++ libraries of OpenFOAM. The ADM-VOF is then employed for an *a posteriori* LES on the phase inversion benchmark (Figure 1) which represents a buoyancy-driven turbulent interfacial flow with several interfacial events such as coalescence and rupture. To investigate the performance of this approach, a series of quantitative comparisons with highly resolved data and conventional LES (i.e. eddy viscosity approach) is conducted based on macroscopic characteristics of the flow including enstrophy and interfacial length (figure 2). The results reveal that the structural ADM-VOF approach improves the prediction of macroscopic flow characteristics associated with unresolved contributions compared to the conventional LES (figure 3). Additionally, we concluded that the choice of functional methods for modelling relaxation term may not be extendable to the two-phase ADM. This approach is intended to be employed for modelling turbulent interfacial flows with industrial applications such as continuous casting and liquid atomization.

Fig.1: Highly-resolved numerical simulation of interfacial turbulence in the phase inversion problem. The images display liquid-liquid interfaces at different stages of the problem.

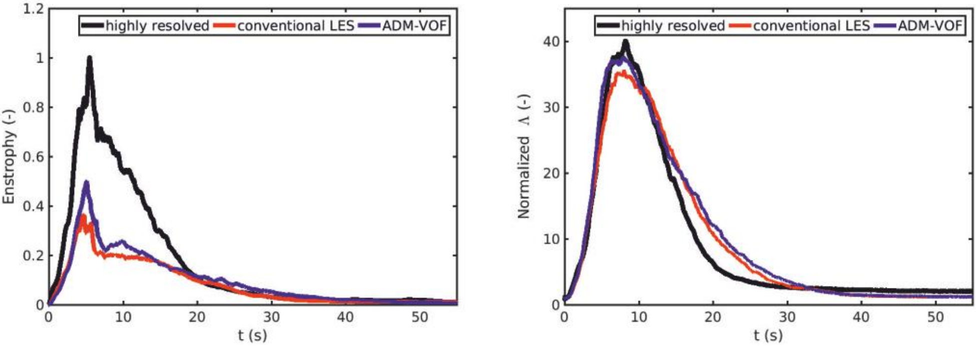

Fig.2: Temporal evolution of heavier fluid enstrophy (left) and normalized interfacial length (right) during the phase inversion for the highly resolved simulation as well as conventional LES and ADM-VOF. The LES grid is 4 times coarser.

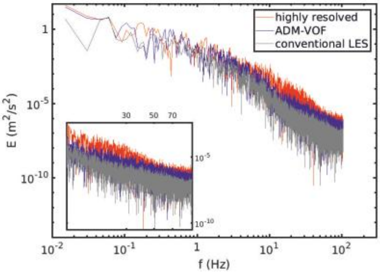

Fig.3: Energy spectra of the highly resolved simulations compared with conventional LES and ADM-VOF on 4 times coarser grid.

[1] Saeedipour, M., Vincent, S., Pirker, S., Large eddy simulation of turbulent interfacial flows using Approximate Deconvolution Model. International Journal of Multiphase flow. 2018.

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EDITORIAL | MESO

Dear Readers,

Like each scientific discipline, research on particulate and multiphase flows on the mesoscale has its own, very specific challenges. On smaller scales, we find the domain of microscopic calculations with hardly any empirical input. They provide accurate insights into problems of small dimension. On the other side, macroscopic simulations describe full-size processes inside industrial plants but rely on phenomenological, sometimes unreliable closures. On the mesoscale, we aim to build bridges between these two extremes. Based on findings from microscopic simulations, clever models are developed for somewhat larger problem sizes to eventually understand the laws of physics acting on the macroscale.

The challenge of mesoscopic research has an additional aspect. Due to their close connection with well-established physics, microscopic models can attract public, scientific funding. Macroscopic simulations, on the other hand, promise practical insights into industrial processes thus being an obvious target for industrial sponsors. In the mesoscale domain, are we caught between two stools? No, we are not. It is because of you, dear Readers! With industrial partners who understand the importance of strategic research, we explore the secrets of physics between very small and very large scales. Our close collaborations guarantee that the goal of our efforts will have a purpose. Furthermore, they allow us to focus on solving problems instead of fulfilling shortsighted paper counts with often hardly any meaningful contents. While being scientists who are proud to present their findings to the public, we do not “publish or perish” but hunt down open questions to systematically answer them.

Sincerely,

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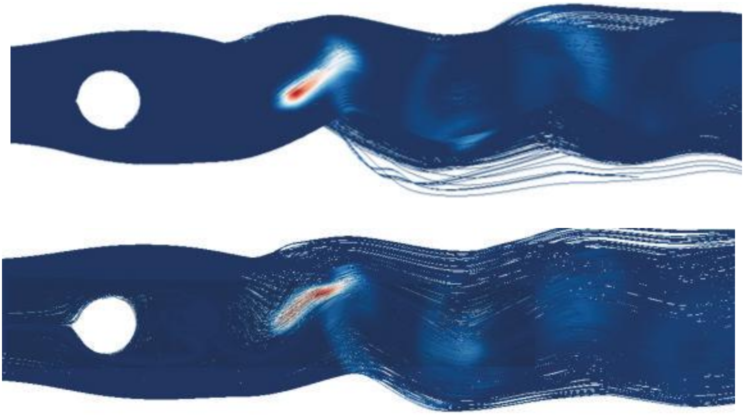

Fig.1: Species transport after a cylinder at Re=3900 with a source in the wake centerline after the recirculation length LES (upper image) and rCFD (lower image) simulations show qualitatively very similar results, where the latter may be obtained on much coarser grids.

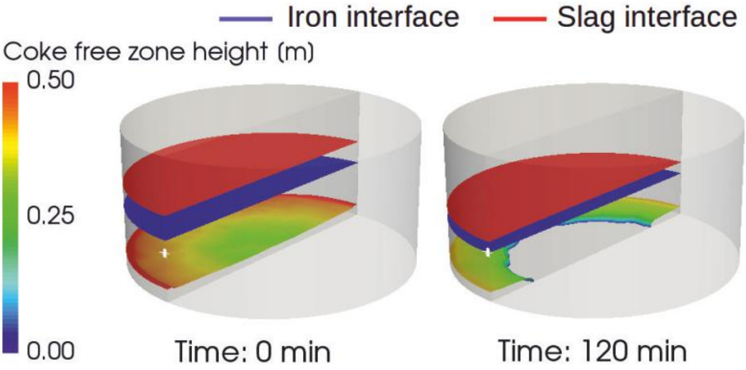

Fig.2: Liquid iron and slag flow in a blast furnace hearth. Depending on the fluid levels, the coke bed (“deadman”) floats or sits, which affects the tapping behavior. The description of the bed’s state in terms of liquid masses leads to a much more efficient model.

MESO | MULTI-LEVEL COARSE-GRAIN MODEL OF THE DEM IN THE MIDREX® PROCESS

The discrete element method (DEM) has proven to be a viable tool for the analysis of granular flows. In a broad range of industries, DEM simulations are successfully used to support process design and optimization. On the downside, the DEM is a computationally demanding method, making it difficult to apply to large-scale systems.

The coarse-grain (CG) model of the DEM relaxes this computational restriction by replacing multiple equal particles by a single coarser (pseudo) particle, thus significantly decreasing the number of particles involved in the computations. However, due to the violation of geometric similarity, this approach fails to capture effects that intrinsically depend on particle size. Particularly, this becomes an issue in multi-scale systems typically found in large industrial facilities.

Seeking for a computationally feasible description of such large-scale systems, we have developed the multi-level coarse-grain (MLCG) model which concurrently couples multiple coarse-grain levels to adjust the resolution of the simulation as required.

Among our targeted applications is the direct reduction of iron ore in a shaft furnace (Fig. 1). One of the most widely used methods for DRI production is the MIDREX® process, which uses a reforming gas made from natural gas to reduce iron ore. The raw material is charged from the top while the reductant gas is blown in from about the middle of the shaft. On its way to the top the gas reduces the iron ore. A cooling gas circulates in the lower part of the furnace.

Currently, in its largest incarnation, the MIDREX® shaft furnace (the SUPER MEGAMOD®) has a production capacity of more than 2.2 million tons per year (i.e. >70kg/s). To achieve this throughput, the SUPER MEGAMOD® has an inner diameter of 7.15m and contains an estimated 500 million iron ore pellets (Fig. 2) – not considering particles smaller than 3mm.

This amount of particles would require a powerful high performance computing cluster to reasonably execute DEM simulations. Using a 3-level setup of our MLCG method (cf. Fig. 3), we are able to reduce the number of particles to simulate in this furnace to about 1-2 million which can be handled by a modern desktop computer or small computing cluster.

To gain a better understanding of the influence of the plant operating parameters on the performance of the furnace is the goal of this study.

Fig.1: MIDREX Super MEGAMOD direct reduction shaft furnace in Corpus Christi, Texas.
Source: Primetals Technologies primetals.com.

Fig.2: Pelletized iron ore with scale (by Arnoldius (CC BY-SA))

Fig.3: 3-level setup of the coupled ML-CG simulation. From top to bottom the coarse-grain ratios 8:4:2 (red:green:blue) are used.

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MESO | MODELLING DIRECT REDUCTION OF IRON ORES IN FLUIDIZED BEDS WITH CFD-DEM

Fluidized beds and moving bed reactors are commonly used in the reduction of iron-ore. However, measurements in these reactors are not that easy. Thus, in research simulation tools can be utilized, such as the CFD-DEM coupling method, where the reacting gas is represented with the Eulerian side and the iron-ore particles in the Lagrangian side. In this project we have implemented the unreacted core model to represent the iron-ore reduction, as it is able to represent the three different interfaces of hematite/magnetite, magnetite/wustite and wustite/iron that occur during the reduction of an iron-oxide. The rate of reduction can thus be determined with considering all the resistances due to the reactions at interfaces, the intraparticle diffusion and the gas film diffusion surrounding the particle. With this rate the mass sources for the gas phase and the particle phase are determined. This procedure posed several challenges such as determining the iron-oxide phases depending on the gas concentrations, the extend of computational time and heat transfer between the two phases.

Through extensive literature review and numerical investigations the most appropriate equilibrium constants that define the iron-oxide phases, as shown in Fig. 1, have been determined and implemented. The determined equilibrium constants and other critical kinetic parameters such as activation energies and frequency factors are then verified with comparing the simulations of a reduction of a single hematitic particle with available experimental data for various gas concentrations, ranging from only CO and N_2 to gas concentrations with CO, CO_2, H_2, H_2O and N_2, as illustrated in Fig. 2. After validating the model with the single particle reductions and verifying that the gas molar fractions are changing according to reactions as shown in Fig. 3, we have carried on investigations with a three-staged fluidized bed, in which the thermodynamic conditions are defined so that only one of the reactions takes place in every stage. To reduce the computation time we have used a coarse graining model where the particles are replaced by larger (pseudo) particles and implemented a scaling factor for the reduction rate that affects only the mass change of particle layers, thereby requiring less computational time. The results are then compared with experimental work for the three different stages, as shown in Fig. 4. For heat transfer between the two phases, we are currently evaluating several approaches such as the heat transfer model proposed by Gunn as well as heat produced due to the chemical reactions.

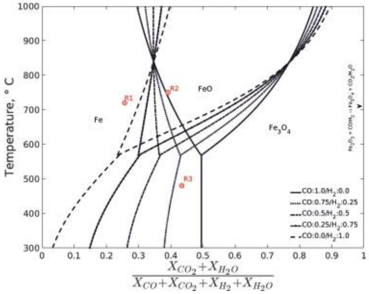

Fig.1 (top): The iron-oxide phases represented in a phase diagram (Baur-Glaessner-Diagram) for various gas compositions with the different reaction points that are used in the experimental and numerical calculations, where a mixture of CO/CO_2 and H_2/H_2O is used as reducing gas at different temperature.

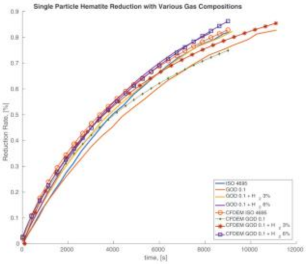

Fig.2 (top): The comparison between numerical and experimental works on the reduction of a single hematitic particle with various gas concentrations. The straight lines are experimental works, and the marked lines are numerical results. It can be seen that the end reduction rate is achieved at the same time for both works.

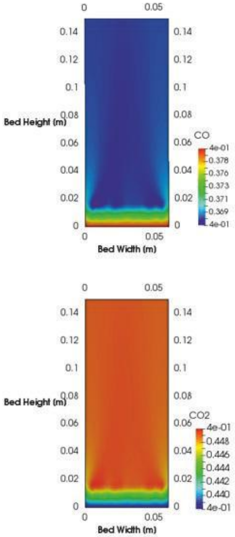

Fig.3: (left):Contour plot for reacting gas molar fraction of CO and product gas molar fraction of CO_2.

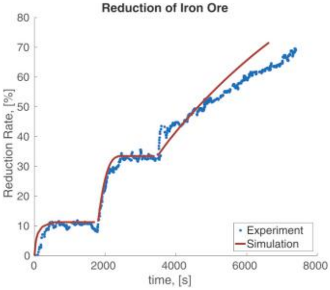

Fig.4 (top-right): Comparison of the total reduction rate of iron-ore through the different fluidized bed stages between experiment and simulation results.

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MESO | MODELLING OF BLAST FURNACE TAPPING

Erosion of the blast furnace hearth is a big problem and is most often the cause of a limited campaign length. In order to obtain information about the state of the hearth, numerical tools have to be resorted to, due to harsh conditions making direct measurements extremely difficult.

In the blast furnace hearth, molten iron and slag fill the voids between a dense porous coke structure, often referred to as the deadman. The deadman is buoyant and its position, shape and porosity distribution varies heavily depending on other operational conditions. While in previous research, the deadman was often treated as a static porous medium and its dynamic nature ignored, we developed a tool to study the blast furnace tapping using a CFD (Computational Fluid Dynamics) – DEM (Discrete Element Method) approach. This method allows for a very detailed study that captures individual coke particle movement at the cost of high computational times. Consequently, it is limited to small-scale systems.

To investigate the tapping of an industrial scale blast furnace, we suggested a pure CFD approach (dynamic void fraction model), where pre-generated deadman states are utilized in a clever way, to in a fast manner take the deadman dynamic behavior into account. In previous work, we performed CFD-DEM simulations of an experiment that we conducted. By employing the dynamic void fraction model we could obtain very similar results with a speedup of *x60,* reducing the total computational time from four hours to four minutes (cf. Fig. 1).

We applied this model to a full-scale blast furnace with a hearth diameter of 12 m, shown in Fig. 2 for two typical deadman states, a sitting (left) and a floating (right). By using the dynamic void fraction model, we could with little effort simulate a full tapping cycle of ca. two hours. Detailed information about the iron and slag flow can then be obtained as shown in Fig. 3, where the flow rates are compared with a static floating deadman. When the deadman movement is taken into account, we observe a higher iron flow rate, a longer slag delay and an increased tapping duration, highlighting the necessity to do so.

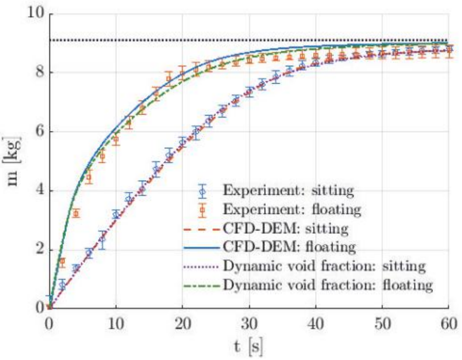

Fig.1: Comparison the simulated experiment drainage between the CFD-DEM and dynamic void fraction models.

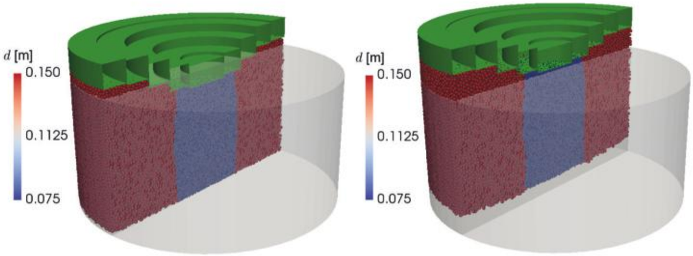

Fig.2: Visualization of a typical simulation setup of a sitting deadman (left) and floating deadman (right), here shown with a dense center of smaller particles.

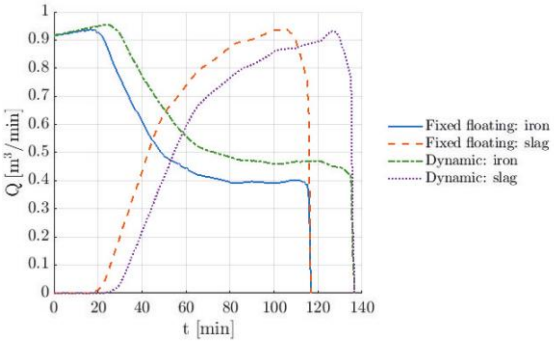

Fig.3: Iron and slag flow rate of the dynamic void fraction simulation, compared with a static floating deadman.

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MESO | RECURRENCE CFD APPLICATION IN TURBULENT FLOWS

Expanding range of the application of Computational Fluid Dynamics (CFD) brings the challenge of reducing the high computational costs especially in complex and large-scale processes along with maintaining the accuracy. Recurrence CFD (rCFD) aims at time-extrapolating a system's behavior according to its dominant reappearing structures in a really fast way.

With the purpose of investigating the potential of rCFD in turbulent flows, we studied passive scalar transport on the turbulent vortex shedding over a circular cylinder at Reynolds number (Re) 3900 by large eddy simulations (LES) as well as rCFD. The computational domain built for LES had approximately 3000000 cells. The distances between inlet and outlet boundaries, upper and lower walls were 30D and 10D, respectively. Also, the span-wise length of the domain was ×D. Then in order to carry out rCFD, we recorded a database for 5 vortex shedding periods after the turbulent flow was fully established and performed recurrence analysis. The computed distance plot is presented in Fig. 1. This plot shows the periodicity of the system and its dominant frequency which corresponds to vortex shedding frequency.

The primary objective of rCFD is to reduce temporal and spatial resolution. Therefore, we created a coarser mesh with 300000 cells for the rCFD simulation and consequently used a time-step 10 times greater than the LES time-step. We time-averaged the results over approximately 75 shedding cycles. Figure 2 depicts the mean species distribution for LES on the fine grid and rCFD on the coarse grid. Besides, to have a quantitative comparison we plotted species profiles at different sections in the wake region in Fig. 3. We can conclude that rCFD has been very successful in predicting the mass transport in the turbulent flow and our results are in a very good agreement.

In addition, a notable achievement of this work is the speed-up of 250 at 1/8 of the required computer power compared to LES. rCFD decreased the computational cost considerably. For our future work, we will apply the rCFD method to complex multi-phase problems.

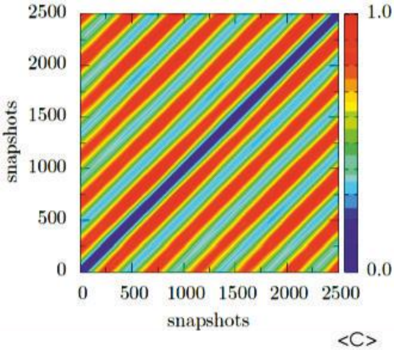

Fig.1: Distance matrix generated according to the velocity profiles for 5 vortex shedding cycles. The blue color refers to the most similar states and the red color represents the highest difference between two states.

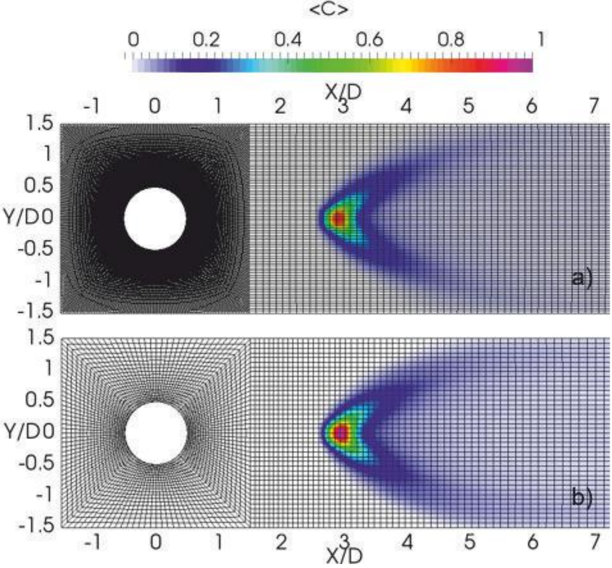

Fig.2: Time-averaged species transport in the wake region of the cylinder over about 75 vortex shedding cycles for a) LES on the fine grid and b) rCFD on the coarse grid. The results are in a very good agreement.

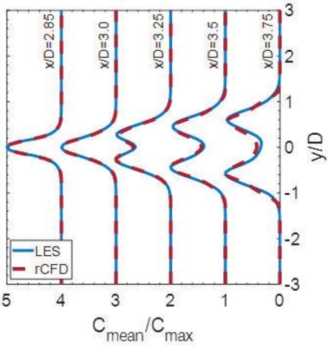

Fig.3: Mean species transport over 75 shedding cycles at different sections of the wake region. rCFD on the coarse mesh is in very good agreement with LES on the fine mesh.

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MESO | BLAST FURNACE SIMULATIONS AND THE ISSUE OF MULTIPLE LENGTH AND TIME SCALES

Particulate systems are frequently described with the discrete element method (DEM). For each single grain, the forces due to its neighbors are evaluated and its position and velocity are updated for a small time increment. With increasing system size, this type of simulation becomes too computationally expensive. Without further improvements, the method is thus limited to particle numbers of order $10^5 – 10^6$ and to investigation times of a few seconds or at most minutes. Straight-forward application to blast furnace modeling is clearly impossible. It takes additional efforts to simplify the equations of motion while retaining the relevant physics.

Recently, we have introduced a generalized coarse-graining strategy that allows to combine particles of various sizes into larger parcels (c.f. Fig. 1) which interact with modified material parameters. This allows for an approximate description of the granular bed inside industrial-size furnaces as depicted in Fig. 2. However, one is still bound to short-term observations. To picture the journey of an ore or coke particle through the furnace, we disregard any irregularities and assume that particles follow their time-averaged velocity field which we can obtain from short DEM simulations. Then, instead of evaluating the forces on each grain, we let them follow the previously calculated streamlines displayed in Fig. 3.

Without the severe restriction to resolve particle-particle contacts, we can use much larger time steps. Essentially, their size is limited by the ability of the non-interacting tracers to properly follow the time-averaged velocity field. Given the slow burden descent, it may be far above any gas-phase time scale. Therefore, to include gas dynamics, we will abandon a time-accurate transient description and assume that the fluid flow immediately adapts to the current solid configuration leading to only one additional, steady-state calculation per particle time step.

The resulting description is numerically very cheap and allows to follow particles from their insertion into the top of the furnace to their consumption in the cohesive zone and in the raceways, respectively.

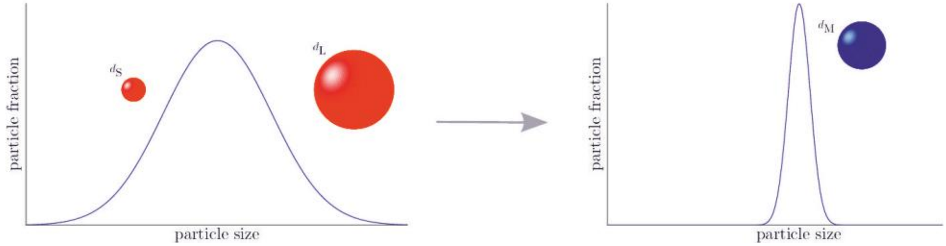

Fig.1: Polydisperse parcel approximation. Particles with a broad size distribution (left) are replaced with parcels obeying a narrower one (right).

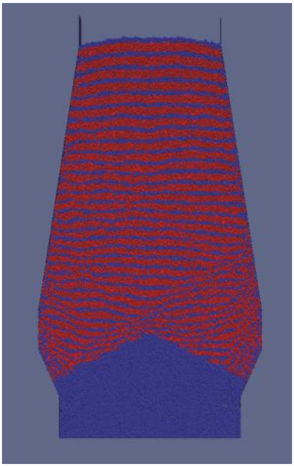

Fig.2: Snapshot of particles in a real-size blast furnace. Coke (blue) and ore (red) form a layered structure in the upper part above the cohesive zone.

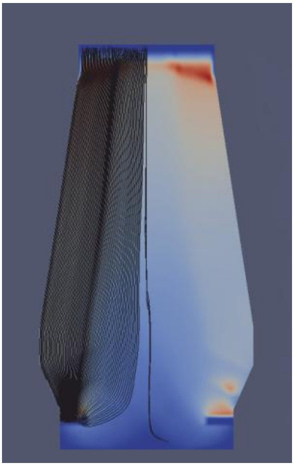

Fig.3: Time-averaged particle velocity field. Streamlines (black; shown for the left-hand side only) move particles towards the raceway where they are consumed.

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MESO | MODELLING OF GAS-SOLID FLOW WITH COHESIVE POWDERS

Fractures of particle assemblies happen frequently in dense gas-solid systems leading to a notable heterogeneity in the particle configuration, especially in case of cohesive powders and non-spherical particle interlocking. This can have a strong impact on the powder behavior in the industrial applications (e.g. die filling).

Experimentally, we have discovered that an initial bed loosening by slight aeration has a tremendous effect on the die filling performance. We hypothesize that this powder pre-conditioning process causes the formation of local fractures, which divide the global powder bulk into smaller pieces that can pour into the slit die without forming arches (Figure 1).

We reproduced this phenomenon in a coarse-grained DEM simulation by provoking active gas channels during the initial aeration step (Figure 2). As with the experiment, the number of filled particles was significantly higher with the procedure applied. These findings might lead to improved die filling operations.

Next, we have investigated the influence of such heterogeneities on the hydrodynamic drag by studying the idealized case of a random arrangement of spheres with a channel like void region. Single-relaxation-time lattice Boltzmann simulations were performed to resolve fluid flow through arrested particle configurations and calculate the corresponding gas-particle momentum exchange and pressure drop (Figure 3.). In the case of heterogeneous particle arrangements comprising a channel-like void region in between two dense bulk regions, our simulations indicate a dramatic decrease in overall pressure drop even for channel widths of only one particle diameter.

Thus, we demonstrate the significance of channel/crack formation on fluid-solid momentum exchange and overall pressure drop in dense particle arrangements. At the same time, sub-grid heterogeneities are commonly neglected in unresolved CFD-DEM simulations.

Fig.1a: As the powder is very cohesive, only the small amount of material is discharged.

Fig.1b: With the gas-induced bed loosening, the powder flowability increased significantly.

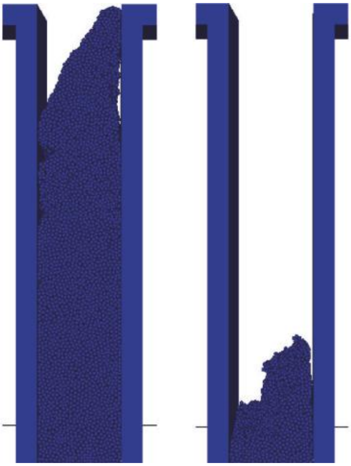

Fig.2: To test our hypothesis of a local fracture formation, we have artificially applied discrete vertical forces strings to the initial powder bulk. We can observe a substantial increase of the disposed material (right).

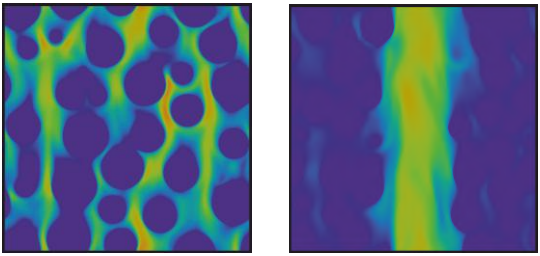

Fig.3: The channel allows for a by-passing of a considerable amount of the flow leading to a reduced overall pressure drop and thereby underestimating the minimum fluidization velocity in a fluidized bed.

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EDITORIAL | MACRO

Dear Readers,

The focus of our macroscale research efforts is laid on industrial scale gas-solid flows (Fig. 3). Thus, the main question is: “ How can we accurately predict those industrially highly relevant flows in a reasonable time?” Hereby, we develop either ”coarse grained” models, where the micro-scale behavior is accounted by proper constitutive relations for the unresolved sub-grid scales or highly efficient time integration methods such as recurrence CFD (rCFD).

Last year we pushed forward the gas-solid turbulence models towards heat and mass transfer. Furthermore, we explored the applicability of new approaches for turbulence modeling such as the approximate deconvolution model (ADM). The main advantage of such a structural model is its purely mathematical nature, which allows the reconstruction of certain unresolved by, for example, de-filtering or Taylor series expansions (Figs. 1 & 2). Finally, we are further developing the rCFD method for large-scale fluidized beds.

In addition to model development, we took the plunge to implement all these developments to open source software, which frees our industrial partners and ourselves from the bonds of increasing license fees.

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

Sincerely,

Simon Schneiderbauer | simon.schneiderbauer@jku.at

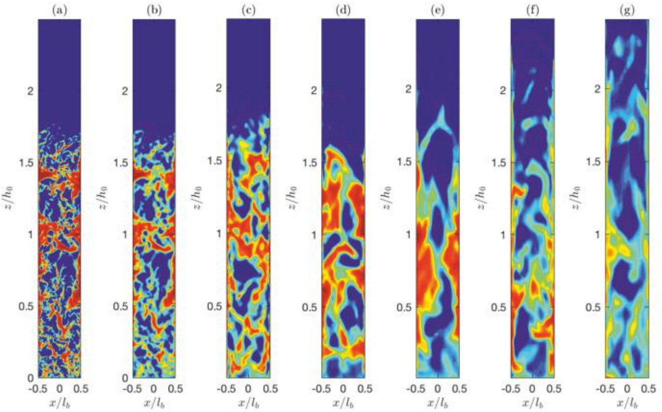


Fig.1: Snapshots of the solids volume fraction: a) fine grid ($\Delta=8d_p$); b) filtered fine grid; c) ADM-TFM ($\Delta=48d_p$); d) ADM-TFM ($\Delta=64d_p$); e) ADM-TFM ($\Delta=96d_p$); f) TFM ($\Delta=64d_p$); g) TFM ($\Delta=96d_p$).

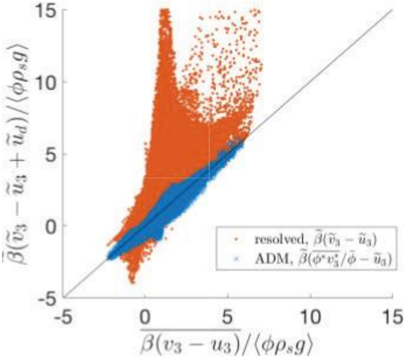


Fig.2: Correlation of filtered drag force measured from fine grid simulation with prediction received from either uncorrected coarse grid or ADM.

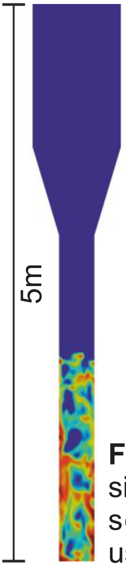


Fig.3: Coarse grid simulation of indus-trial scale fluidized bed using ADM-TFM

MACRO | CLUSTER INDUCED TURBULENCE FOR MOMENTUM AND HEAT TRANSFER

Gas-solid flows, like fluidized beds or risers, are used for a wide range of applications, from food drying and polymer production to the direct reduction of iron ore. While for small scale fluidized beds, simulation is quite feasible, the occurring physical phenomena cannot be fully numerically analyzed in large scale reactors yet, due to a large range of involved scales. In fluidized bed reactors of several meters in height, the smallest stable structures are usually only several particle diameters wide [1]. By employing coarse enough grids to make the simulation of full-scale reactors possible, mesoscale structures and, thus, their contributions to the macroscale flow properties are not resolved (Fig. 3). The unresolved heterogeneous structures, however, have a significant influence on the flow properties. The velocity fluctuations around particle clusters give rise to turbulence, i.e. cluster induced turbulence [6]. An overestimation of the gas-solid drag force by not accounting for this turbulence leads to an overestimation of the bed expansion [5].

A model accounting for the unresolved terms can be derived by spatiallyaveraging the kinetic theory based two-fluid model equations [4]. The filtered gas-solid drag can be, for example, approximated by the resolved drag coefficient times the resolved slip velocity corrected by a drift velocity [2, 3]. The drift velocity can be viewed as the gas-phase velocity fluctuations seen by the particles. Similarly, the filtered interphase heat transfer can be approximated by the resolved heat transfer corrected be a drift temperature.

We developed closure models for the drift velocity and drift temperature, as well as for the other unresolved terms in the filtered energy equations. Thereby, the scale-invariance of the correlation coefficients present in the models is used (Fig. 2). A comparison of the presented closure models with filtered fine grid simulation data shows good agreement (Fig. 1)

[1] Agrawal K, Loezos PN, Syamlal M, Sundaresan S. The role of meso-scale structures in rapid gas-solid flows. J. Fluid Mech. 2001;445:151–185.

[2] Ozel A, Gu Y, Milioli CC, Kolehmainen J, Sundaresan, S. Towards filtered drag force model for non-cohesive and cohesive particle-gas flows. Phys. Fluids 2017;29:103308.

[3] Schneiderbauer S, Saeedipour M. Approximate deconvolution model for the simulation of turbulent gas-solid flows: An a priori analysis. Phys. Fluids 2018;30:023301.

[4] Schneiderbauer S. A spatially-averaged two-fluid model for dense large-scale gas-solid flows. AIChE J. 2017;63(8):3544-3562.

[5] Schneiderbauer S, Puttinger S, Pirker S. Comparative analysis of subgrid drag modifications for dense gas-particle flows in bubbling fluidized beds. AIChE J. 2013;59(11):4077-4099.

[6] Fox RO. On multiphase turbulence models for collisional fluid-particle flows. J. Fluid Mech. 2014;742:368-424

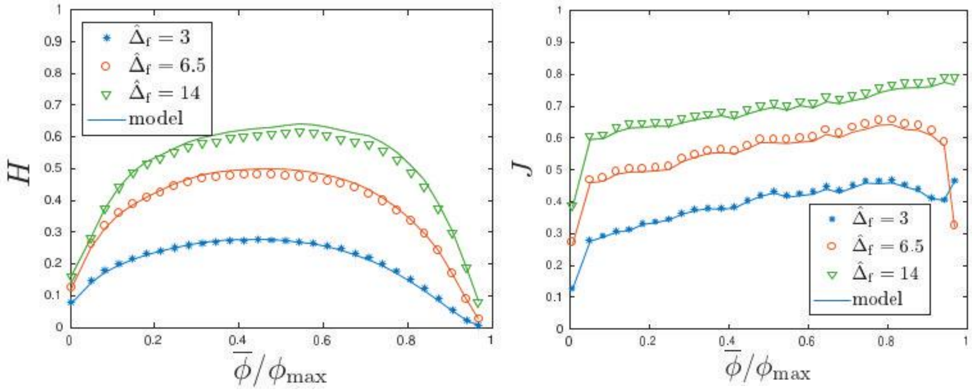
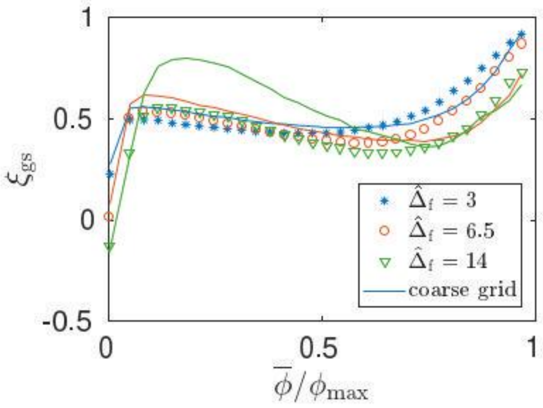


Fig.1: Fractional correction functions H for the drag force and J for the interphase heat transfer, measures for the overestimation of the drag force and heat transfer by not accounting for mesoscale structures, as a function of the normalized filtered solids volume fraction. The symbols represent filtered fine grid simulation data, the lines the proposed models for the filtered interphase transfer terms.



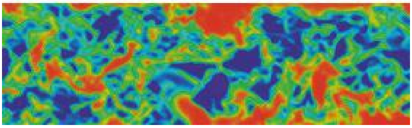


Fig. 3: Clustering

Fig. 2: Correlation coefficient calculated on the fine grid (symbols) and on the coarse grid (lines).

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MACRO | DEFLAGRATION

In the past, we as a research group nearly exclusively focused on the behavior of inert particles and their (multi-scale) interaction with an interstitial fluid phase. Beyond that, we looked in awe at those huge numbers of species and reaction mechanisms scientists from the combustion community are dealing with. This just seems too complex to touch!

Consequently, we clearly communicated our doubts when we were approached by colleagues from HOERBIGER Wien GmbH, asking for a feasibility study on numerical modelling of deflagration events. However, they insisted that we should have a modelling try ‘from a particles’ perspective’.

We finally agreed to approach this topic on senior-postdoc level. While Stefan Puttinger collected literature on the physical core phenomena and on characteristic deflagration experiments, Simon dug into single particle combustion and I tried to set-up an ‘umbrella’ simulation framework for a macroscopic representation of deflagration events. For the latter, I opted for a combination of Lagrangian prediction and Eulerian relaxation, yielding an efficient and robust simulation tool.

In figure-1 deflagration is considered in two connected chambers. After ignition in the top chamber a pressure wave travels towards the bottom chamber. Once, the combustion process reaches the bottom chamber a counter pressure wave propagates upward again. In this test configuration (as well as in others) we could produce plausible results in affordable time.

Encouraged by these first results, we decided to dig a little bit deeper into this topic by setting up an experiment, picturing the turbulent intensity and heterogeneity in typical deflagration calibration tests (figure-2). In parallel to these experimental activities, Simon performed two-fluid simulations, evaluating the generation and decay of turbulence and heterogeneity of particle concentration (figure-3).

Particulate Flow Modelling

Fig.1: Two snap-shots of a macroscopic simulation of deflagration in a two-chamber geometry, picturing particle and gas temperature during (left) downward and (right) upward pressure waves.

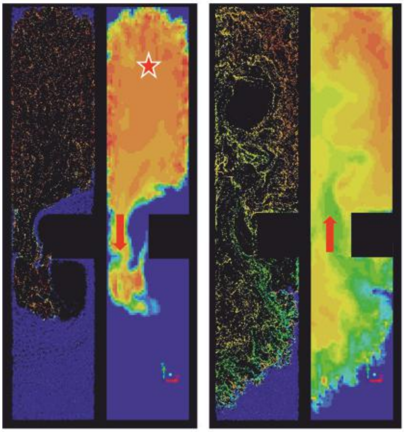
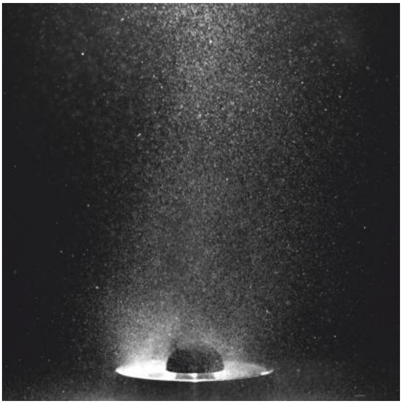
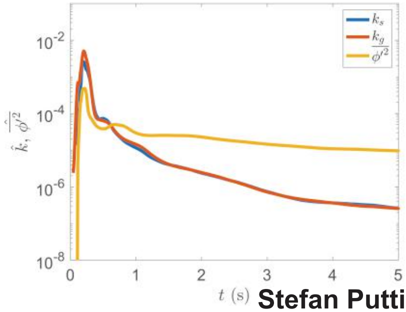


Fig.2: (right): Snap-shot of a dust dispersion experiment, picturing dust concentration and turbulence pattern prior to ignition.





Stefan Puttinger | Simon Schneiderbauer | Stefan Pirker

Fig.3: Decay of turbulence and heterogeneity of particle concentration.

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MACRO | TOWARDS A FAST FLUIDIZED BED SIMULATION USING RECURRENCE CFD

The dynamics in fluidized beds reveals a complex physics because of the variety-multiscale interactions between the solid-fluid phases (*e.g*. particle-particle, particle-fluid, solid-clusters, bubbles and slugs). This diversity of scales has constrained the numerical simulations of sizeable fluidized beds to a short-term duration, making the slow processes such as heat and mass/species transfer, out of reach.

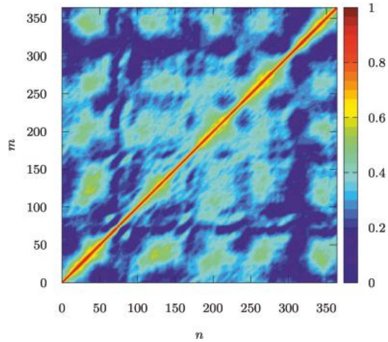
As a remedy, some of us † have proposed the novel approach of recurrence CFD (**rCFD**) as an efficient time-extrapolating method for a fast simulation of passive transport. Therein, the pseudo-periodicity of a system is measured by a recurrence norm (rNorm), which has to be based on a subtle active field.

In an initial stage, we have restricted ourselves in investigating the rNorm at different regimes of fluidizations (see Figs.1,2). The outcomes have emphasized on the proper relevance of the *uniform* flow dynamics in computing the rNorm.

In an advanced step, the transport-based **rCFD** † is applied to simulate the propagation of a passive concentration on gas-phase, considered as chemical species in fluidized beds. Following a Lagrangian shift-positions history, stored in memory and tracked on the gas-phase, the transport of species is fairly predicted within few seconds run-time in comparison with several hours full-CFD simulation in ANSYS/Fluent (Fig. 3).

As future concerns, we will account more efforts on the accuracy of the transport-based **rCFD**, On the other hand, we aim to study the species transport on the solid-phase as well, using this fast methodology.

Pirker & Lichtenegger, ChES, 188, 65-83, (2018).



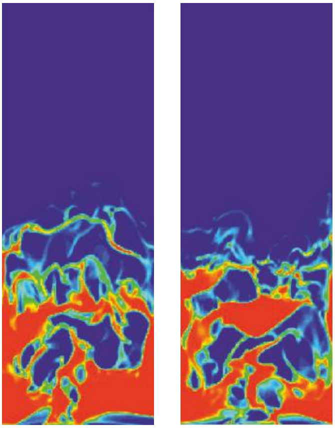
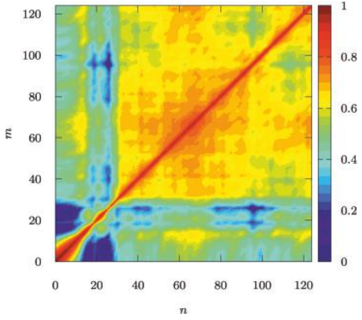
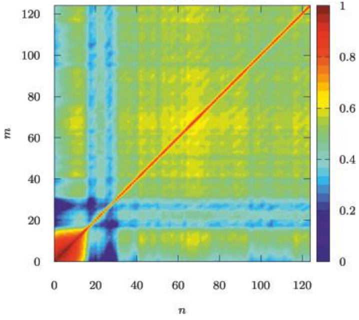


Fig.1: rMatrix of solid volume fraction rNorm for bubbling fluidized bed together with the corresponding states (270,140).



(a)

Fig.2: rMatrix of solid flux rNorm in turbulent fluidized beds (a) and its counterpart of the magnitude gradient tensor flux (b).



(b)

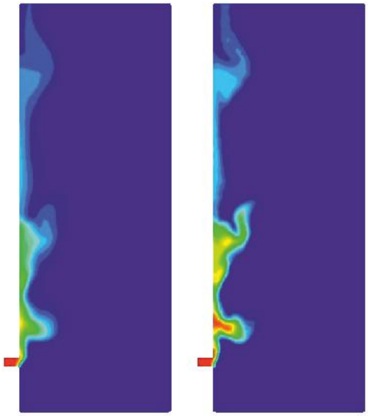


Fig.3: Species full-CFD simulation (left) together with the predictive concentration using transport-based rCFD (right), at an instant in a bubbling fluidized bed.

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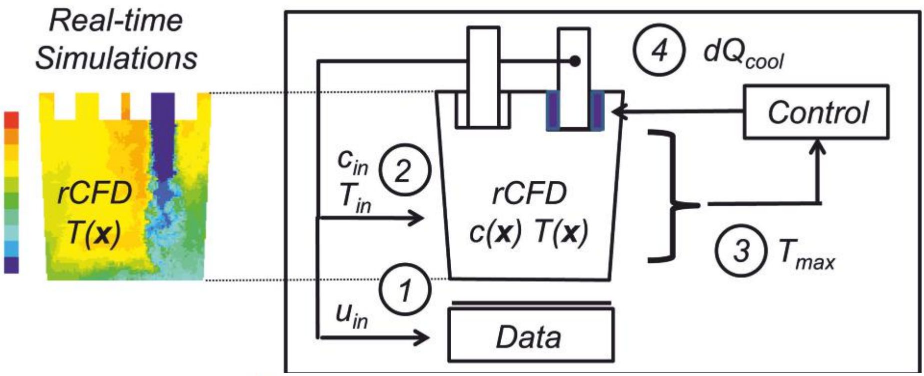
MACRO | RECURRENCE CFD

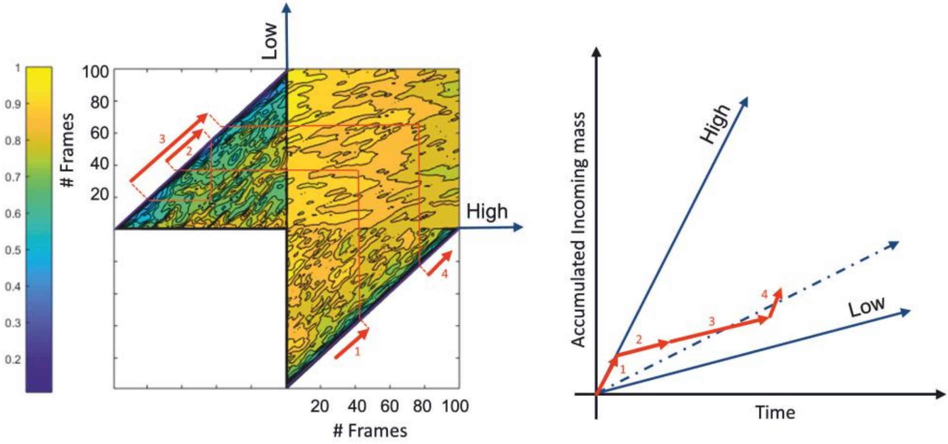
The tremendous speed-up of recurrence CFD (rCFD) opens the door towards bridging between classical (offline) CFD simulations and online process control. We could use high-resolution and real-time simulations of (multiphase) flows in order to observe and control our industrial process under consideration.

On the way towards this logical next step, we have to meet two main challenges: First, we need an interpolation strategy for the case our process runs in-between two pseudo-periodic states (which are covered by corresponding recurrence databases). Here, we could show that an alternating sequence methodology in the sense of pulse-width-modulation could do the job (see figure-1, middle).

Second, we have to define a stringent methodology for the interplay of (i) real-world point probes, (ii) real-time rCFD simulations and (iii) process control. For this, we propose a four step procedure as sketched in figure-1, top. At first (1) we choose recurrence databases depending on the dynamic process state. Based on this fast dynamics, we (2) extrapolate real-world point probes of incoming scalars (e.g. species concentration and temperature) to field information (i.e. concentration and temperature fields). Based on this comprehensive three-dimensional information, we (3) deduce characteristic scalars (e.g. maximum temperature), which then (4) triggers process activation.

In a recent publication (Pirker & Lichtenegger, *Chem. Eng. Sci.*, 2018b), we exemplified this approach for the case of exothermic reactive species transport. After validation (see figure-1, bottom), we used real-time rCFD simulations of species concentration and temperature in order to detect local hot spots of excess temperature. In case of hot spots, we switch on additional cooling in a critical region of the reactor (i.e. we activate the process), thus avoiding local overheating of the liquid.





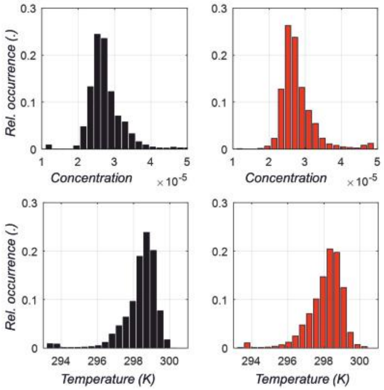


Fig.1: Concept of rCFD in process control (top) based on **Fig.2:** Interpolation of recurrence databases (middle), and **Fig.3:** Real-time simulations of reacting species transport (bottom).

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EDITORIAL IV | EXPERIMENTS & DATA ANALYSIS

Dear Readers,

the past year we did not spend so much time with doing experiments. It was mainly characterized by lots of data processing and documentation of our activities within the K1Met projects during the first funding period. The Experimental activities during this period contributed to 12 conference proceedings and four Journal papers. Another journal paper about interfacial flow modelling and validation is currently under review.

Experimental techniques like time resolved PIV (TR-PIV) produce a tremendous amount of data and lead to similar processing times than highly resolved CFD simulations. So, like large eddy simulations, TR-PIV is a big data business and we put a lot of efforts into postprocessing of PIV and LES data over the last year. However, the results are really convincing and demonstrate a huge step forward in the validation of LES sub-grid models.

The raceway monitoring project together with voestalpine Donawitz is now in its know-how transfer phase to the industrial partner. A first quasi-online system is running at VASD and constantly processing two blast furnaces to acquire long term statistics about raceway blockages.

Experimental projects not always run smoothly and this holds especially true for new prototypes in an industrial environment. The first electrical capacitance tomography sensor (ECT) for voestalpine Linz experienced some delay due to manufacturing problems with the pressure resistive encasing. However, the sensor is now almost finished an will soon be installed in the main conveying pipe of the pulverized coal injection (PCI) plant at voestalpine Linz.

Sincerely,

Stefan Puttinger | stefan.puttinger@jku.at

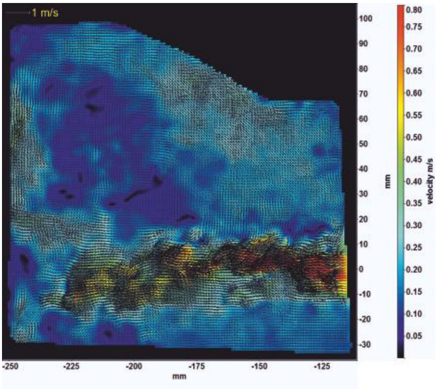


Fig.1: : Snapshot of the flow field in our benchmark experiment for liquid-liquid interfacial flows. It shows the deflection of the incoming jet upwards causing a deformation of the oil-water interface. The vector field has a spatial resolution of 0.5mm and was captured with a sampling rate of 1kHz.

Fig.2: ECT sensor demonstration in the Lab. Online reconstruction of two polyethylen rods in the sensor volume.

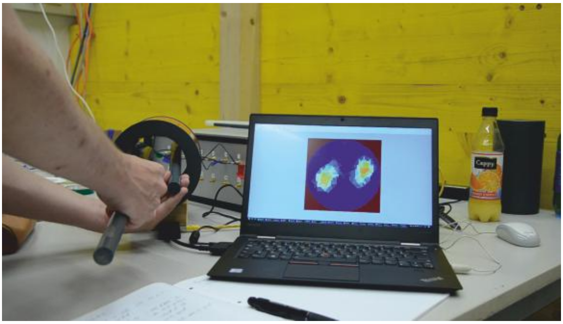
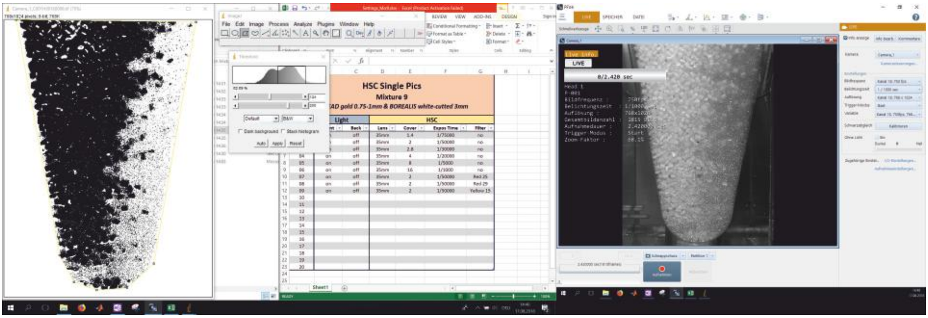


Fig.3: Investigating mixing and segregation of bi-dispers particle systems under various mass flow conditions.



EXPERIMENTS & DATA ANALYSIS | TIME RESOLVED PIV AND INTERFACIAL FLOWS

The latest developments in sub-grid modelling for large eddy simulations (c.f. page 8) brought the need for highly resolved validation experiments. Time resolved PIV (TR-PIV) can bridge the gap between obtaining turbulence statistics for Reynolds averaged models (RANS) and full or partly resolved turbulence models (DNS and LES). However, doing highly resolved PIV experiments also brings the need to achieve a very high spatial resolution. The example in **Fig.2a** shows a vector field snapshot with 0.5mm spatial resolution which matches the grid size of the corresponding CFD simulations.

In combination with shadowgraphy images we can analyse the different time scales of the main flow as well as the interface deformations (**Fig.2b**). The latter are actually two orders of magnitude slower than the fluid flow in the bulk liquid. Thus, this setup can be considered a multiscale approach for stratified liquid-liquid flows. On one hand we can fully resolve the turbulence spectra (**Fig.3**) of the flow and on the other hand we can record the long term behavior of the liquid-liquid interface (**Fig.4**).

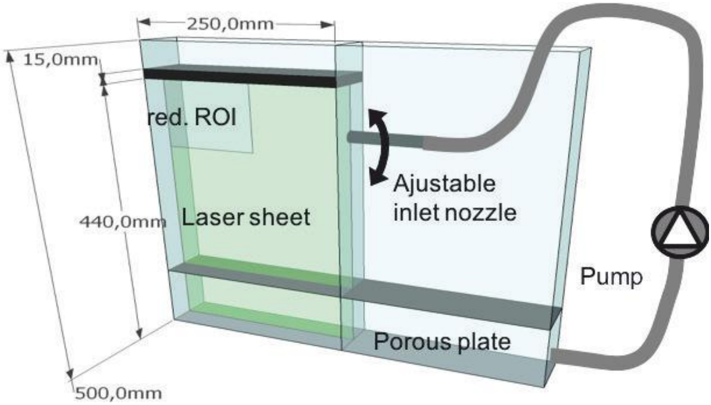
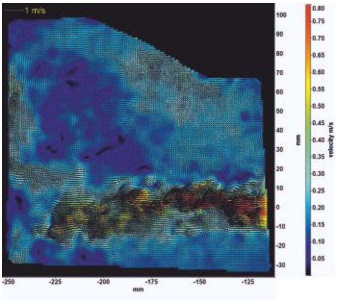
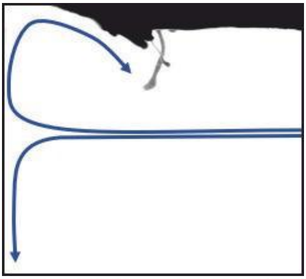


Fig.1: Benchmark experiment for investigating interfacial behavior in stratified two-fluid systems.

Fig.2: Example of a highly resolved PIV vectorfield recorded with 1kHz (left). In addition to the PIV recordings we use an ordinary video camera for shadowgraphy recordings. A homogeneous background illumination allows a precise analysis of the interface deformations (right).





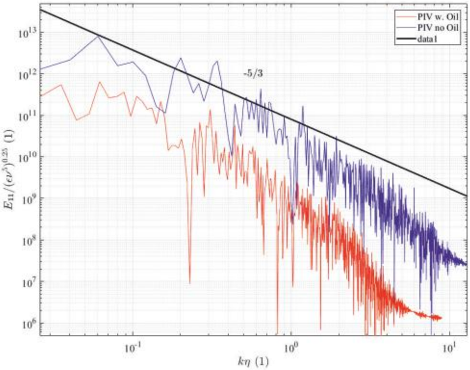


Fig.3: Power spectral density plot close to the interface with and without oil layer. The presence of the oil layer obviously dampens the turbulent fluctuations in the interface region.

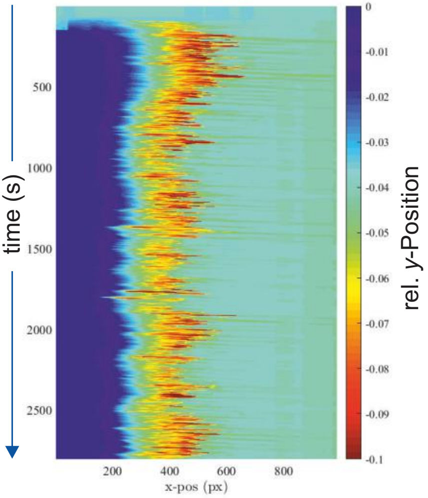


Fig.4: Visualization of the relative oil-water interface dislocation over time.

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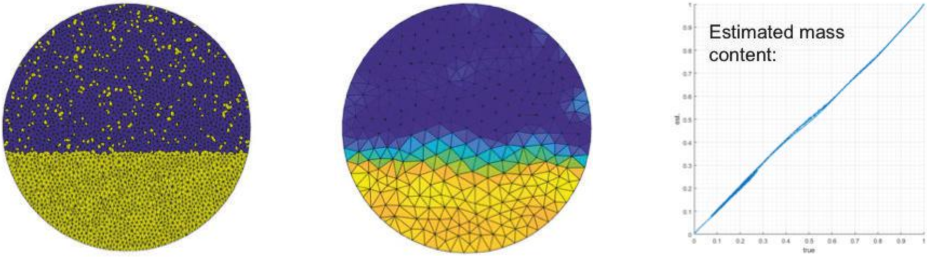
EXPERIMENTS & DATA ANALYSIS |ELECTRICAL CAPACITANCE TOMOGRAPHY (ECT)

The ECT system used in the laboratory is constantly being improved. In a joint effort with the colleagues from the Institute of Electrical Measurement and Measurement Signal Processing (EMT) at Graz Technology University we are working on new reconstruction algorithms and new lab experiments to test their results.

A new test rig (**Fig.1**) was designed for detailed measurements on particle flows in pipes. The topology of particle conveying inside a pipe differs significantly from a vertical pipe to a horizontal pipe. While a vertical transport is characterized by a more or less centrally located strand or homogeneous particle distribution, a horizontal pipe usually shows strand conveying with varying heights of the particle strand. To capture this switch in flow topology and all states in between (e.g. mixed strand and dilute conveying), we built a tiltable test rig which can cover the whole range from vertical to horizontal pipe orientation in a reproducible manner. In addition we can modulate the height of the particle strand by pressurizing the particle hopper. This allows to capture valuable data for optimizing the reconstruction algorithms in addition to artificially generated test data (**Fig.2-3**). Beyond algorithmic improvements we also worked on the usability of the system and implemented a GUI for an easy to use workflow (**Fig.4**).

Fig.1: Snapshot of the new lab test rig to investigate particle flows in pipes. The setup can be tilted from a vertical to a complete horizontal position and by pressurizing the storage hopper we can modulate the height of the particle strand.



(a) (b) (c)

Fig.2: Testing of reconstruction algorithms. (a) Artificially generated data representing a combination of strand conveying and suspended particle transport. (b) Reconstruction result. (c) Accuracy of predicted mass concentration.

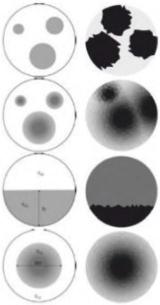
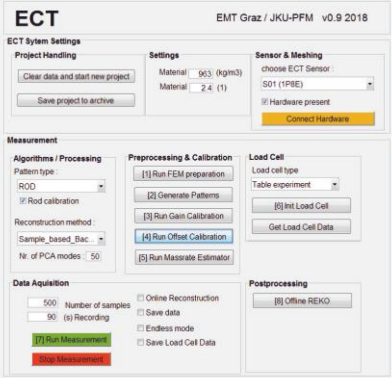


Fig.3: Different types of data reconstruction tests for vertical and horizontal particle strands.


ECT
EMT Graz / JKU-PFM v0.9 2018

ECT Sytem Settings

Settings: Material 963 (kg/m3); Material 2.4 (1)

Sensor & Meshing: choose ECT Sensor : S01 (1P8E); ☑ Hardware present

Measurement

Algorithms / Processing: Pattern type : ROD; ☑ Rod calibration; Reconstruction method : Sample_based_Bac...; Nr. of PCA modes : 50

Load Cell: Load cell type Table experiment

Data Aquisition: 500 Number of samples; 90 (s) Recording; ☐ Online Reconstruction; ☐ Save data; ☐ Endless mode; ☐ Save Load Cell Data

Fig.4: Graphical user interface to operate the ECT system.

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EXPERIMENTS & DATA ANALYSIS | RACEWAY MONITORING OF BLAST FURNACES

Operating a blast furnace at maximum pulverized coal injection (PCI) rates demands a more sophisticated process control to ensure stable BF operation. One part of such a system is a reliable raceway monitoring to detect erratic burden movements and blockages around the tuyere areas (**Fig.1**).

In this project we tested several approaches for raceway blockage detection based on signal and image processing. A universal testbench (**Fig.2**) provides a common framework to test various algorithms and obtain objective quality measures on their results.

The extensive work of this K1Met project has been documented in a series of three journal papers which have been accepted for ISIJ International.

A first test installation has been implemented at voestalpine Donawitz and is processing the hot blast pressure data of BF1 and BF4 to collect long term statistics about the frequency of occurrence of raceway blockages at different blast furnace operating conditions (**Fig.3**).

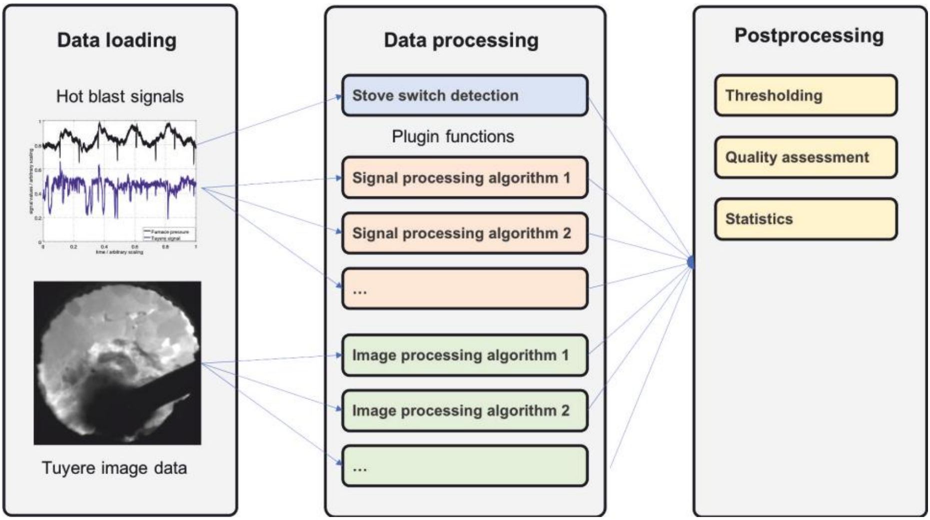

Fig.2: Outline of the modular software testbench for raceway monitoring.

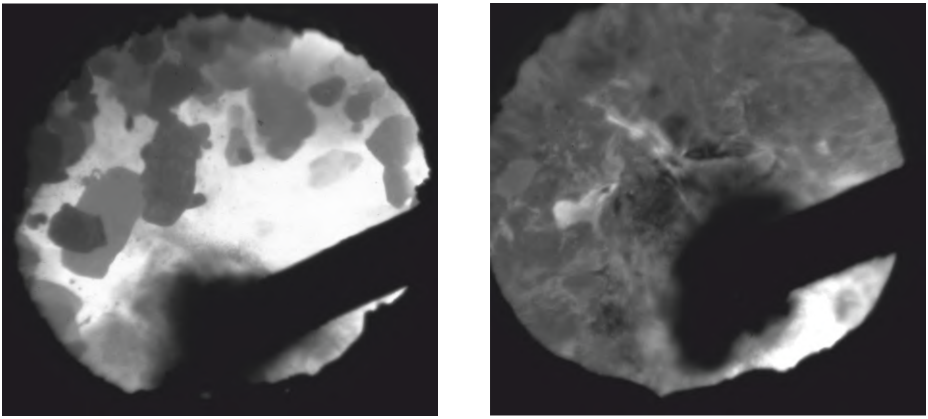

Fig. 1: Ordinary operation (left) and entire blockage of the raceway (right) in a blast furnace for ironmaking.

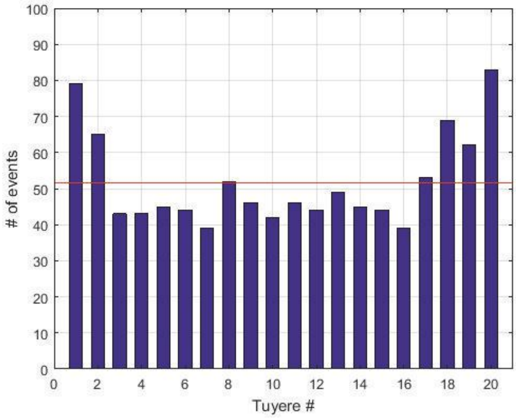

Fig. 1: Long term statistics of BF1 at voestalpine Donawitz for 1500 hours of blast furnace operation. The plot shows a higher frequency of occurence for raceway blockages for the neighboring tuyeres 15-2.

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SCIENTIFIC FRIENDS | BERT BLOCKEN TU/e

“What can basic research do for society?” Some years ago, I was asked by the president of the CDG research association to deliver a lecture on just that topic. What a challenge!

While we feel very close to our industrial partners knowing their needs, we honestly do not see a direct connection between our research and society. However, this lecture request seeded a persistent idea/wish not only for me but for our whole group. There should be a way to transfer our group’s expertise towards society!

After intense discussions, we chose “pollutant dispersion in urban environments” as our favorite societal topic, which we would like to attack beyond our daily process-industry related research. In the following years, we organized two seminars in order to get familiar with this new topic. Finally, we came to the idea that we could apply recurrence CFD for the real-time assessment of pollutant dispersion from point sources in urban environments.

While we were enthusiastic by our own idea, we were realistic enough, that we won’t be able to do serious research (and rise funding) in that field without a knowing partner. What a great luck that I could meet Bert Blocken – one of the most distinguished experts in urban flow modelling! During several hours of discussions, I could transmit our spark of enthusiasm. We should give rCFD simulations a try and go for real-time and high-resolution simulations of pollutant dispersion!

The rest was very encouraging: Together with Bert I submitted a scientific proposal targeting the modelling of pollutant dispersion at the Linz/Westring tunnel portal (figure-1) to the Linz Institute of Technology. After several months we received four overwhelmingly excellent reviews together with a two years’ funding for a postdoc researcher. With Yaxing Du we could attract a recognized postdoc to actually work on this project (first results are depicted in figure-2).

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Particulate Flow Modelling

Fig.1: Linz/Westring configuration, showing a point-source of pollutants (future tunnel portal, marked by yellow ellipse), a bluff body obstacle (public building Wissensturm) and a residential area (in the wake of Wissensturm).

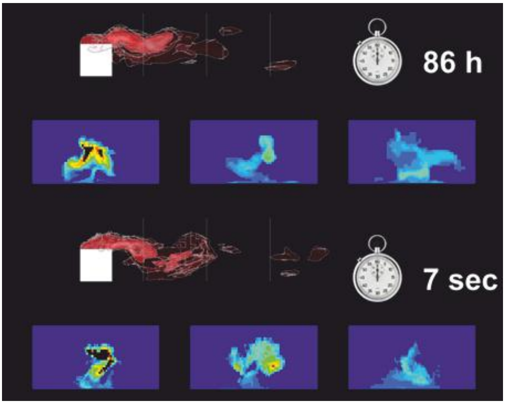

Fig.2: Snapshots of full CFD (top) and rCFD (bottom) simulation of ´cube with roof stack‘ wind-engineering benchmark showing iso-surfaces and concentration contours together with simulation times.

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