



JYU | Department of Particulate Flow Modelling

Annual Report | 2017

JKU DEPARTMENT OF PARTICULATE FLOW MODELLING

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Front cover: High resolution VOF simulation of a phase inversion benchmark test (representing e.g. oil rising to water surface); such benchmarks serve as validation base for the development of novel multiphase LES models, which are urgently needed for modelling for e.g. liquid metal/slag processes
© M. Saeedipour & S. Vincent (Paris)

EDITORIAL

Dear Readers,

Joint research is more efficient than just cooking your own soup. Last year we enjoyed a couple of fruitful collaborations, I would like to bring to stage. With Hans Kuipers from Eindhoven and Stefan Heinrich from Hamburg we further developed recurrence CFD (rCFD), Stephane Vincent from Paris guided us towards novel multiscale LES models and Johan Padding from Delft helps us with cohesive drag models. We, in turn, commit our software base which we jointly maintain and further develop. Maybe, this works out so well, because we minimized administration and didn't wait for specific funding. We collaborate because we want to collaborate – joint research is rewarding and more than that it is fun!

For the future we are full of new ideas: We definitely want to further explore rCFD and other cutting edge models, which can accelerate classical CFD(-DEM) simulations by orders of magnitude. We like to break new and challenging grounds. In doing that, we stick to our mission of developing efficient and applicable multi-scale models for multiphase processes!

With these introducing words I wish you a pleasant reading!

Sincerely,



EDITORIAL | NEW CD-LAB

Dear Readers,

Last October the Christian Doppler Laboratory for “Multi-scale modeling of multiphase flows” successfully went through its two years’ evaluation. We received outstanding feedback from the international evaluator Prof. Sasic from the Chalmers University of Technology in Gothenburg, who was very impressed of the outcome of the group during the first two years.

In particular, this laboratory stands for new challenges in field of multiphase processes with special attention on multi-scale aspects. For example, we significantly contributed to the research on gas-solid turbulence and we developed novel and efficient models for the numerical simulation of liquid-liquid emulsions in stirred tank reactors, a particle magnification lens method for the numerical simulation of particulate processes. Finally, we are heading for an efficient numerical tool for the numerical assessment of industrial scale iron ore reduction.

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,



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EDITORIAL | MICRO

Dear Readers,

During 2017, we continued our rather new research activities focusing on modelling interfacial flows with the application from small-scale (e.g. microfluidics) to large-scale (e.g. metallurgical processes) engineering applications. Although seem different from each other, these two research worlds have a major characteristics in common: the presence of a distinct interface between the phases which makes the physics of flow more complex.

Together with **K1-MET**, we proceed further with modelling and characterization of the turbulent interfacial flow in the continuous casting mold. We focus on subgrid modelling in large eddy simulation of multiphase flows in parallel with time-resolved PIV experiment to obtain a better understanding of the interaction of turbulence with interface as well as the effect of small-scale physical phenomena on large-scale flow characteristics.

Within the **MicroNeedle** project, we work on modelling the capillary-driven flow in micro-channels with application in transdermal drug delivery. We also came up with the idea of improving the conventional VOF method for efficient simulation. Inspiring from these activities, once again we found the opportunity to do applied research on an interesting topic in life science. Our new PhD student **Achuth B. Nair** will investigate the complex biological flow in microfluidic devices.

Let's keep walking on the "interfaces"!

Sincerely,



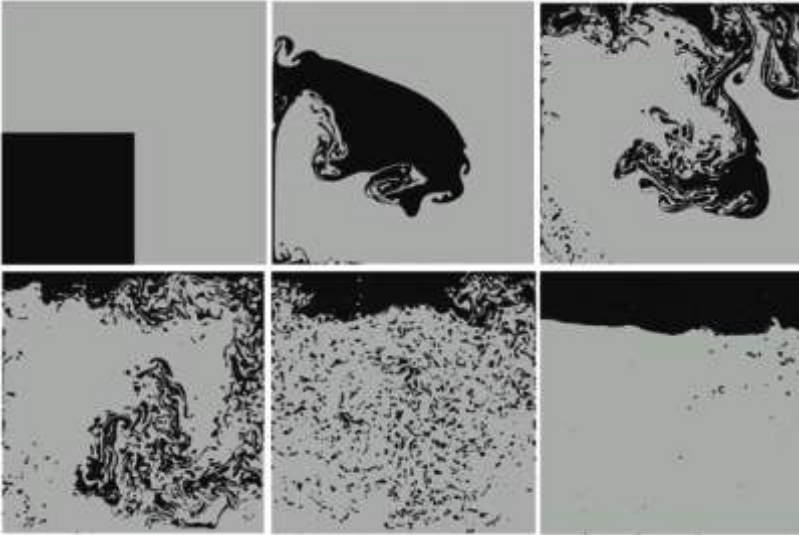


Fig.1: Quasi-direct numerical simulation of interfacial turbulence in the oil-water phase inversion problem. The images display how the liquid-liquid interface evolves as time elapses ($t= 0, 2.2, 4.5, 6.5, 14$ and 40 s). Different micro-scale phenomena such as rupture and breakup occur due to the interaction of turbulence with the interface. The oil and water phases are colored in black and gray, respectively.



Fig.2: Numerical simulation of liquid transport in complex microchannels. The images display the moment the interface reaches the sharp edges from both sides (left), and the moment the interface is pinned at one edge and moves on the other edge (right). This flow behaviour has application in uni-directional liquid transport through microfluidic devices.

MICRO | MODELLING SLAG ENTRAINMENT IN CONTINUOUS CASTING MOLD

Slag entrainment is a challenging problem to control during continuous casting process. From fluid dynamics viewpoint, it mainly occurs due to (i) the instability of the fluids interfaces at the top of the mold and (ii) vortex formation around the sub-merged entry nozzle (SEN). Both mechanisms are complex phenomena involving surface instability, vortex interactions with the metal-slag-air interface, deformation of the slag layer and its entrainment into the molten metal in the form of small droplets.

Numerical modelling of such multiphase flow still remains challenging due to different physical scales involved in the real process. To better investigate the flow characteristics, a large eddy simulation - volume of fluid (LES-VOF) approach is employed to investigate the flow behavior upon injection into the mold. The preliminary simulation results are compared to a water/oil benchmark experiment using PIV. A promising agreement is revealed on the macroscopic flow characteristics such as velocity fields and interface displacement [1]. For instance, the maximum slag entrainment depth for different nozzle injection angles correspond quite well between CFD and experimental results (Figure 1). Nevertheless the current LES-VOF model has several limitations. For instance, it is not capable of picturing micro-scale physics such as interface rupture and droplet formations out of interface in the more rigorous cases (e.g. upward injection) as shown in Figure 2.

To improve the numerical simulation, we further focus on two steps: (i) modelling all the subgrid terms in two-phase LES, and (ii) multiscale (Eulerian-Lagrangian) algorithm for picturing the oil droplet inclusion in the water phase. For the former aspect, we currently concentrate on structural turbulence modelling (i.e. Approximate Deconvolution Model [2]), while for the latter one an Eulerian-Lagrangian technique will be developed for identification and tracking subgrid-scale slag droplets coupled with continuous phase.

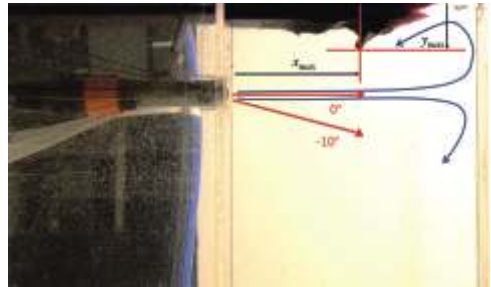
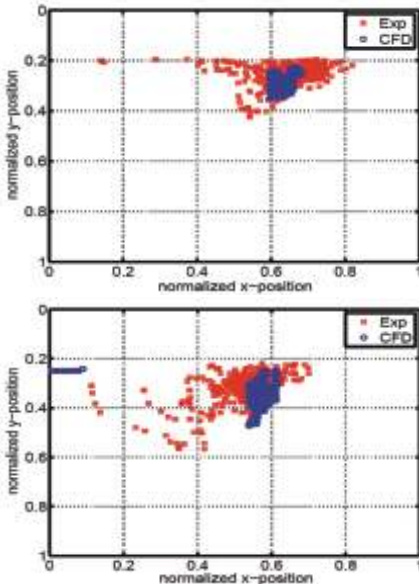


Fig.1: The mold flow experiment showing the position of maximum slag layer entrainment (right), and the comparison of maximum slag entrainment positions during the the simulation and experiment at -10° and 0° (left).

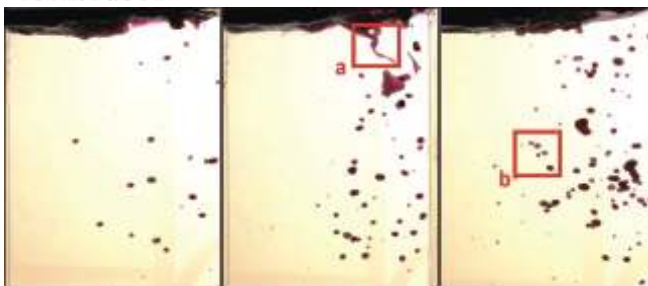


Fig.2: Sequence images of mold flow experiment at $+10^\circ$ which leads to an unsteady turbulent flow with several (a) interface deformation and ruptures as well as (b) droplet formations.

[1] Saeedipour, M., Puttinger, S., Pirker, S., LES-VOF simulation of turbulent interfacial ow in the continuous casting mold. In: 12th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries. Trondheim, Norway, 2017.

[2] Stolz, S., Adams, N. A.. An approximate deconvolution procedure for large-eddy simulation. Physics of Fluids 11, 1699–1701, 1999.



EDITORIAL | MESO

Dear Readers,

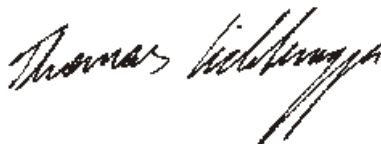
What does it mean to model and simulate mesoscopic systems? For us, it is certainly more than just aiming at rather small to medium problem sizes without too high a resolution. Quite the opposite is the case! Ideally, the art of meso-scale modeling consists of two phases: First, a thorough analysis of the relevant physics involved in a problem needs to be carried out in order to understand how detailed microscopic mechanisms can be simplified for an approximate treatment at medium scales. After a successful validation, in the second step a strategy is outlined how to incorporate the information obtained so far into macroscopic descriptions.

While some of the various PhD projects in the mesoscopic group of our department are currently in the first phase, others have already tackled the second one in 2017. **Mathias Vangö**, for example, derived a stable simulation strategy for drainage from particle beds, which he can now apply to full-scale blast furnace tapping with the aid of clever physical modeling. On a more algorithmic side, **Daniel Queteschner** embeds highly detailed particle simulations into coarse-grained ones to allow for a look through a "magnification lens".

While these projects are approaching their completion, others have just started. Our newest group member **Sanaz Abbasi** joined us in August. She will develop strategies to describe large-scale transport phenomena in turbulent flows governed by microscopic equations of motion.

I hope that you, dear Readers, enjoy seeing the progress of our projects which are as diverse as the persons working on them. I certainly do!

Sincerely,



Thomas Lichtenegger | thomas.lichtenegger@jku.at

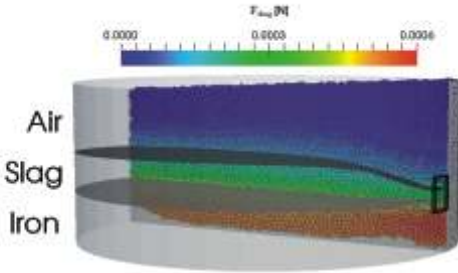


Fig.1: Multiphase flow in a blast furnace hearth. A partly floating coke bed called the deadman poses resistance to outflow of liquid iron and slag through the tap hole.

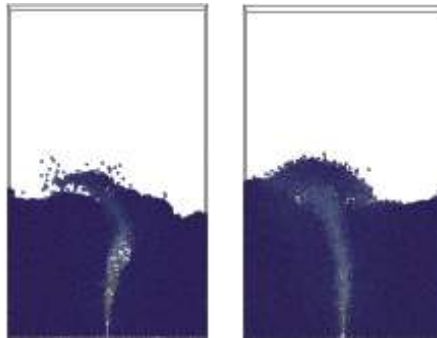


Fig.2: Spout bed simulations. While dry, non-cohesive particles (left) lead to a relatively narrow, uniform channel, wet, cohesive ones (right) give rise to block-like material motion with a heterogeneous spout structure.

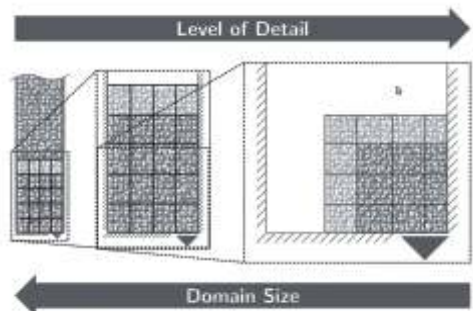


Fig.3: Multi-level coarse graining. A highly resolved DEM simulation (right) is embedded into a mildly coarse-grained one (middle) which again is part of a strongly coarsened particle bed.

MESO | TOWARDS A UNIFIED MODEL FOR LARGE-SCALE PROCESSES

Simulations of large-scale industrial processes are extremely challenging for several reasons: Firstly, the relevant length and time scales exceed the capabilities of modern hardware when using state-of-the-art methods like CFD and DEM. Secondly, besides particle and fluid flow, many other phenomena like heat transfer or chemistry need to be modelled. In this project, we aim at creating a modelling framework that allows us to (a) run simulations for longer times using alternative time integration methods and (b) incorporate existing models to create a complete picture of the process, and apply it to a direct reduction shaft (Fig. 1). This poses several challenges, two of which will be discussed below: initialization and time integration.

We evaluated the available algorithms and computational demand to create the initial conditions for simulation of a large system, and found that the currently available particle insertion algorithms are not able to produce a dense packing of millions of particles in a complex geometry in reasonable time. To improve this, we implemented the more sophisticated dense packing algorithm by Lozano et al. [1] which generates the packing by geometrical considerations, and is able to achieve solid volume fractions up to $f_s=0.57$ in complex geometries in shorter time. A comparison of runtimes for filling a cylinder is shown in Fig. 2.

For time integration, we are currently in the concept phase, where we evaluate the capabilities of several approaches. One promising candidate, outlined on the opposite page, is a predictor-corrector approach in which heat transfer, chemistry, fracture etc. are computed on tracers that are integrated on flow fields obtained from a steady-state simulation (predictor). Periodically, the predicted configurations are mapped back to a full CFD-DEM simulation to obtain a physically correct state that is then used for further prediction (corrector). But other approaches, such as using the contact network of the granular material to propagate information, are being investigated.



Fig.1 (above): A direct reduction shaft. Image source: midrex.com

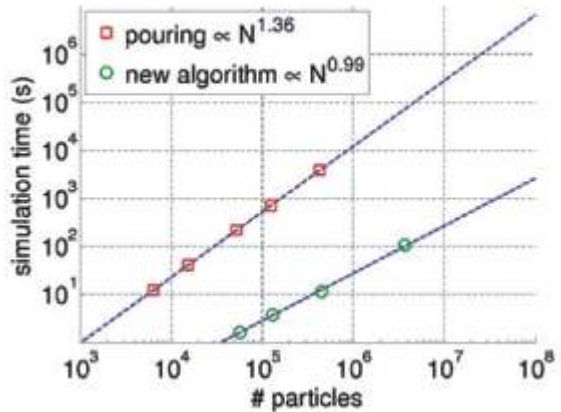
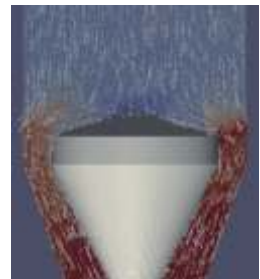


Fig.2 (above): Runtime for filling a container with the available algorithm (red squares) and with the new algorithm by Lozano et al. [1] (green circles). The new algorithm is substantially faster and allows us to create initial conditions for large simulations.

Fig.3: Illustration of the time extrapolation algorithm. First, obtain steady state from full DEM simulation (left). Then, get granular velocity field averaged to CFD grid (right). Convert DEM particles to non-interacting tracers, integrate them along velocity field, and compute other properties on them. Periodically, convert the tracers back to DEM particles, let them relax and perform a few seconds of full DEM simulation.



[1] Lozano et al., Computers & Mathematics with Applications, 71(8):1568-1601, 2016.

MESO | MULTI-LEVEL COARSE-GRAIN MODEL OF THE DEM

The discrete element method (DEM) is a well-established but computationally demanding method for simulating granular systems. The DEM coarse-grain (CG) model alleviates the computational costs by replacing a number of original particles by a larger (pseudo) particle, thus effectively reducing the number of simulated particles. However, scaling the particles while keeping the same boundaries in the system violates the geometric similarity and as a consequence this CG model may fail to correctly describe the system.

To improve this situation we have introduced a technique to concurrently couple differently resolved DEM simulations. With this method, we embed a sub-domain with a more detailed representation of the particles wherever the CG model is insufficient. Now we have extended this method to work with multiple nested coarse-grain levels to further improve the balance between speedup and accuracy. Furthermore, we have added the option to use a separate simulation instance for each coarse-grain level so that simulation settings can be tuned individually at each level.

As we have demonstrated before using the setup shown in Fig. 1a, we are able to achieve a speedup that is nearly proportional to the saved number of particles. Here we show that this still holds for the multi-level coarse-grain (ML-CG) extension of the method. To this end we measure the discharge rate of the rectangular bin with 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 1 mm.

We conducted a reference simulation consisting of 960.000 particles resulting in an initial bed height of about 500 mm. Then we repeated the simulation using the original CG model with a coarse-grain ratio of 4, i.e., 15.000 particles with a diameter of 4 mm. Figure 2 shows a significant discrepancy between the predicted mass flow rates.

We set up the same case with three coupled coarse-grain levels, combining the coarse-grain ratios 4:2:1 as illustrated in Fig. 1b. This way we are able to correctly predict the discharge rate (Fig. 3, Table 1) using a total of about 60.000 particles and achieving a relative speedup of more than 11 compared to the reference simulation.

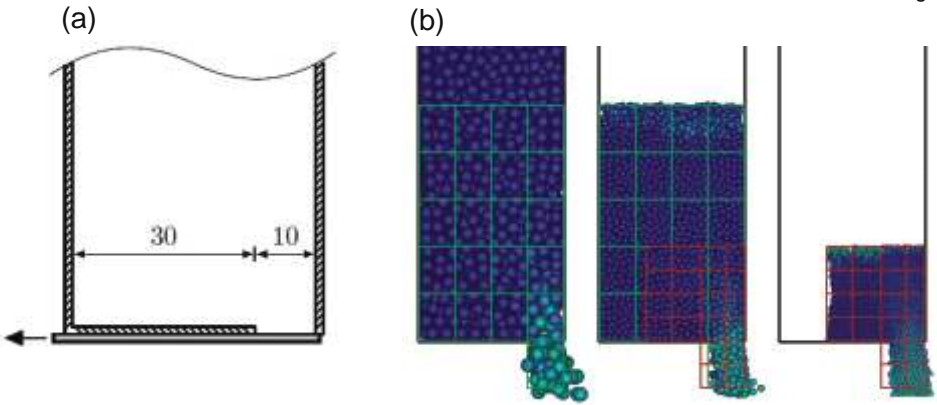


Fig.1: (a) setup with the outflow orifice at the bottom right of the bin, (b) 3-level coupled simulation with coarse-grain ratios 4:2:1.

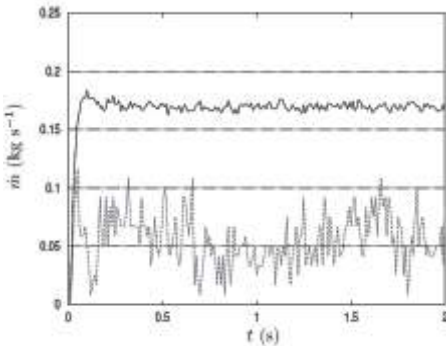


Fig.2: The rate of discharge in kg s^{-1} of 1 mm particles using the default model and the original CG model.

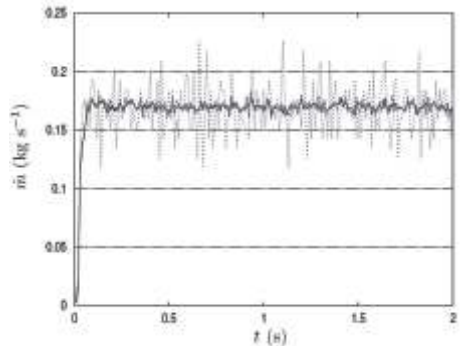


Fig.3: The rate of discharge in kg s^{-1} of 1 mm particles using the ML-CG model.

Simulation	$\langle \dot{m} \rangle$	$\sigma(\dot{m})$	speedup
reference	0.169	0.003	1x
ML-CG ($\alpha=1$)	0.170	0.003	11.1x
ML-CG ($\alpha=2$)	0.170	0.005	
ML-CG ($\alpha=4$)	0.168	0.022	

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



MESO | DIRECT REDUCUTION OF IRON ORES IN FLUIDIZED BEDS

As one of the advantageous direct reduction process, the fluidized bed technologies have become quite significant in the iron- and steel-making industries. With the depletion of natural resources, the deterioration of ore quality due to high cost, as well as the usage of scrap and scrap substitutes as a replacement for the conventional route of steel-making, advances in the direct reduction process has gathered more attention [1]. Efficient investigation of these reactors can be carried through numerical simulations such as the CFD-DEM coupling method, since measurements inside these reactors are highly complicated.

The two models that represent the solid-fluid reaction are the shrinking particle model, where the particle reacts and shrinks without forming a product layer, and the unreacted core model, where the particle reacts and shrinks leaving a product layer behind [2]. The shrinking particle model is a basic model that can be used for establishing communication and stability, however it is not able to represent highly complicated reactional models like the iron ore reduction. Therefore, we are using the unreacted core model, where the different reactions steps between hematite/magnetite, magnetite/wustite, wustite/iron, can be represented with three layers. The gaseous reactant diffuses through the porous layer of iron shell, wustite and magnetite layers, while simultaneously reacting with these layer, and finally reaching the hematite core. This process can be represented as an electrical network circuit in which the resistances are defined as the chemical reaction resistance, diffusion resistance, and mass transfer resistance terms.

The unreacted core model is thus implemented into the CFD-DEM library, with the relative correlations for the resistances that affect the reduction process. The implementation is carried out so that only the required data is communicated between the two phases with an adaptable communication interval. A validation case where only a single iron-ore particle is reacting with a gas mixture of CO and N₂ is carried out, and the results are compared with available experimental data that uses the ISO 4695 conditions at 950°C and 50 NI/min [3]. The possible parameters that affect the reduction process such as the particle porosity, pore diameter and tortuosity, as well as the gas composition and velocity are investigated for a broad spectrum of variables by comparing the simulation results for fractional reductions with the experimental data. These results give us insights about the total reduction process.

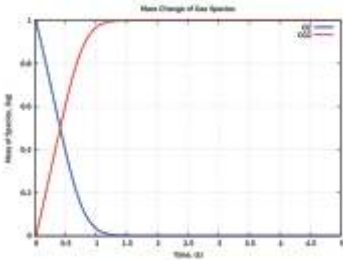


Fig.1: Results for the verification case with shrinking particle model, where C is reaction with incoming O₂ to produce CO₂. The mass changes of relative species are verified.

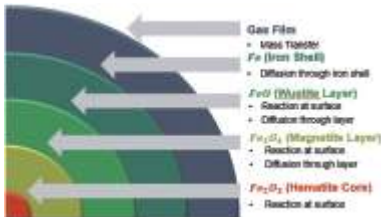
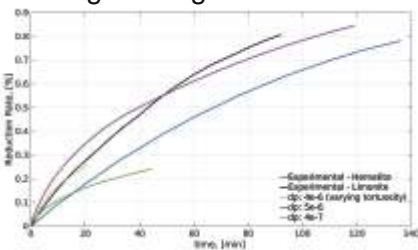


Fig.2b: Graphical illustration of the various layers of iron-ore and the steps the reactant gas has to go through.



[1] Habermann, A. et al. An Experimental Study on the Kinetics of Fluidized Bed Iron Ore Reduction. ISIJ International, 40(10):935-942. 2000.
 [2] Octave, L. et al. Chemical reaction engineering. Vol. 2. New York etc.: Wiley, 1972.
 [3] Hanel, M. B. Characterization of Ferrous Burden Material for Use in Ironmaking Technologies, PhD Thesis, Montanuniversitaet Leoben, 2014.
 [4] Turkdogan, E.T. "Physical chemistry of high temperature technology", 1980.



Fig.2a : Snapshot of a sintered iron ore pellet reduced 30%, where every layer with various pore structures are visible [4].

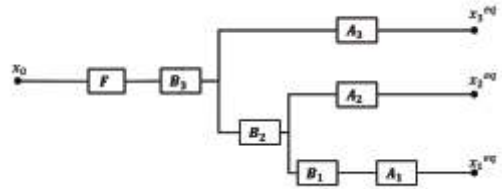


Fig.3: The combination of each resistances need to be solved to determined the mass source terms. The easiest way is to consider the reduction process as a combination of electrical resistance network.

Fig.4: Comparison of the reduction rates from experimental values with various simulation results, where the pore diameter has been diversified and new correlations for tortuosity tested.



MESO | MODELING OF BLAST FURNACE TAPPING

Understanding the lower part of a blast furnace (hearth) is essential in order to ensure stable operation and optimize the campaign length. In the blast furnace, iron ore is chemically reduced by charging iron and coke pellets from the top and injecting reacting gas from tuyeres located above the hearth. The resulting molten iron settles at the bottom of the hearth with a slag (bi-product from the reduction) layer on top due to their different specific gravities. Additionally, a dense porous structure of coke particles (deadman) is present, whose position and shape varies over time between a fully sitting, partially floating or fully floating (cf. Fig. 1). Due to the harsh conditions in the hearth with temperatures exceeding 1500°C , measurements and general insight are limited, hence numerical methods are necessary.

To simulate the tapping process we developed a fully coupled multiphase CFD (Computational Fluid Dynamics) – DEM (Discrete Element Method) model. While there have been several previous studies on the subject using pure CFD, the deadman is often treated as a static homogeneous porous medium. To account for the deadman dynamics we modeled it with the DEM.

To validate our model, we performed a lab-scale experiment, in where water was drained from a tank filled with buoyant particles. The simulation domain shown in Fig. 2 illustrates the initial condition where the particle bed has reached a buoyancy equilibrium. During the first seconds of draining, the particles were descending with the water and dragged towards the outlet. This formed a characteristic shape of the lower part of the particle bed which we managed to successfully reproduce in the simulation, which is depicted in Fig. 3. Additionally we measured the drainage rate in the experiment and compared it with the simulation. The total drained mass is visualized in Fig. 4, where we observe very good agreement between the simulation and experiment.

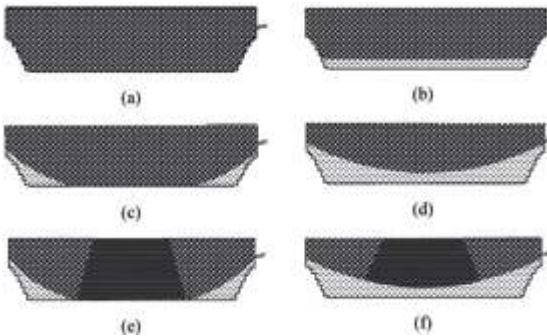


Fig.1: Illustration of varying deadman shape and permeability from a homogeneous sitting- (a) to a floating deadman with a denser core (f) [1].

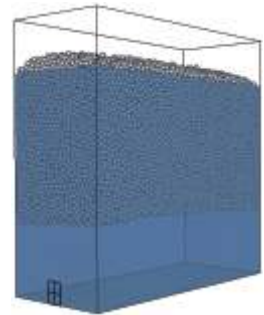


Fig.2: Simulation domain of the experimental setup. The particle bed is initially floating and the outlet is located on the bottom left.

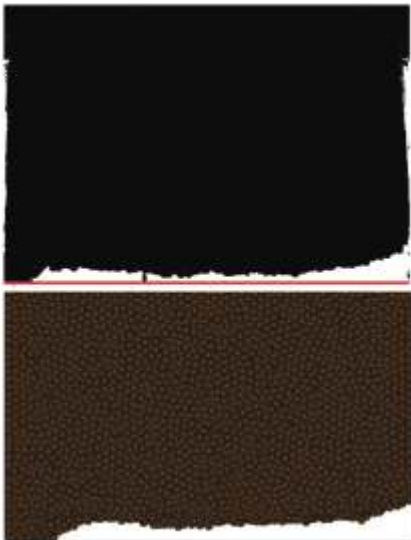


Fig.3: A snapshot comparison of the lower particle bed shape between experiment (top) and simulation (bottom).

[1] Guo et. al., CFD Modelling of Liquid Metal Flow and Heat Transfer in Blast Furnace Hearth, ISIJ Int. (2008)

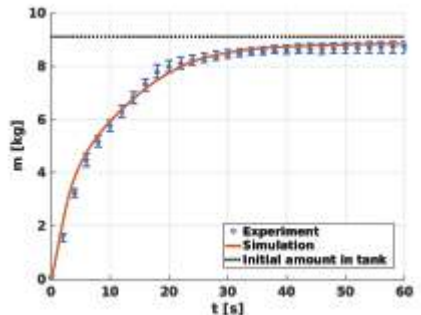


Fig.4: Drained mass over time for experiment (error bars) and simulation (solid line). The dotted line indicates the initial amount in the tank.



MESO | MODELING STRONGLY POLY-DISPERSE GRANULAR SYSTEMS

Particulate systems can be readily modeled and simulated with the discrete element method (DEM). Large ranges in grain sizes, however, pose a serious challenge: The number of particles per volume increases significantly, computational time steps need to be reduced (particle collision times scale with their diameter) and an efficient bookkeeping of neighbor lists becomes more complicated.

For broad or not-too-strongly separated size distributions, we introduced an "effective parcel model" (c.f. Fig. 1), where smaller particles are combined with larger ones into polydisperse parcels analogously to ordinary coarse graining where several particles of the same size constitute a grain. In this regard, two questions arise: First, what is the impact on the granular mechanics? Do effective parcels behave like actual particles with modified material parameters like coefficients of friction? Second, how does the particle-fluid interaction depend on the composition of a parcel?

The second question can be answered quite simply. Widely accepted correlations for particle-fluid momentum exchange and pressure drop like the Ergun equation depend on the local mean Sauter diameter and the packing fraction of the particulate phase. Thus, an effective parcel needs to have the same diameter as the mean Sauter diameter of its sub-particles and it needs to occupy the same amount of volume.

The first question, on the other hand, is much more difficult. Small-scale simulations of the full size distribution allow for a comparison with effective parcels to investigate which material parameters lead to similar macroscopic properties, such as the angle of repose. However, effects like segregation are not straight-forward to incorporate and will require extensive research.

For the application to dense beds, e.g. in blast furnaces, our simple model turns out to be sufficient. We compared simulations of a bidisperse mixture (size ratio 5 : 1, mass ratio 3 : 1) with monodisperse effective parcels in a part of a blast furnace geometry Fig. 2. Time-averaged quantities like the granular velocity field in Fig. 3 agree astonishingly well given the highly dynamic raceway region, where our approach is clearly challenged by segregation and a complicated dense-dilute crossover regime.

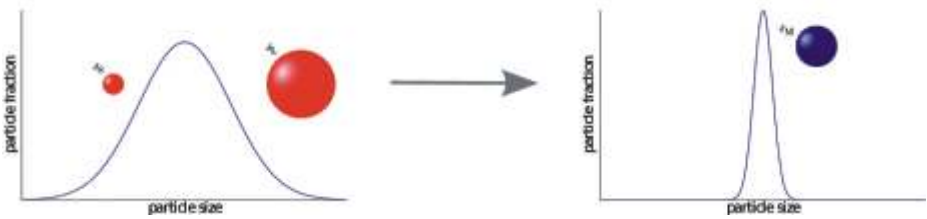


Fig.1: Idea of effective parcels. Instead of a broad size distribution (left), a narrower one (right) with adapted material parameters (effective volume, coefficients of friction etc.) is used.

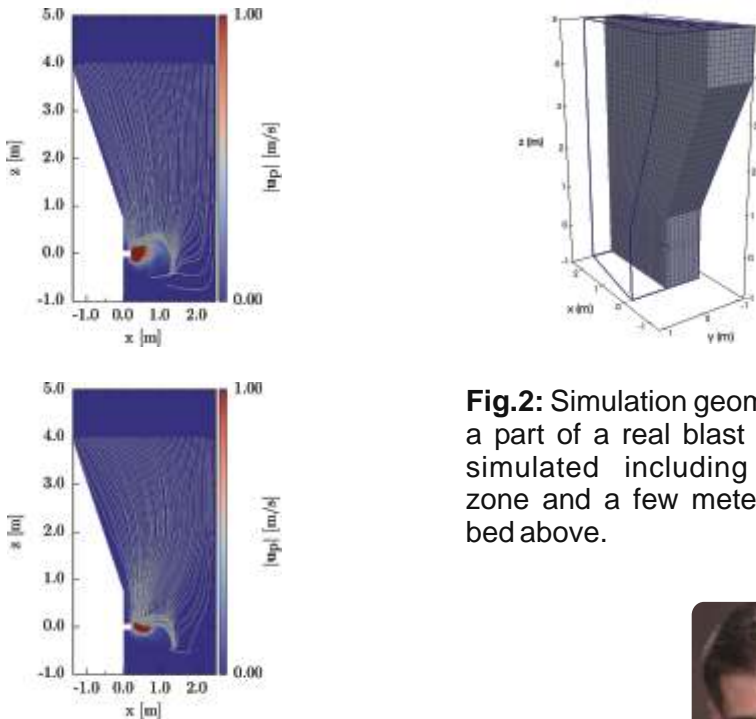


Fig.2: Simulation geometry. Only a part of a real blast furnace is simulated including raceway zone and a few meters particle bed above.

Fig.3: Time-averaged particle velocity fields. For both a bidisperse mixture (top) and monodisperse effective parcels (bottom), a qualitatively similar behavior can be seen.



MESO | TURBULENT FLOW OVER A CIRCULAR CYLINDER

Computational Fluid Dynamics (CFD) techniques such as Large Eddy Simulations (LES) are computationally expensive and make long-term investigations impossible. Due to these high numerical costs, recurrence CFD (rCFD) has been introduced for flows with recurring patterns like turbulent flows. This method is aimed at reducing the high temporal and spatial resolutions.

For the purpose of proper functionality of rCFD, as the first step I modeled the turbulent flow over a circular cylinder at Reynolds number (Re) 3900 using OpenFoam. Since this case has been studied well in the literature, there are available experimental data to compare the results. I built the computational domain which has 2800000 cells. The distances between inlet and outlet boundaries, upper and lower walls are $30D$ and $10D$, respectively. Also, the span-wise length of the domain is $\times D$. LES along with the conventional Smagorinsky Subgrid-Scale (SGS) model has been carried out for this case. In Fig.1, streamlines of the flow with the velocity magnitude are shown after approximately 60 vortex shedding cycles. As presented in Fig. 2, the mean stream-wise and transverse velocities at different locations in the wake centerline of cylinder are in good agreement with the experimental results.

In the second step, I added a passive transport equation to the solver in order to monitor mass transfer. Figure 3 displays the time-averaged magnitude for the species transport.

The next phase will be identifying the recurring pattern of this flow and carrying out rCFD for passive transport with the focus on efficiency, i.e. temporal and spatial resolutions.

References:

- [1] Parnaudeau, P., Carlier, J., Heitz, D., Lamballais, E.: Experimental and numerical studies of the flow over a circular cylinder at Reynolds number 3900. *Physics of Fluids* 20, 085101 (2008)
- [2] Lourenco, L.M., Shih, C. Characteristics of the plane turbulent near wake of a circular cylinder. A particle image velocimetry study (1993)



Fig.1: Streamlines of the turbulent flow past cylinder at $Re=3900$. The red color refers to the highest velocity, and the dark blue colors the lowest.

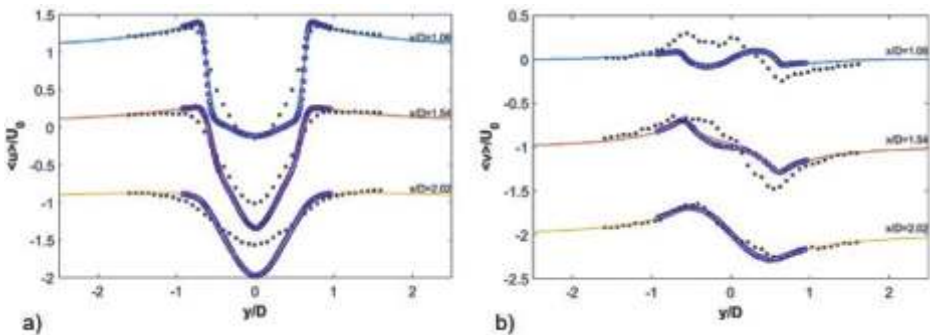


Fig.2: Velocity profiles at various locations in the wake region at $Re=3900$. a) and b) depict mean stream-wise and transverse velocities solved by LES. Experimental data by Lourenco and Shih and Parnaudeau et al. are illustrated by symbols.

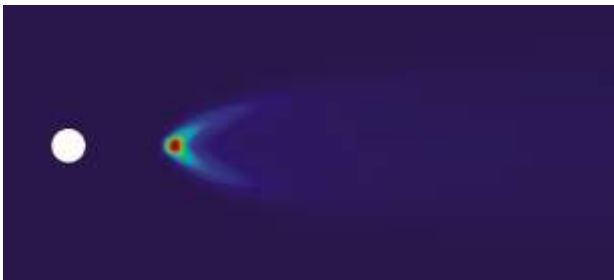


Fig.2: Mean species transport at $Re=3900$ after 45 vortex shedding cycles. The source is placed in the wake centerline after the recirculation length.



MESO | MODELING OF GAS-SOLID FLOW WITH COHESIVE POWDERS

In industrial applications, particle cohesion is a very common occurrence and it can lead to the formation of heterogeneities in particle distribution. In rapid distortion regime of non-cohesive powders with instantaneous inter-particle collisions, such heterogeneities might establish in a form of particle clusters. In cohesive powders where long-enduring inter-particle contacts prevail, it might lead to the formation of block-like structures divided by gas tunnels.

We conducted the experiment measurements in lab-scale pseudo-2D spouted bed facility with dry and wet particles. Interstitial liquid added cohesive effects between particles what lead to formation of channels, limited spout movement and very prominent dilute phase inside the bed. A noticeable difference between results obtained for cohesive and non-cohesive particles was observed.

The motivation behind the procedure was to obtain a quantifiable indicator of block-like movement expected in cohesive flows and create the basis for validation of the numerical simulation. Data was processed and particles velocity vectors obtained by PIV (particle image velocimetry) method.

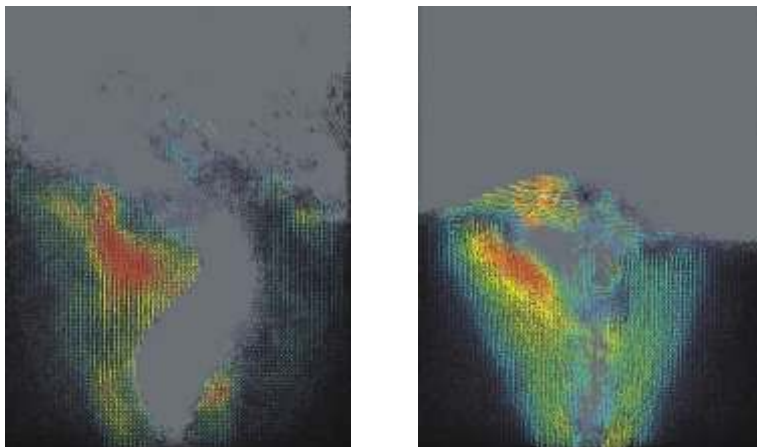


Fig.1: Post-processing snapshots for dry (left) and wet (right) particle experiment.

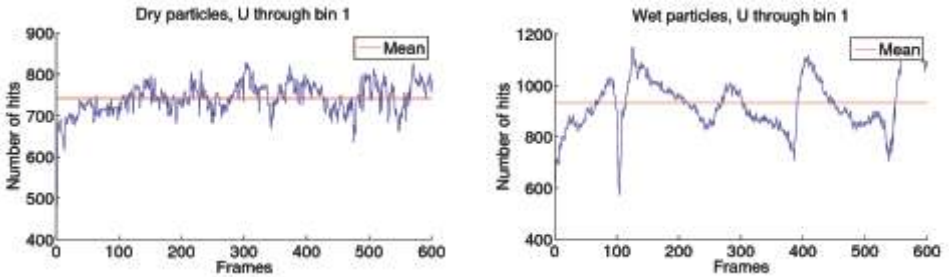


Fig.2: The number of vectors inside the lowest velocity range for each of the recorded frames. We track the number of intersections between vector count (blue) and mean vector number (red) for the chosen velocity range. In the cohesive (wet) particle-gas flow, the relative number of intersections is significantly lower—indicating block-like particle movement.

Coupled CFD-DEM numerical simulation was set for non-cohesive and cohesive particles. The model was achieved with a solver developed at the our department and contact models in CFDEMcoupling environment. Granular Hertz model is included to describe contact forces between spherical particles. Simplified Johnson-Kendall-Robert cohesion model is implemented in LIGGGHTS and it adds an additional normal force to particle equations.

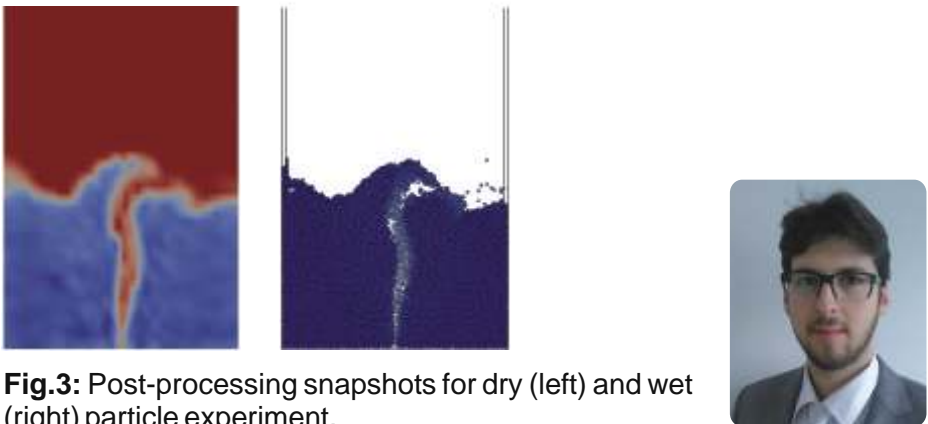


Fig.3: Post-processing snapshots for dry (left) and wet (right) particle experiment.

EDITORIAL | MACRO

Dear Readers,

Macroscale flow problems especially include industrial scale processes. Hereby, we develop "coarse grained" models, where the micro-scale behavior is accounted by proper constitutive relations for the unresolved sub-grid scales. Particularly, we aim to derive physically sound theories, which include as few as possible fitting parameters. This concept is 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. However, originally we developed theories for the coarse grid simulation, when using Eulerian-Eulerian methods.

Currently, our research efforts are dedicated to the validation of those macro-scale models, which includes, for example, the numerical simulation of gas-solid risers (Figure 2) and the extension of these theories to Lagrangian parcel methods (Figure 1).

Furthermore, we study the formation of emulsions in agitated tanks. Last year we made considerable progress in describing the influence of changes of the operating conditions (e.g. speed of the stirrer) on the final droplet size distribution. Here, the appropriate modelling of the coalescence of droplets is of vital importance (Figure 3).

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

Sincerely,



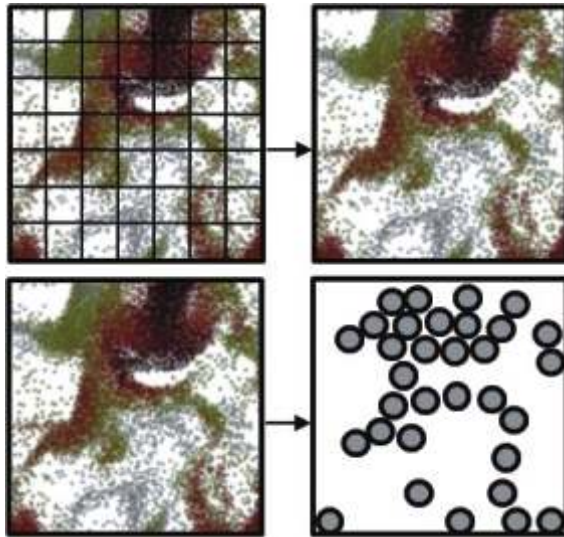


Fig.1: Direct reduction of iron ore in a fluidized bed; left: particle volume fraction; middle: mass fraction of CO, which is consumed in dense regions due to reduction; right: fractional reduction of individual parcels.

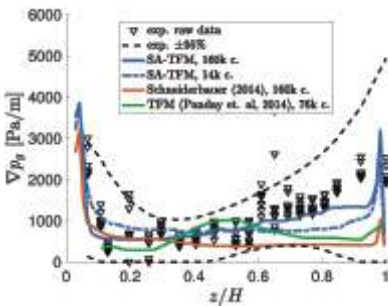


Fig. 2: Pressure gradient profile of the gas-solid flow of Geldart A particles in a riser of 15 m height. The new theory (blue) performs considerably better than previous models (blue, red).

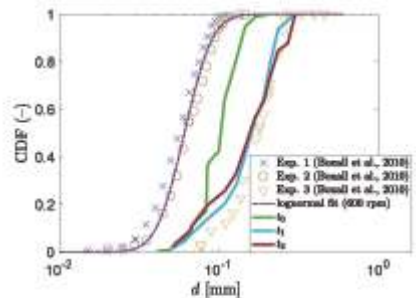


Fig.3: Final droplet size distribution in a liquid-liquid stirred tank after an abrupt change of the operating conditions.

MACRO | MODELING OF EMULSIONS IN STIRRED TANK REACTORS

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. 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, we extracted data regarding to DSD (Fig.2) employing image processing. Furthermore, we developed a correlation for the local Sauter mean diameter D_{32} based on the Kolmogorov turbulence theory and Prandtl mixing length which reads,

$$\frac{D_{32}}{l_m} = 0.08 We^{0.6} (1 + 9.9 \left(\frac{\rho_c}{\rho_d}\right)^{1/2} \frac{\mu_d}{\gamma} (D_{32}^2 l_m \dot{\gamma}^3)^{1/3})^{0.6}$$

μ_d : Viscosity of dispersed phase
 ρ_d : Density of dispersed phase
 ρ_c : Density of continuous phase
 $\dot{\gamma}$: Shear rate
 γ : Interfacial tension

l_m : Mixing length

$$We = \frac{\rho \dot{\gamma}^2 l_m^3}{\gamma}$$

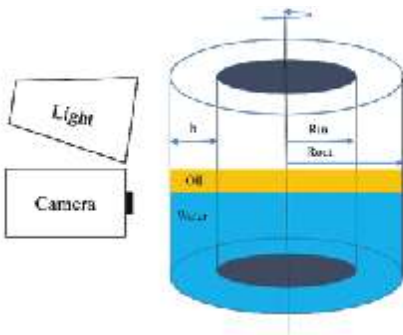


Fig.1: Schematic view of Taylor-Couette flow experiment.

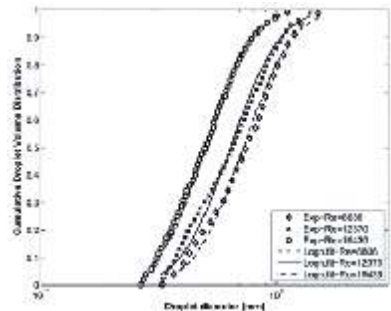


Fig.2: DSD of Soybean oil-in-Water at different rotational speeds.

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-Eulerian-Lagrangian scheme along with the K-ε 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 600 μm were injected at t=0. The simulation was performed for 300 rpm and it stopped when the final drop size distribution did not change any more. Fig.4 shows the cumulative drop size distribution for 300 RPM. As it can be seen in the figure, the simulated results and the experimental data are in a good agreement.

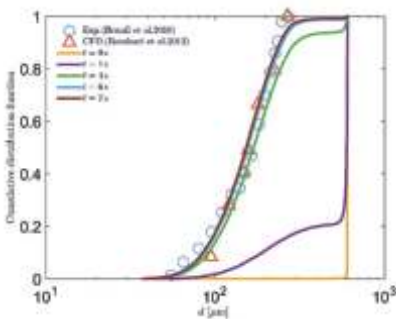


Fig.4: Cumulative drop size distribution, simulation results vs experimental data by Boxall et al. (2010)-300 RPM.

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

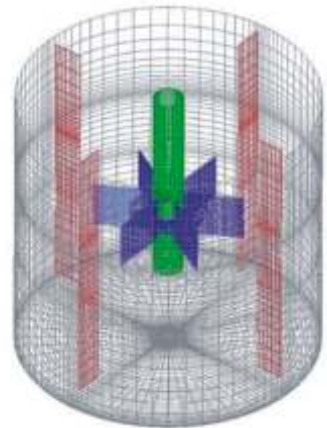


Fig.3: Stirred tank reactor mesh the same as Roudsari et al (2012).



MACRO | RECURRENCE CFD

Well, there is some way to go from a striking idea to an applicable simulation tool. In the last year we dedicated quite some efforts to stepwise transform **rCFD** from concept stage towards a scientifically described and validated simulation methodology.

Two of the major steps on this way are depicted in Fig.1. In long-term simulation of species transport (in this case we considered hydrogen transport in a steelmaking ladle) our fast **rCFD** version exhibits an unacceptable error accumulation (second line of histograms). These deviations can be attributed to the non-conservative nature of memory shifts, which constitute the main ingredient of transport based **rCFD**.

As a remedy we introduced a conservation controller on a coarse compartment level. With this 'global balance safety belt' our long-term **rCFD** simulation results could be significantly improved (third line of histograms).

Next, we successfully reduced the sheer amount of recurrence data by Lagrangian coarse graining of our data shift operations. Obviously, even a fourfold data reduction (last line of histograms) doesn't deteriorate results, while speeding up **rCFD** simulations to breath taking five orders of magnitude – more than an order of magnitude faster than real-time.

Beyond that, we applied transport based **rCFD** to CFD-DEM simulations of heat transfer in a fluidized bed. Here, we had to track two interacting passive properties (i.e. the temperatures of the gas and the discrete particles). Also in this case we reached acceptable agreement, while dropping simulation times below real-time (i.e. five orders of magnitude faster than full CFD-DEM simulations).

Finally, I am very happy that our novel **rCFD** method survived a plenary lecture at Particles conference in Hannover, receiving rewarding feedback from the scientific community.

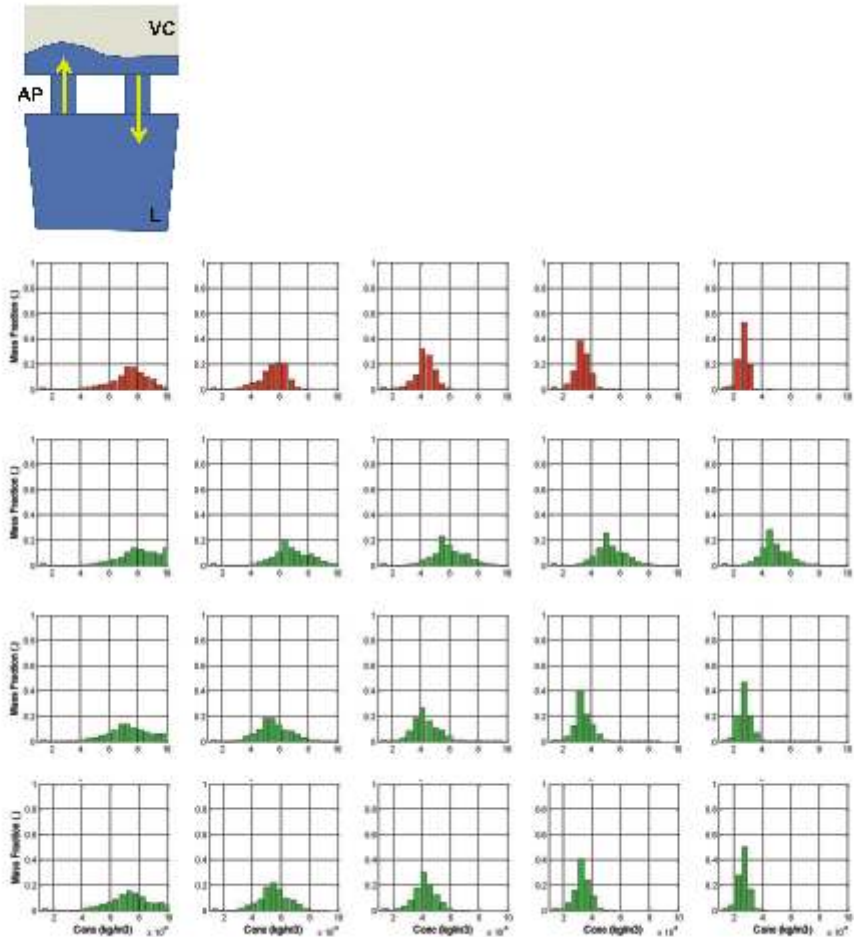


Fig.1: Long-term simulations of hydrogen concentration in a steel ladle (very top) as result of (from top to bottom) full CFD, transport based rCFD w/o and with safety belt and coarse grained; Simulation times for 5 minutes process time account to 85 h, 8 sec, 34 sec and 10 sec respectively.



EDITORIAL IV | EXPERIMENTS & DATA ANALYSIS

Dear Readers,

the past year has also brought some new activities in our laboratory. We were able to enhance the capabilities of our PIV system with a new continuous wave laser and are now able to do time resolved PIV up to approximately 5m/s in in gases and liquids.

Classic PIV (at low pulse rates) is perfectly suited for the validation of CFD models based on Reynolds averaging. However, low speed PIV does not provide the quantities needed for the validation of LES based modelling activities. Hence, we are now able to bridge this gap and do multiscale experiments (in time and space) for new subgrid model approaches like ADM (Approximate Deconvolution Method).

Currently the first field capable ECT sensor to monitor the pneumatic conveying of pulverized coal is being installed at the voestalpine plant in Linz. After a successful prove of concept and the operation of a similar system in lab scale experiments we now have a well organized phase of know how transfer towards our industrial partner.

As we are eagerly waiting to see the first measurement results from real plant operation, this project is also a perfect example, that, beside our experimental work at PFM, my activities have shifted closer towards plant data analysis over the last years.

Sincerely,





Fig.1: New CW Laser for time resolved PIV and a snapshot of shear layer turbulence in a free jet.

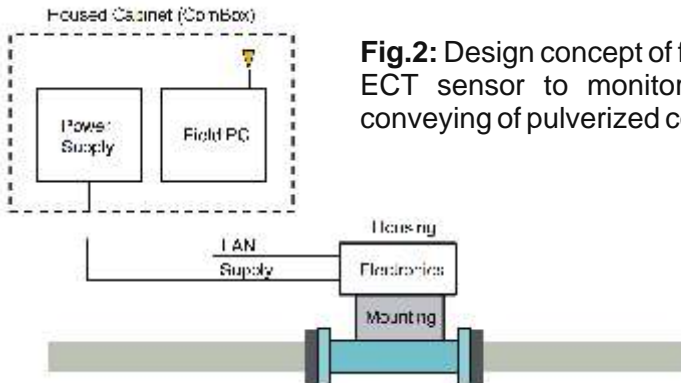


Fig.2: Design concept of field capable ECT sensor to monitor pneumatic conveying of pulverized coal.

Fig.3: Exemplary reconstruction patterns in ECT processing for different flow regimes in pneumatic conveying.



(a) Exemplary pattern for a dispersed flow.



(b) Exemplary pattern for a stationary flow.



(c) Exemplary pattern for a stratified flow.



(d) Exemplary pattern for a stratified slug flow.

EXPERIMENTS & DATA ANALYSIS | RACEWAY BLOCKAGE DETECTION PART I – SIGNAL PROCESSING OF AVAILABLE PLANT DATA

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 raceway blockage detection. This can either be based on already available plant data or on digital image processing of tuyere camera data (see next page).

Figure 1 shows that pressure difference on a tuyere blow pipe (represents the hot blast flow rate) shows significant dips. These signal dips correlate in most cases with blockages of the raceway of various kinds as could be evaluated from a test installation of a tuyere camera. the blow pipe sensor 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.

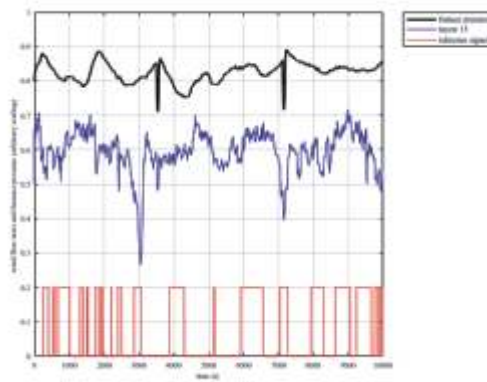


Fig.1: Pressure difference on a specific blow pipe (blue) in comparison with the main blast pressure (black) and the identified blockage signal (red), obtained by manually checking tuyere camera images. The dips in the black curve represent the events of switching the hot blast stove.

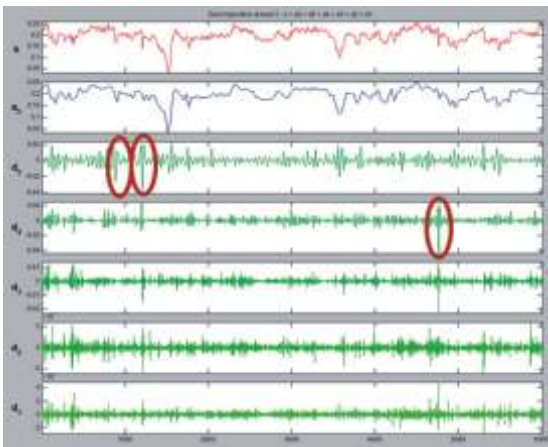


Fig.2: Result of wavelet decomposition into different scales. The blockage events differ strongly in their length (from ~10s to 10min). For such signals wavelet transform is a powerful tool to detect these different time scales (like the marked examples on scales 4 and 5).



EXPERIMENTS & DATA ANALYSIS | RACEWAY BLOCKAGE DETECTION PART II – VISUAL BLOCKAGE DETECTION

As camera technology has evolved rapidly over the last two decades, it is nowadays feasible to equip every tuyere on a blast furnace with a raceway camera. The visual impression of the tuyeres adds valuable information about what’s going on in the raceway regions of the blast furnace.

Hence, it is also an interesting question if raceway blockages can be detected automatically via digital image processing. In fact this is not a trivial task as the visual impression of various raceway conditions differ quite significantly as can be seen in **Fig.1**.

We have tested different algorithms and implemented a common quality assessment for the results which derives a digital 0/1 signal via a final thresholding step. These yes/no signals can be compared with manually defined reference signals to automatically count the found, missed and false positive results (**Fig. 2**).

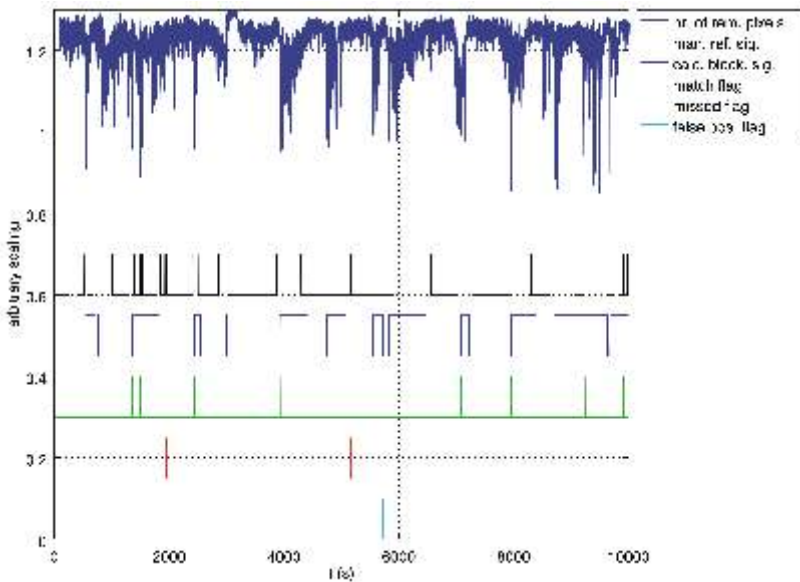


Fig.2: Quality assessment of image processing results based on a final thresholding step and comparison with a reference signal.

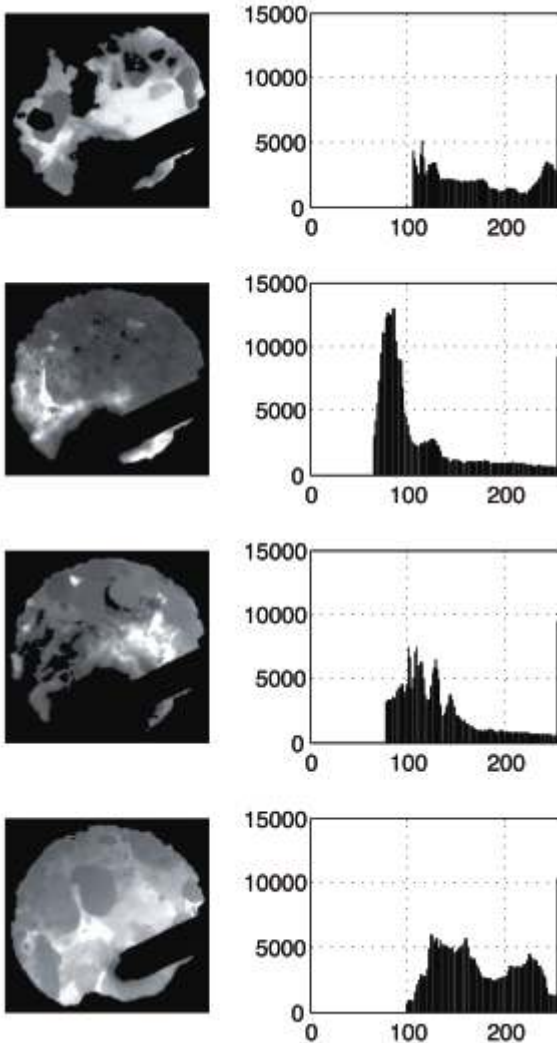


Fig.1: Example of various raceway conditions after cutting of the grey level histogram based on the threshold level calculated by Otsu's method. The top image shows ordinary raceway operation, the second and third image show different types of blockages and bottom image a situation where the PCI branch was switched off.



EXPERIMENTS & DATA ANALYSIS | MULTISCALE EXPERIMENTS OF SLAG ENTRAINMENT IN CONTINUOUS CASTING

Our in-house validation experiments are strongly driven by the latest developments in CFD modelling. Basically all current modelling activities are in one way or another dealing with the macroscopic impact of unresolved physics. Hence, this also drives the need to resolve finer time and length scales in lab experiments.

Last year we had the chance to upgrade our PIV System for time resolved measurements of liquid systems. For the mold flow activities in the frame of K1Met P4.4 we are now testing advanced PIV setups with either time resolved PIV of the liquid-liquid interface (representing liquid steel and slag) and/or multiscale measurements with two cameras (**Fig.1** and **Fig.2**), where one camera is capturing the complete flow field, while a second camera zooms in to the interface region with highest shear rates in the top right corner of the basin. This will give more precise data for the calculation of turbulent quantities and energy spectra.



Fig.1: Two camera PIV setup to acquire flow field data at different spatial resolutions simultaneously.

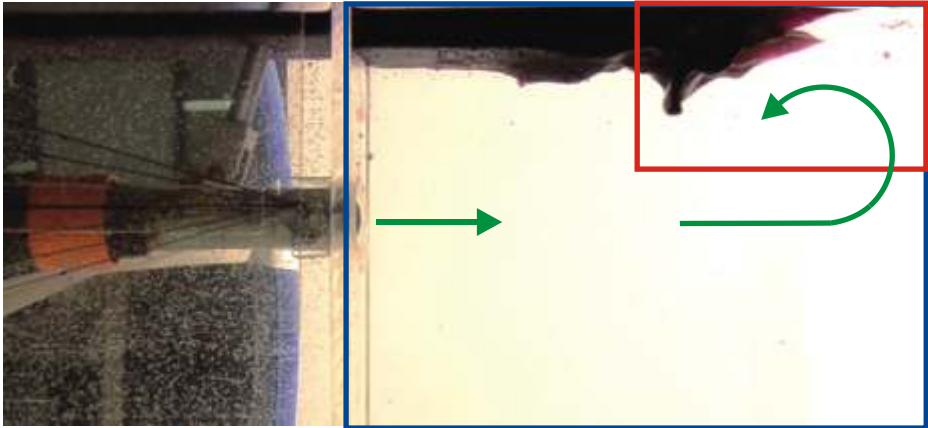
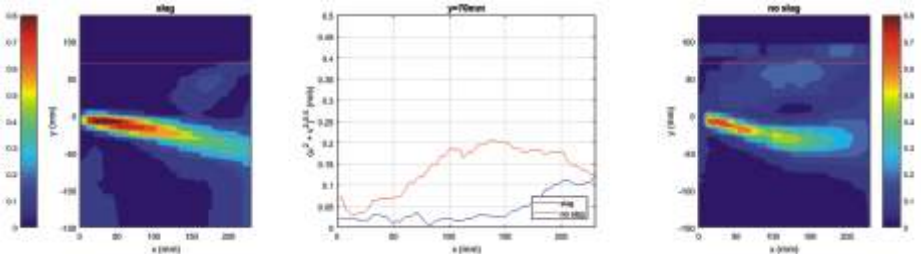


Fig.2: Multiscale setup of a PIV setup for the water/oil experiment for mold flow modelling in continuous casting. One camera can capture the complete flow field (blue area), while a second one zooms in to the interface region with highest shear forces caused by the recirculating vortex in the top right corner (red area).



Stefan Puttinger | Nikolaus Doppelhammer

Fig.3: Damping effect of the oil layer (representing the slag phase) on the complete flow field at an inlet angle of -10° . the center image shows the averaged velocities on a horizontal line close to the water/oil interface (red line in left and right image).



EXPERIMENTS & DATA ANALYSIS | 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 (**Fig.1**).

Since then we were able to extend our measurement capabilities to real 3D problems. The tomographic reconstruction is able to run online (with real time visualization) and allows insight to e.g. pneumatic conveying of granular materials in pipes (**Fig.2**) or small fluidized bed experiments.

Together with EMT/Graz and voestalpine we managed to acquire additional funding for a FFG/Bridge project to develop a field applicable version of the ECT system. The first sensor is currently being installed at a conveying pipe for pulverized coal at the voestalpine plant in Linz. The construction of this field sensor is based on an inner glass cylinder sealed and housed in a pressure resistive steel pipe.



Fig.2: Single plane ECT sensor on our hopper discharge experiment in the PFM lab. The grey box is the main hardware unit of the ECT system which sends its raw data via network connection to a PC running Matlab for three-dimensional data reconstruction.

Fig.2: Two plane ECT sensor in a horizontal conveying pipe of 50mm diameter. The transported material are glass beads with a mean diameter of $\sim 50\mu\text{m}$. The insert shows the online visualization of the reconstruction software. As expected a moving strand at the bottom of the pipe can be seen along with some dilute conveying patterns above this strand.

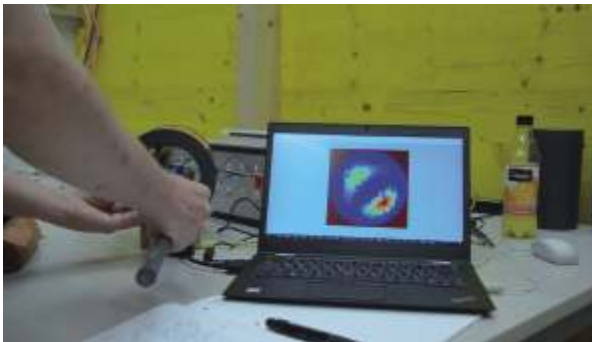
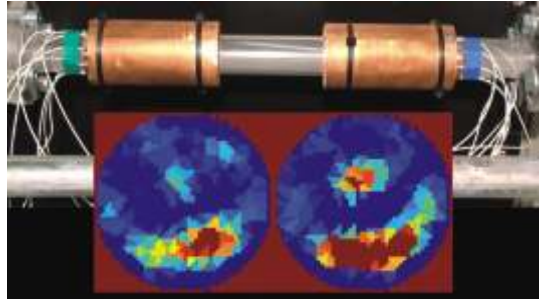


Fig.3: Prototype of a completely sealed ECT sensor at first sensitivity tests. A first version of a field capable sensor is currently being built and installed in a conveying pipe for pulverized coal at voestalpine in Linz.

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SCIENTIFIC FRIENDS | P. KIECKHEFEN, S. PIETSCH & S. HEINRICH

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Spray coating of particles is commonly performed in spouted beds. Numerical simulations are required for the accurate design of such apparatuses.

The variety in flow regimes present in the system requires the accurate, but numerically expensive CFD-DEM method to be used. The present lab-scale system (500k particles) requires about 1 day wall time per second, which is prohibitive for describing the spray coating process that takes hours. All of these constraints make spouted beds a prime target for rCFD.

To enable the treatment of complex geometries, the Lagrangian rCFD implementation of T. Lichtenegger was ported from CFDEM & LIGGGHTS to the OpenFOAM Lagrangian Particle Tracking framework. Here, the efficient wall treatment and inter-processor communication were leveraged to yield a speedup of around 2100x CFD-DEM, or 2.4% real-time.

Comprehensive validation regarding the reproduction of bed distribution and mixing behavior as judged by residence time within a spray cone (Figure 2) were performed, showing good agreement.

Coating was simulated by injecting Lagrangian droplet parcels and using a filter correlation to model the deposition of droplets on a Eulerian grid, avoiding costly contact detection. Simulations for an unstabilized and a draft plates-stabilized spouted bed were performed. The resulting surface coverage distributions are shown in Figure 3. The installation of draft plates reduce homogeneity due to inhibited mixed while slightly reducing overspray.

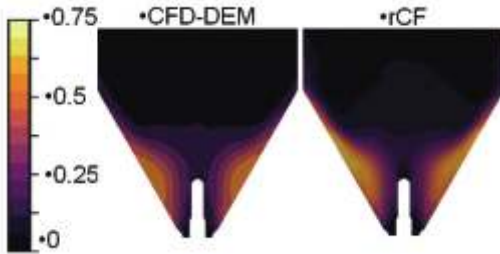


Fig.1: Time-averaged particle volume fractions derived from CFD-DEM simulations and subsequent rCFD simulations.

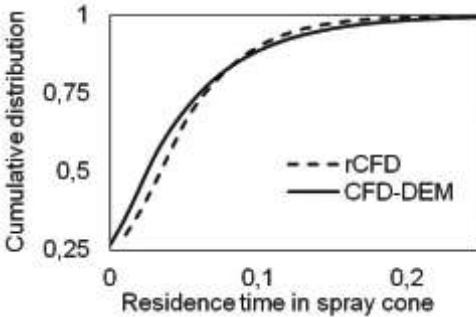


Fig.2: Particle residence time distributions within a fictitious spray cone after 10 s of simulation time, indicating an accurate representation of mixing patterns by rCFD.

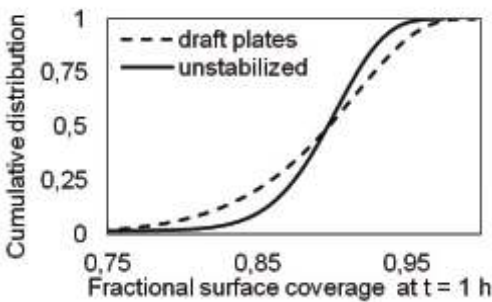


Fig.3: Surface coverage distribution after 1 hour of process time as simulated by rCFD.



Supervision:
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SCIENTIFIC FRIENDS | STÉPHANE VINCENT, PROFESSOR UNIVERSITÉ PARIS-EST MARNE-LA-VALLÉE, LABORATOIRE MSME UMR CNRS 8208

Whereas Large Eddy Simulation (LES) of single-phase flows is already widely used in the CFD world, even for industrial applications, LES of two-phase interfacial flows, i.e. two-phase flows where an interface separates two immiscible fluids (liquid or gas phases), still remains a challenging task. The main issue is the development of subgrid scale models well suited for two-phase interfacial flows.

Introducing spatial filtering to the continuous media governing equations of the interfacial flows results in appearing various subgrid terms that should be modelled via subgrid closures. Whereas the well-known subgrid contribution of the non-linear convective term is modelled using eddy-viscosity approach (e.g. Smagorinsky model for example), the other subgrid terms such as the contribution of surface tension force and transport of interface are usually neglected in the current state of the art of LES of two-phase flows. According to the *a priori* studies [1], these terms are not always negligible and their contribution can be of great importance especially when the viscosity and the density ratio of two fluids are close to unity (e.g. water-oil systems).

A recent *a-priori* study [2] also presented a comparison study between different sub-grid closure models in the literature such as Smagorinsky, WALE, Bardina and ADM. It is clearly concluded that the subgrid model of Approximate Deconvolution Model (ADM) [3] shows the best performance to predict the sub-grid contribution of those terms (Figure 1). ADM is a structural subgrid modelling with a purely mathematical nature. Since no prior knowledge of the physics of the interaction between resolved and non-resolved scales is needed, ADM seems a potential candidate for developing subgrid closure for LES of interfacial flows.

The first steps of this scientific collaboration have been taken during the research visit of Mahdi Saeedipour at the group of Prof. Stéphane Vincent at the “Laboratoire de Modélisation et Simulation Multi Echelle”, University of Paris-Est Marne La Vallée (UPEM). Currently, we are working on the *posteriori* large eddy simulation of interfacial flows with including all the subgrid contributions modelled by the structural model of ADM (Figure 2). This will serve as an important step toward the multiscale modelling of turbulent interfacial flows such as the slag-molten metal interaction in the continuous casting model flow.

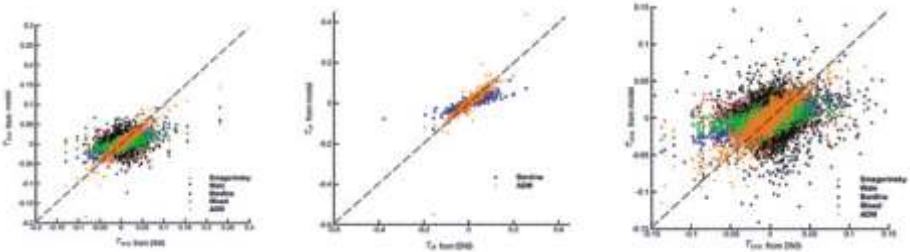


Fig.1: Spatial correlation of two-phase LES subgrid terms. The subgrid terms computed by LES models and filtering the DNS data are shown on vertical and horizontal axis, respectively. More details are provided in [2].

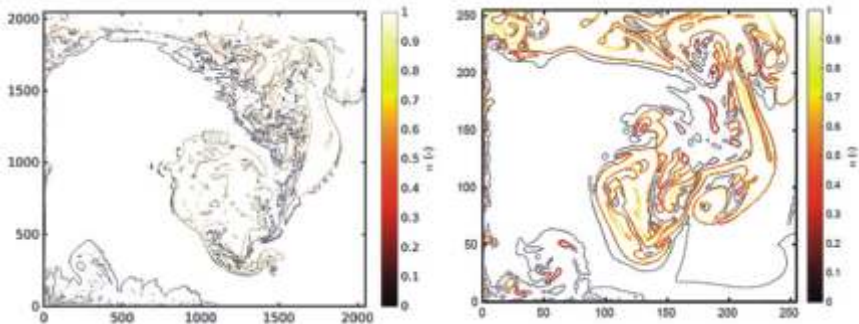


Fig.2: Snapshot of interface profiles of quasi-direct numerical simulation of interfacial turbulence in the oil-water phase inversion process (left) and *a-posteriori* LES using ADM on 8 times coarser grid (right) at the peak of enstrophy.

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