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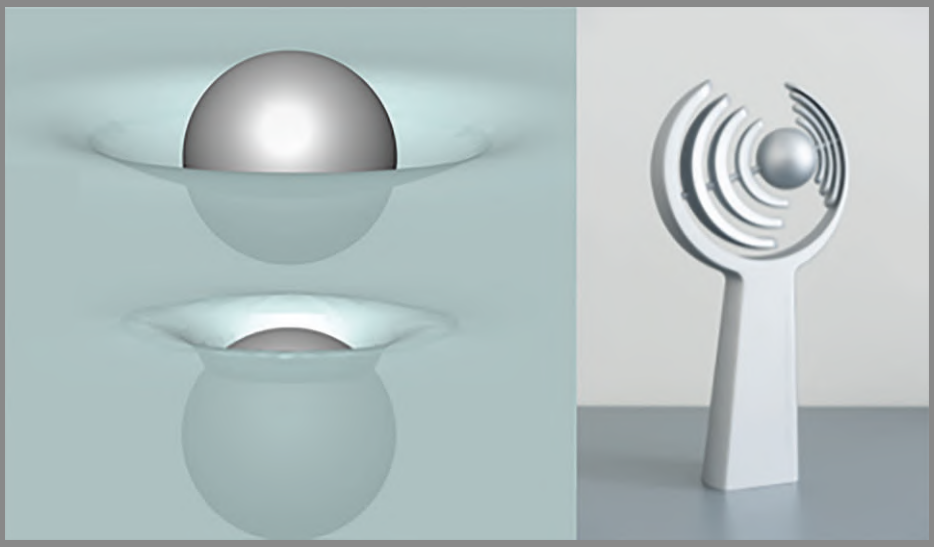

JKU | Department of Particulate Flow Modelling

Annual Report | 2021

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Front cover: A hidden champion siding with our Christian Doppler Award: Numerical simulation of particle behavior at metal-slag interface – while dominant capillary forces govern particle capture, Marangoni convection triggers separation. © X. Zhang, M. Saeedipour & S. Pirker

EDITORIAL

Dear Readers,

In the second year of our corona restricted life, we received a prestigious governmental award for what they called outstanding scientific achievements. In a rare period of free gatherings, we could celebrate this together with our industrial partner – reflecting on a successful twelve years' research journey.

In terms of current scientific developments, we pushed further our data-assisted recurrence CFD method, aiming to bring it closer to potential applications. However, this fancy mainstream topic shouldn't drown other important developments of classical methods like the novel powder characterization techniques of Tobias and Thomas, advanced filtered Two-Fluid models of Stefanie and Simon or the microscopic capillary-driven flow models of Xiaomeng and Mahdi, to just name three of those hidden champions.

Looking at our last year's achievements, I see a balanced mixture between significant advancements of classical methods and a general drive for novel avant-garde explorations.

With these introducing words, I wish you a pleasant reading!

All the best,

Stefan Pirker | stefan.pirker@jku.at

EDITORIAL

Dear Readers,

Last November the Christian Doppler Laboratory for “Multi-scale modeling of multiphase flows” successfully gone through its five year’s 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 last 3 years.

Currently, the focus of the CD-Laboratory is laid on extending the concepts of multiphase turbulence to heat and mass transfer. Especially, in gas-particle flows heat transfer and the chemical reaction rates significantly depend on the heterogenous structures, such as clusters and streamers.

A second focus of this CD-Laboratory is recurrence CFD, which has been successfully applied to a reactive pilot scale polymerization fluidized bed. Other projects include the efficient numerical simulation of the transport and mixing of cohesive particles, the impact of cohesion on fluidization, the generalization of turbulence models for multiphase flows.

Finally, I want to thank my team for their great work and their engagement and I am looking forward to the final phase of this CD-Laboratory!

Sincerely,

Simon Schneiderbauer | simon.schneiderbauer@jku.at

CONTENTS

EDITORIAL | MICRO

Dear Readers,

In the past year and under the shadow of pandemic, we continued our research on different aspects of interfacial flows. From attempts toward performing volume of fluid-based DNS of interfacial turbulence to develop and test new subgrid models for two-phase LES. From resolved immersed boundary-based simulation of solid particles in two-phase gas-liquid and liquid-liquid flows to implication of such techniques to blood flow, bubbly flow, and Marangoni-driven systems.

Achuth B. Nair has successfully finished his PhD on blood flow modelling, and could further adopt the reduced-order RBC model to industrial application of plasma separation (Figure 1). Besides, we developed a coupled VOF-fictitious domain method for the resolved simulation of droplets and bubbles with solid particles. This resolved CFD-DEM method has been tested for droplet-particle collisions at different regimes (Figure 2), and will be the numerical basis for our new research project on capillary-based blood separation.

Besides, **Xiaomeng Zhang,** in her PhD research on resolved simulation of particles in the vicinity of fluid-fluid interfaces, has reached essential conclusions about the role of hydrodynamic forces and Marangoni stresses on the destiny of micron-sized particles at the steel-slag interface (Figure 3).

Our research focus on interfacial turbulence has further evolved through the ongoing collaboration with Prof. Stephane Vincent from Paris by performing enstrophy-resolved simulations for well-known Phase Inversion benchmark (Figure 4). In next year, we plan to further analyze the physics of turbulence in two-phase flows based on high order moments such as enstrophy.

Let's have a tour together to our
research activities on interfaces and particles!

Mahdi Saeedipour | mahdi.saeedipour@jku.at

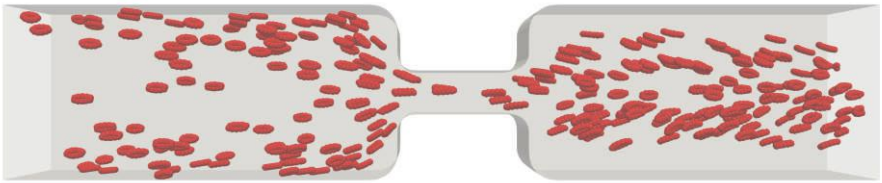

Fig.1: Resolved CFD-DEM simulation of blood flow across a micro-channel with constriction and the the cell-free layer enhancement applicable to plasma separation.

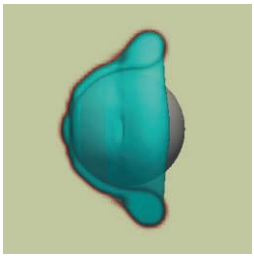

Fig.2: A snapshot of fully resolved VOF-IB simulation of droplet-particle collision at We = 69.

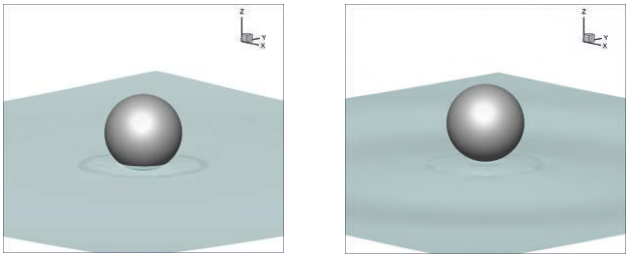

Fig.3: VOF-overset grid simulation of non-metallic inclusion behavior at the steel-slag interface with different wettability: entrapped at the interface (left), and separated toward slag (right).

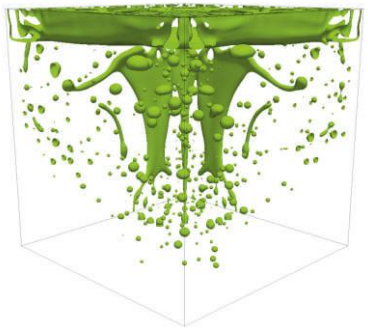

Fig.4: A 3D snapshot of the interfacial flow in the enstrophy-resolved VOF simulation of the phase inversion problem.

MICRO | INCLUSION SEPARATION AT STEEL-SLAG INTERFACE

As one common strategy in steel cleanliness control, removing non-metallic inclusions in molten steel has been widely studied. However, the removal efficiency tends to be overestimated due to insufficient consideration of inclusion separation behavior (trapped at the interface or completely entering into slag) at the steel-slag interface. This interfacial phenomenon not only affects the subsequent dissolution kinetics but is also closely associated with phenomena such as inclusion re-entrainment into the steel and agglomeration at the interface. Therefore, an understanding of the fundamental aspects of inclusion separation at the interface is essential to achieve better control on steel cleanliness.

For this purpose, we have conducted numerical simulations to investigate the dynamics of a spherical particle interacting with the steel-slag interface using the Volume of Fluid method in combination with the overset grid technique to account for particle motion. As shown in Fig. 1, the simulations have shown a detailed particle's separation process in the vicinity of the steel-slag interface and successfully captured the formation and continuous evolution of a meniscus in the course of particle motion. Besides, the simulation results indicate that a complete separation for the spherical inclusion occurs when θ_{IMS} is about 20. For less slagophilic inclusions, they end with trapped at the interface in a very short time.

On the basis of that, we believe the Marangoni convection induced by interfacial tension gradient due to particle dissolution may further enhance inclusion separation. At present, we have successfully implemented the solutal Marangoni effect by incorporating the species transport model and a tangential source term at the interface by user-defined functions. A process combining solute diffusion, interfacial flow and particle motion is shown in Fig. 2. Nevertheless, it is still a work in progress to verify and eventually quantify the influence of the solutal Marangoni flow on the context of inclusion separation.

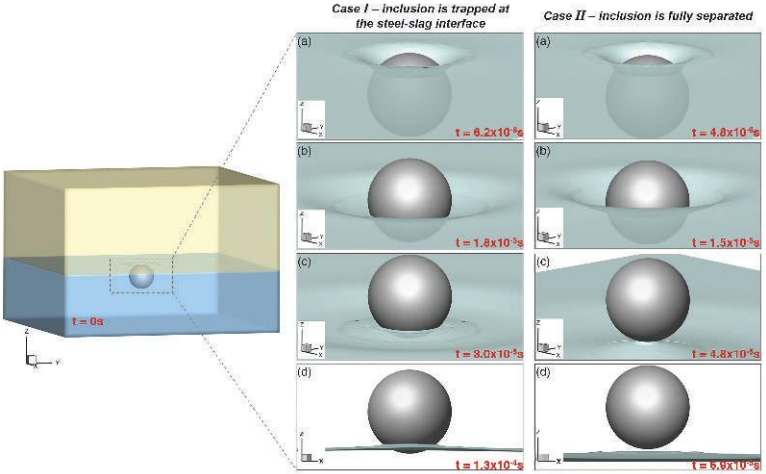

Fig.1: Evolution of particle motion across the steel-slag interface at θ_{IMS} = 40° (Case I) and 20°(Case II). Snapshot on the left provides a full view of the initial state (particle just touches the flat interface). Details on subsequent motion are shown in closeups (a)-(d) in chronological order.

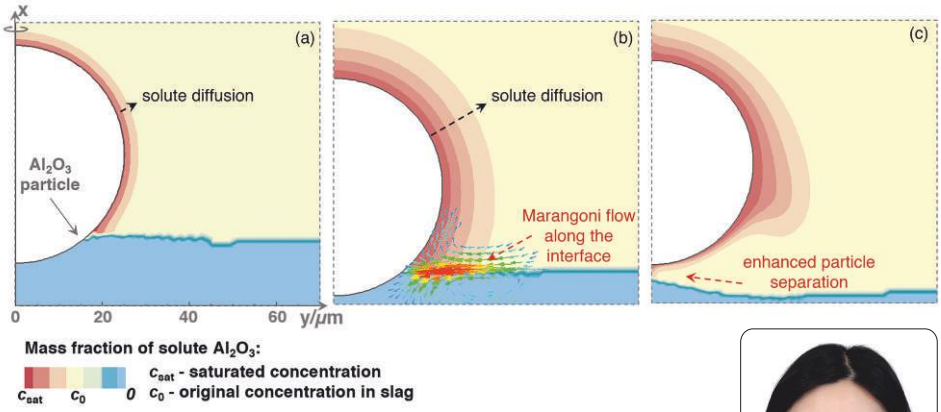

Fig.2: Marangoni convection and the resulting particle motion. Color transition in the slag phase represents the diffusion of solute coming from the dissolved particle. An interfacial flow arising from concentration gradient further enhances particle motion.

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MICRO | A COUPLED VOLUME OF FLUID-FICTICIOUS DOMAIN FOR RESOLVED SIMULATION OF DROPLET-PARTICLE INTERACTIONS

Dispersed multiphase flows involving both fluid interfacial elements (droplets and bubbles) in the presence of moving solid particles are frequently encountered in many different chemical and metallurgical industries. In such multiphase systems, the microscopic interactions of droplets/bubbles with particles influence the evolution of macroscopic characteristics of multiphase flow. Thus, a fully resolved small-scale description of such interactions is essential to understand the process and propose multiscale simulation methods.

We recently developed a coupled volume of fluid-fictitious domain method for the fully-resolved interaction of fluid-fluid interfaces with solid particles. We employ the VOF method to capture the interface between the interfacial structures, and adopt an immersed boundary concept to account for the presence of solid particles. In this fictitious domain approach, the particle-covered finite volume cells are identified, and the hydrodynamic forces acting on the particle are computed separately While the particle motion is governed by the Newton's second law, a continuous force field is applied at particle-covered cells as a penalty term in the momentum equation. To guarantee the mass conservation of the method, the VOF algorithm is also adjusted to prevent penetration of the interface into the particle region. This method is developed and implemented by coupling the VOF and immersed boundary libraries of OpenFOAM and LIGGGHTS. The schematic of the coupled solver is presented in Figure 1.

This method is employed to study the droplet-particle interactions where a water droplet and a solid particle constitute a heads-on binary collision in the surrounding air [1]. The collision behavior at different impact Weber numbers and are simulated (Figure 2). The particle-coated area is used as one of the measures to identify different outcome regimes (Figure 3). Besides the rebound and fully-coated regimes reported by the existing literature, we could observe some new regimes such as partial coating and sudden wash-off at higher Weber numbers (We > 250). This approach will be further improved by including the wetting phenomenon into the code and increasing the number of interacting droplets and particles.

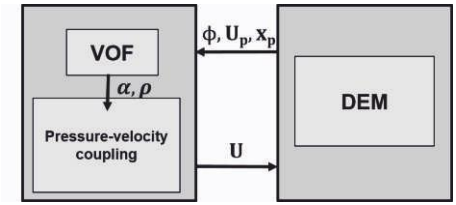

Fig.1: Schematic of the developed coupled VOF-DEM solver.

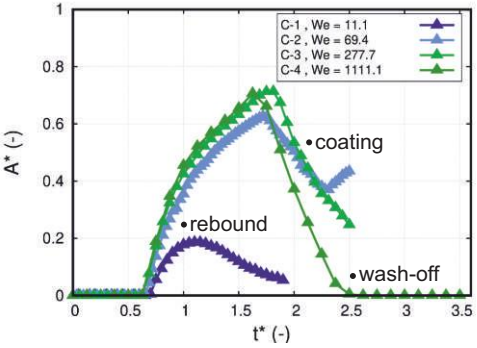

Fig.3: Temporal evolution of dimensionless particle-coated area for different We numbers, and different outcome regimes.

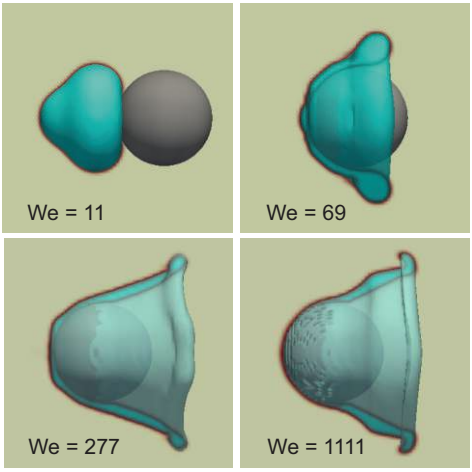

Fig.2: Snapshots of droplet-particle collisions at dimensionless time t* = 1 for different impact Weber numbers. At low We, the collision results in rebound, while at higher We different coating regimes are observed.

[1] Saeedipour M., Balachandran Nair A., Pirker S., A coupled volume of fluid-fictitious domain method to study droplet-particle interactions at different impact conditions. *International Conference on Liquid Atomization and Spray Systems (ICLASS-2021), 2021*.

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MICRO | TOWARD FULLY RESOLVED VOLUME OF FLUID SIMULATION OF INTERFACIAL FLOW BENCHMARK

Modelling and simulation of turbulent interfacial flows is important for many industrial applications such as atomization, emulsification and bubble columns. The physical complexity and multiscale nature of such flows entail a crucial challenge to experimental validation of models. As the alternatives, highly resolved and direct numerical simulation (DNS) are necessary to serve as the numerical benchmarks to evaluate the accuracy and performance of new models for other affordable approaches such as large eddy simulations (LES), and multiscale simulation techniques.

One such problem is the interfacial homogeneous isotropic turbulence (HIT) which consists of the evolution of an initially flat interface in interaction with an isotropic turbulent flow. This problem has been used in our recent model validation for two-phase LES [1]. Nevertheless, the current DNS of this problem is restricted to capillary forces in interfacial flow with no density and viscosity contrasts. The other potential benchmark is the well-known phase inversion (PI) problem. This buoyancy-driven interfacial flow features several large and small-scale interfacial processes such as deformation, ligament formation, interface rupture, and coalescence. Even though this problem has been subject to many a priori and a posteriori LES studies, so far no fully resolved simulation for this problem has been reported in which all low and high order moments reveal grid independence.

During our ongoing research collaboration with two research groups in France [2], we recently proposed a new enstrophy-resolved configuration for this problem by reducing the Reynolds and Weber numbers. The new setup reaches grid convergence for all the flow characteristics, including enstrophy, on a 512^3 grid. Also, we analyze the temporal evolution of interfacial structures and size distribution of the droplets. The results highlight that (i) the enstrophy converges for these moderate Re and We numbers, and (ii) the convergence of the total interfacial area is sensitive to the choice of initial and wall boundary conditions. Finally, a new setup with new initial and boundary conditions is proposed (Figure 1) that succeeded in full convergence for enstrophy and a partial convergence for the total interfacial area (Figure 2).

Although for a fully turbulent phase inversion the Re and We number should further increase, the new setup provides insight into the possible directions toward a DNS for such a problem.

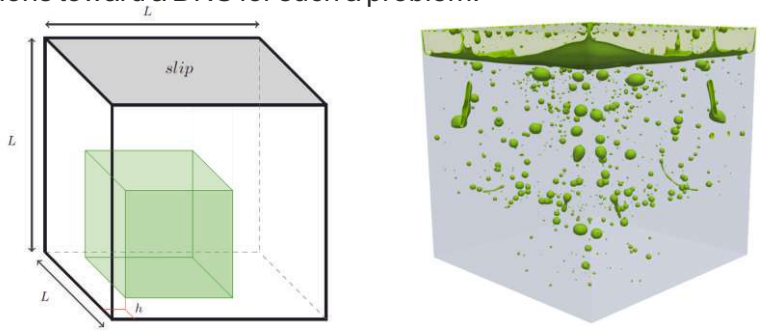

Fig.1: Schematic of the initial condition of the proposed phase inversion problem (left), a 3D snapshot of the fully resolved PI at t* = 2.5 with new initial conditions (right). At this instant, the enstrophy and total interfacial area reach grid-independent results at 512^3 grid [2].

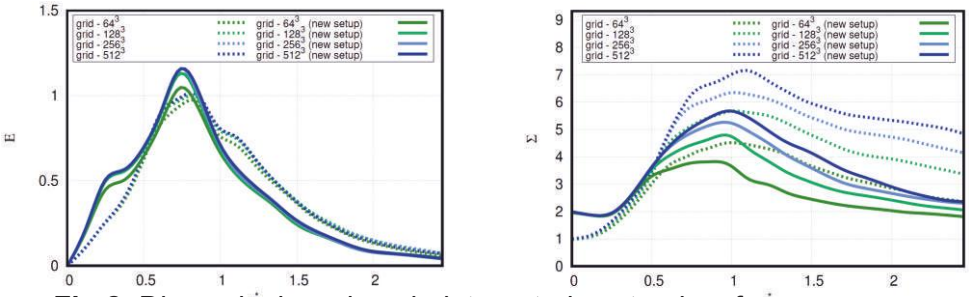

Fig.2: Dimensionless domain-integrated enstrophy of heavier fluid (left), and interfacial area (right) on different grid resolutions for the new configuration (solid lines) compared to the original case with no-slip walls (dashed lines) [2].

[1] Saeedipour M., Schneiderbauer S., Favre-filtered LES-VOF of two phase flows with eddy viscosity-based subgrid closure models: An a-posteriori analysis, *International Journal of Multiphase Flow* 144 (2021).

[2] Saeedipour M., Vincent S., Estivalezes J-L., Toward a fully resolved volume of fluid simulation of the phase inversion problem. *Acta Mechanica* 232 (2021).

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EDITORIAL | MESO

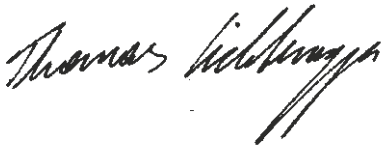
Dear Readers,

Yet another year impacted by the pandemic has passed. In some regards, the return to a more regular life as we knew it from before 2020 has slowly started to take place, and we have been returning to our offices to conduct research side by side and exchange ideas with each other, at least temporarily. Nevertheless, most part of the previous twelve months was characterized by working from home only with video conferences to stay in touch. Especially for our PhD students who usually support each other with the everyday struggles of research life, this posed a significant burden. I think we can be especially proud of the fact that some of our group members finished and successfully defended their dissertations in the previous year – congratulations to **Sanaz Abbasi** (meso team) and **Achuth B. Nair** (micro team) –, and others, who started their work only recently, made remarkable progress.

Even though we, like everyone else, try to make the best of the current situation, we feel enthusiastic about the hope that we can function as a scientific group again to inspire each other side by side. Equally important, we are looking forward to meeting you, our valued partners, again face-to-face to discuss our both's perspective on the upcoming topics in our joint collaborations and to shape the future of PFM!

Dear Readers, I hope these lines have awakened your interest and you enjoy reading about the scientific highlights of our group members!

Sincerely,



Thomas Lichtenegger | thomas.lichtenegger@jku.at

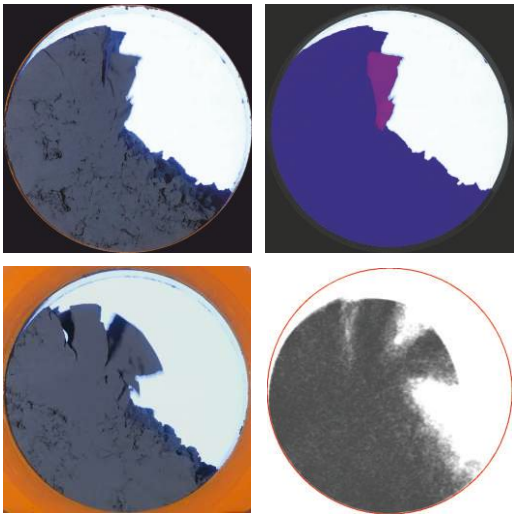


Fig.1: Characterization and simulation of cohesive powder in a rotating drum. Automated block identification (upper row) allows to extract material properties towards which DEM parameters can be calibrated. The agreement between experiment and simulation (lower row) demonstrates the power of the method.

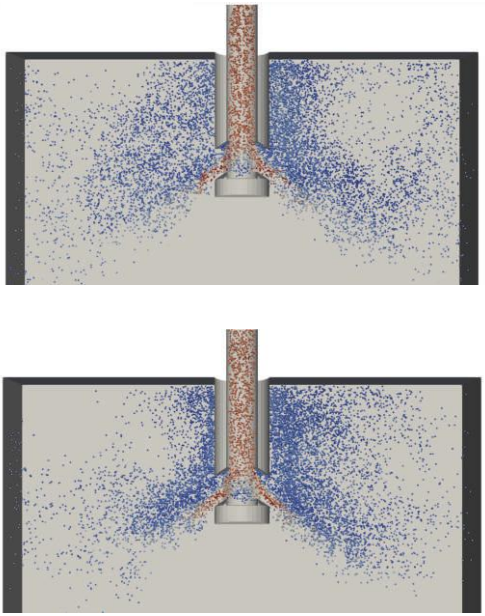


Fig.2: Bubble injection by a turbulent double jet. While large-scale flow patterns give rise to macroscopic transport behavior of the bubbles, small-scale fluctuations disperse them. Detailed large-eddy simulations (upper figure) can predict the bubble distribution reasonable well but require long run times. Recurrence CFD (lower figure) provides results of similar quality at fractions of the runtime.

MESO | HEAT TRANSFER IN UNRESOLVED CFD-DEM SIMULATIONS USING THE MULTI-LEVEL COARSE-GRAIN MODEL

The sheer amount of particles in DEM or CFD-DEM simulations of large-scale industrial systems makes it necessary to introduce certain model simplifications. An eligible candidate is the coarse-grain (CG) model of the DEM which lowers the computational demand by using coarser (pseudo) particles to represent a certain number of original particles. However, due to the violation of geometric similarity, this simple coarse-graining approach fails to capture effects that intrinsically depend on particle size.

To overcome these deficiencies and increase the applicability of DEM coarse-graining we have introduced the multi-level coarse-grain (MLCG) model of the DEM. In this approach, multiple coarse-grain levels are coupled to spatially adjust the resolution of the simulation as required. We have previously shown that the MLCG model can be extended to fluid-particle systems using CFD-DEM. To round out the method we have added heat transfer mechanisms (particle fluid heat convection as well as particle-particle heat conduction) and chemistry models.

To illustrate the heat transfer mechanisms in CFD-DEM simulations we use the setup shown in Fig. 1(a). The silo has a maximum diameter of 270 mm and a height of 425 mm. Starting at a height of 200 mm the container narrows to a diameter of 40 mm at the bottom. The bin is initially filled with 75000 coarse-grained particles with a diameter of 5.6 mm coupled to an original-size subdomain containing about 41000 particles of diameter 2.8 mm. The particles have an initial temperature of 180°C. A steady supply of cooling gas with 25°C is flowing into the bin right above the conical section and leaves the container at the top while the particles leave the silo through the bottom outlet.

The particle temperature at the boundaries of the embedded fine-scale simulation is deduced from the overall coarse-grain simulation. Subsequently the particle temperature is calculated from particle-fluid heat convection as well as particle-particle heat conduction.

The influence of the particle phase on the fluid phase is calculated from the fine-scale domain at the bottom of the simulation and the coarse-grained domain in the rest of the domain.

Figures 1(b)-(d) and 2(a)-(c) show the temperature of the fluid and particle phases, respectively, after 1, 2 and 3 s of particle outflow. Figure 3 depicts the average particle temperature below the orifice during the outflow and demonstrates that the temperature evolution is in good agreement for both representations of the system.

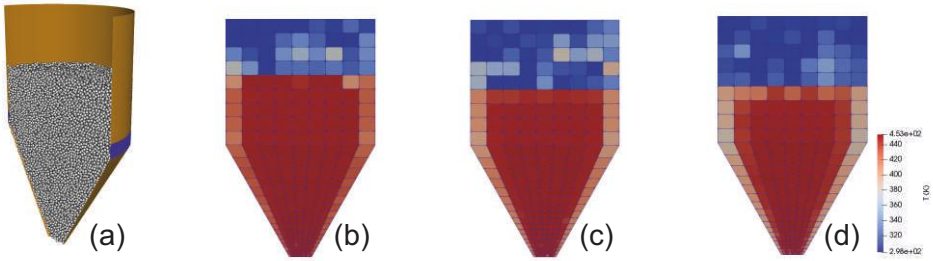


Fig.1: (a) Cutaway view of the simulation setup with the gas inlet above the conical part of the bin (blue), (b) - (d) cross section of the gas temperature field after 1s, 2s, and 3s.

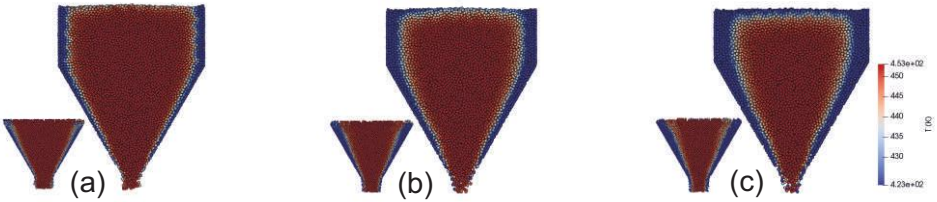
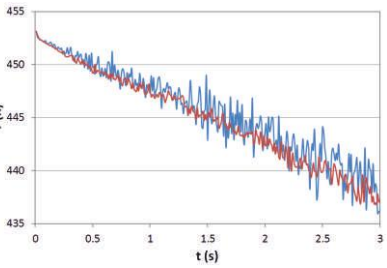


Fig.2: Cross section of the particle bed colored according to their temperature after 1s (a), 2s (b), and 3s (c), with the subdomain of the original-sized particles on the left and the coarse-grained particles on the right.

Fig.3 Average temperature of the original-sized (red) and coarse-grained (blue) particles at the outlet.



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MESO | CHUTE FLOW SIMULATION OF POLYDISPERSE PARTICLES

Particles are present in many industrial processes such as gasification, coating, and powder metallurgy. Discrete element method (DEM) is a powerful tool to simulate the particles. This method calculates the location, velocity and contact forces of individual particles in a Lagrangian field. Due to this lagrangian nature, the computational cost increases as particle number increases and this is a main challenge for simulating particles on industrial scale. Coarse graining (CG) is a method that can reduce the computational cost by far. In this method, small particles are modeled by larger particles in a way that mass and energy remain conserved. However, some size-dependent parameters such as packing density and frictional forces do not match exactly with the fine grain (original) system.

Our research is divided into two main part: first, the numerical results of fine-grained and coarse-grained model for a polydispersed system with 1mm and 5mm particles was investigated to find model parameters that produce consistent results. Second, a set of experimental tests were carried out in an inclined chute to validate the numerical results.

Velocity, mass flow rate, volume fraction and the height of particles, are the parameters that used for the comparison. As an example, the velocity magnitude at a section of inclined chute is shown in fig (1) for different cases. A good agreement can be seen between tuned fine grain and coarse grained velocity. Volume fraction values (fig (2)) show a same trend.

In the chute experiments, smaller particles tend to go near wall and lower regions fig(3.a). To show this segregation pattern, the volume fraction of larger (5mm) particles divided by the total volume fraction of particles is shown in fig (3). CG particles (2×1mm) cannot penetrate the gap between larger particles (5mm) as much as original fine grain particles (1mm). This results to a different segregation pattern (fig(3.c)). To solve this problem another parameter is used to let CG particles overlap large particles during collisions. By using this overlap factor (β) fig(3.d), the segregation pattern is more similar to fine grain results.

α: Coarse graining factor
β: Overlap factor
Fr: Sliding friction factor

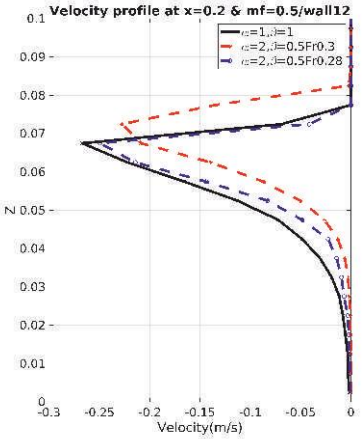


Fig.1: Velocity profile for fine grain, coarse grain and tuned coarse grain model.

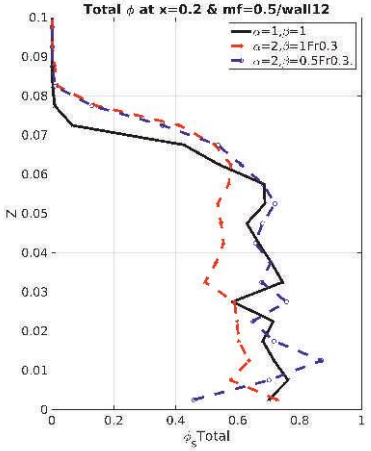
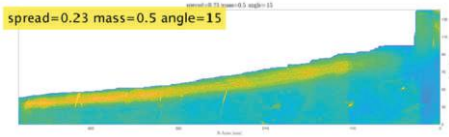
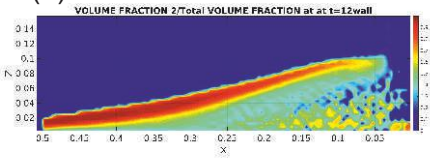


Fig.2: Volume fraction for fine grain, coarse grain and coarse grain with overlap factor.

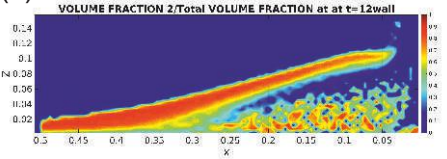
(a)



(b)



(c)



(d)

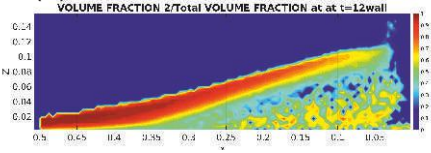


Fig.3: Volume fraction of larger particles divided by the total volume fraction. (a) experimental results. (b) fine grain model. (c) coarse grain (factor 2). (d) coarse grain (factor 2) and overlapping factor (0.5).

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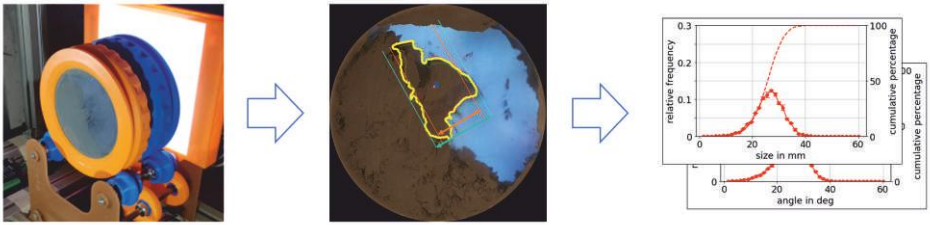
MESO | MODELING OF FINE COHESIVE POWDERS

Industrially used powders, especially metal powders for PM processes, often consist of small, irregular grains, which can cause strong cohesive forces between the individual particles. The importance of these attraction forces can even be observed in everyday life, if you think of crystal and powdered sugar with completely different flow behavior for the same material. Understanding and predicting the flow behavior, as well as the reaction to changes in environmental conditions, is challenging due to these properties.

As a first step, we developed a novel characterization technique that tries to describe the behavior of strongly cohesive powders in a more immediate way. It makes use of the avalanche-dominated flow dynamics of these particles, which can be expressed by block-like motion. Therefore, the flow of the material in a rotating drum device is analyzed for these block-structures. This method has proven to be sensitive on even small changes in the flow behavior but delivers robust and reliable data.



(a) Rotating drum experiment (b) Block evaluation (c) Block value result

Fig.1: Block analysis based characterization process.

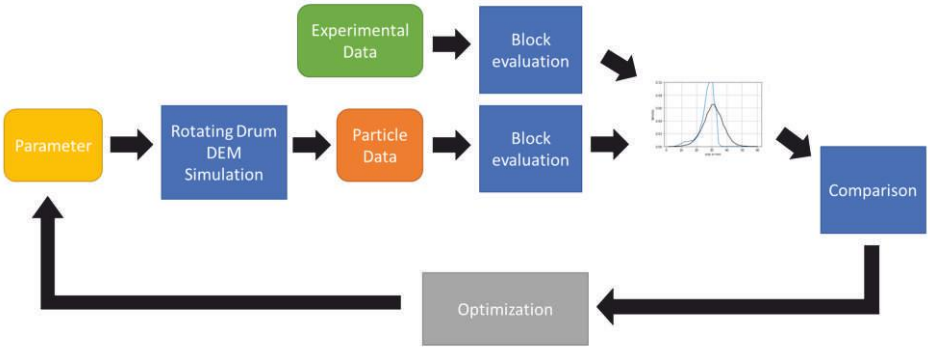


Fig.2: Optimization loop for estimating material parameters from characterisation results.

The modeling of the flow behavior for such materials can be done by the discrete element method, a simulation tool which uses distinct particles to represent the material and is therefore well suited for powders. For fine materials additional techniques are used to overcome the computational cost limitations, especially needed for industrial scale simulations. These came with the difficulty that the material parameters for the simulation particles are hard to estimate. Here, our characterization of the material comes into play, which can be used to calibrate the material parameters of the model so that it mimics the real material behavior. For this purpose, an optimization approach is used, which uses the same setup as the characterization experiment and determines the similarity based on the block evaluation.
With the gained material parameters, simulations of industrially relevant process can be carried out.

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MESO | BUBBLE MOTION DRIVEN BY A TURBULENT DOUBLE JET

Turbulent flows are prime examples for **highly dynamic multiscale systems**. While small-scale, short-lived fluctuations cause a locally erratic behavior, large-scale transport over longer durations can produce rather smooth structures. Nevertheless, detailed knowledge about the microscopic details of the flow is necessary to obtain the correct macroscopic properties. Detailed calculations attempt to resolve at least the most important scales (large-eddy simulations). This makes them very time consuming and suitable only for investigations of short duration. Long-term processes cannot be pictured in a straight-forward way.

Over the last few years, we have developed a new simulation paradigm called **recurrence CFD** (rCFD). This technique allows to time-extrapolate the dynamics of systems characterized by recurring patterns. Using time series of flow fields, the method identifies the **nearest neighbor in the previously recorded database** to the current flow state and uses the already known temporal evolution of this similar state.

The application of rCFD to turbulent flows is demanding for several reasons: (i) Even though reappearing patterns are observed on mesoscopic scales, overall recurrences are disguised by turbulent fluctuations. (ii) Memory demand is very large because of the required high spatial resolution of the database. (iii) Besides fast short-term processes, slow long-term dynamics might be present, which is beyond any feasible database duration.

In our test case of a turbulent double jet that carries bubbles into a large container, we had to address all three of the above points. Concerning (i), it turned out that the method **works even in the absence of pronounced recurrences**. It still produces a time series that has the same statistical moments as the underlying database. It also works well if the flow fields are **mapped onto a much coarser mesh** reducing memory demands (ii). The most challenging issue was connected to very slow “wobbling” oscillations of the jets superposed to their short-term fluctuations. A single time series of a few seconds could only picture the state of one jet facing somewhat more downwards while the other one faced upwards. We solved this problem by **augmenting our database with a mirrored time series** such that overall, reflection symmetry was restored. This allowed us to obtain surprisingly accurate results for the bubble distribution with speed ups in the range of 500.

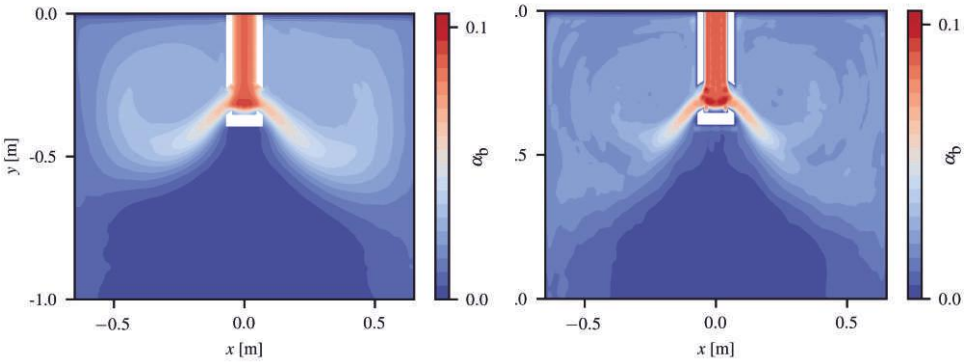

Fig.1: Bubble concentration in a turbulent double jet. LES results (left) are slightly smoother than those from rCFD (right), but the spatial distributions show strong similarities. Results have been averaged over 20 sec.

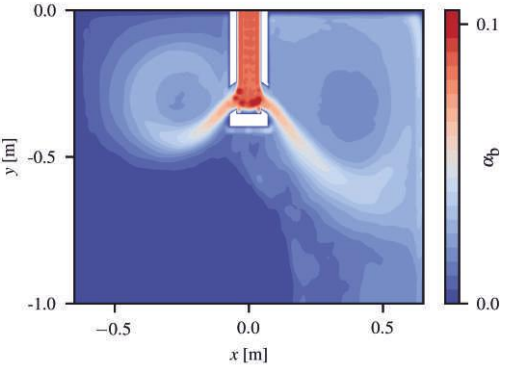

Fig.2: rCFD calculations without symmetry-based data augmentation. The jets point in different directions leading to enhanced downward bubble transport on the right-hand side.

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MESO | INFLOW CONTROL WITH rCFD FOR FLUIDIZED BED

In this project, which is a collaboration with the Hamburg University of Technology (TUHH), we seek to create a framework for inflow control in fluidized bed spray granulation. Recurrence CFD (rCFD) will be used to predict a realistic evolution of the system using real-time measurements, and to guide the control actuation. There are two main challenges. Firstly, recurrent simulations need to be accurate for the polydisperse case because segregation due to different particle size is a key phenomenon in spray granulation. Secondly, the overall time spent for data acquisition, for the recurrence simulations, and for the actuation, needs to be low enough so that the control is effective.

Recurrence CFD based on cell-to-cell operations (Figure 1) will be used to predict particle distributions. The main steps of rCFD are 1) the creation of a dataset, 2) the identification of recurrent processes, and 3) the evolution of the particle phase. In velocity-based rCFD, step 3) is performed using a representation of the particle velocity, which is straightforward but requires standard particle tracking. In the cell-to-cell framework, an index map is used instead, resulting in lower computational cost for the recurrence simulation.

The control actuation will modify the air velocity in different regions of the bed inflow. A preliminary set of simulations will be carried out to describe the impact of non-uniform inflow conditions. The results of a small test case with arbitrary domain size and particle properties are illustrated here. Three different inflow conditions are considered, with the same total flow rate. Figures 2 and 3 show the mean flow in the direction parallel to the inlet and the mean void fraction, respectively. To quantify how the inflow affects mixing, we compute the average probability for a particle to move from one half of the chamber to the other half for a short time scale (Figure 4), denoted by P. Due to the stronger crossflow that appears in Figure 2, P is significantly higher for the two cases with non-uniform inflow, showing how variation of the inflow velocity distribution can affect the particle dynamics.

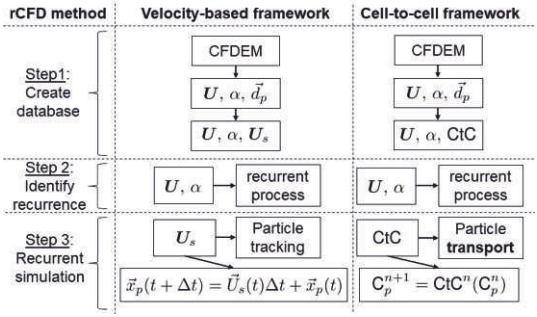

Fig.1: (on the left): Main steps in rCFD in the field-based and cell-to-cell frameworks.

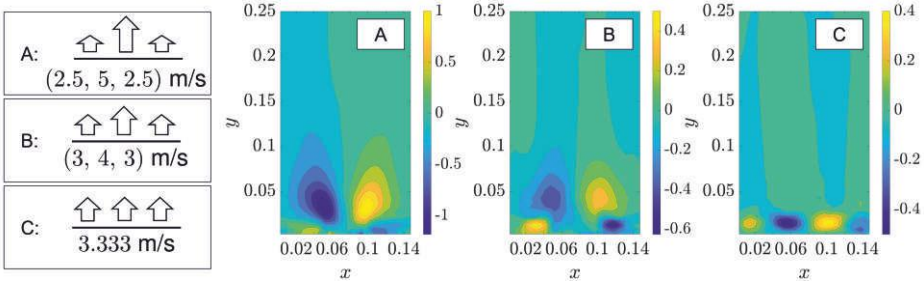

Fig.2: Horizontal mean velocity component for inlet configurations A, B, and C.

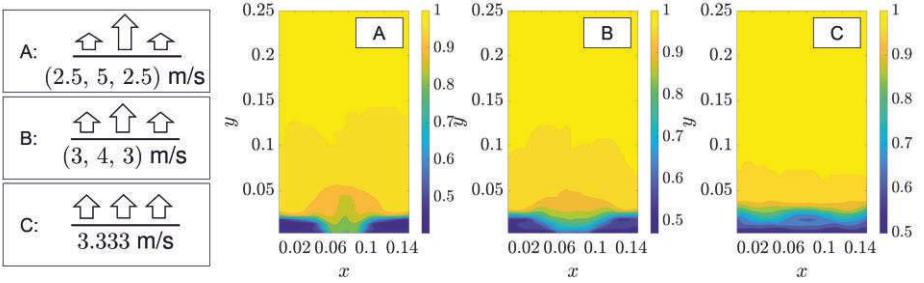

Fig.3: Mean void fraction for inlet configurations A, B, and C.

Fig.4: (on the right): Probability of migrating from the left to the right half of the chamber (or vice versa) for the three inlet configurations.

Case	P
A	*0.5*
B	*0.42*
C	*0.24*

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MESO | EXTENSIONS TO rCFD

Industrial scale processes are still a challenging task to simulate. Potentially millions of particles and hours of processing time require specialized methods to enable us a proper digital reproduction.

Transport based recurrence CFD (rCFD) time extrapolates fields of short runs given by established methods like discrete element method (DEM). This extrapolation method enables a possible speed up by up to 4 order of magnitudes in comparison to DEM for the calculation of passive transport processes.

However, rCFD still suffers from several limitations.
rCFD causes some numerical diffusion. It depends on the actual process if some physical diffusion occurs. While adding some additional diffusion to the simulation is straight-forward, some considerations are required for processes with less physical diffusion than numerical diffusion. Novel methods for different cases alleviate rCFD from this limitation (Fig. 1).

Secondly, in my studies I came across some issues, when some exchange of field values between different phases occurs. In Fig 2. one recognizes the thermal transfer coefficient of a solid and a liquid phase. This thermal transfer coefficient depends on various parameters, especially of the liquid phase. A combination of precalculated parameters with parameters calculated directly within the rCFD framework enables proper simulation of thermal heat transfer, which is mandatory for many applications.

Up to now, the complete rCFD database must be loaded from a file to main memory in the very beginning of the algorithm. Some adaptions allow to reduce the loading time by several order of magnitudes, which means the loading time is negligible in comparison to solving the transport equation (Fig. 3). This allows to fetch each single frame, just when it is required. The so called just in time frame fetching adaptions allow for much larger databases, which was one of the main limitation of rCFD.

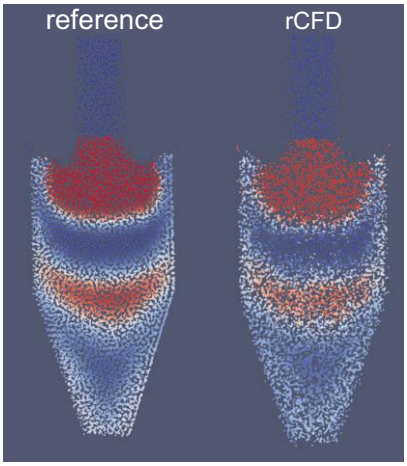


Fig.1: Adaptive Diffusion DEM reference vs rCFD.

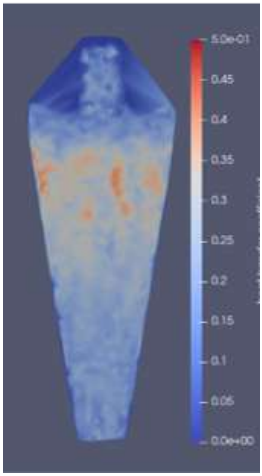


Fig.2: Thermal heat transfer coefficient in a counter flow hopper example case. Heat transfer depends i. e. on the density but also other properties.

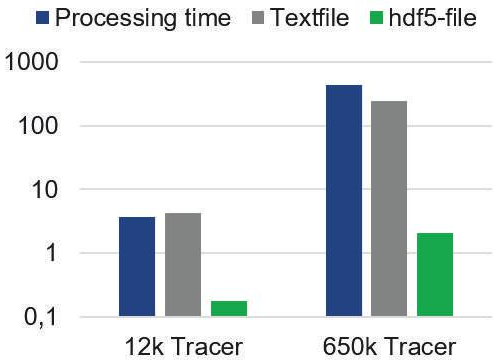
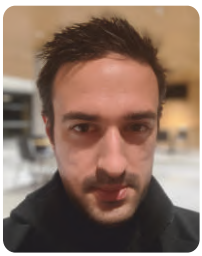


Fig.3: Time in ms for processing and loading one rCFD frame.



David Haider | david.haider@k1-met.com

EDITORIAL | MACRO

Dear Readers,

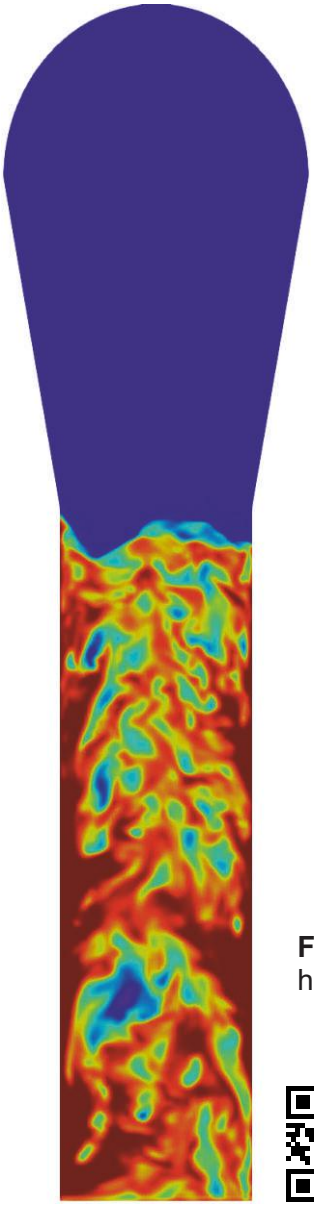
Within the last year we have welcomed two new PhD students, Varun Dongre from India and Behrad Esgandari from Iran, which attend the European training network TUSAIL, where six European academic partners and nine industrial partners are involved. While Varun will further develop the rCFD method with special application to spout beds (Fig.1), Behrad will develop a DEM magnification lens method for large-scale two-fluid model simulations of gas-particle flows. The latter is particularly interesting for regions exhibiting strong gradients, such as spouts (Fig.1).

Furthermore, we made a big steps towards feasible, cheap and reliable industrial scale simulations. For example, we tested our OpenFoam solver for large-scale multiphase flows, `twoPhaseEulerTurbFoam`, in the case of an industrial-scale gas-phase polyproylen reactor (Fig. 2 & 3), which has a height of 28 meters and a diameter of about 5 meters. Results show good agreement with reference data even though we solely used 232,000 to 1,260,000 cells, which is more than a factor 1000 less than required by standard methods. Additionally, we are working on the reactive rCFD simulation of this reactor extrapolating its operation to several hours. First results look quite promising.

Finally, I want to thank my team members for their encouragement and their excellent work, which has been honoured by high impact publications in Chemical Engineering Science, Physical Review Fluids and the International Journal of Multiphase Flow.

Sincerely,

Simon Schneiderbauer | simon.schneiderbauer@jku.at



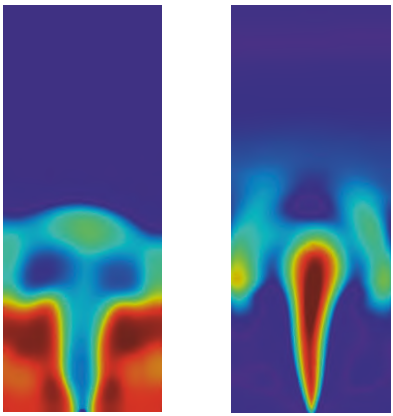


Fig.1: Two-fluid model simulation of a spout bed; left: particle volume fraction; right: particle velocity.

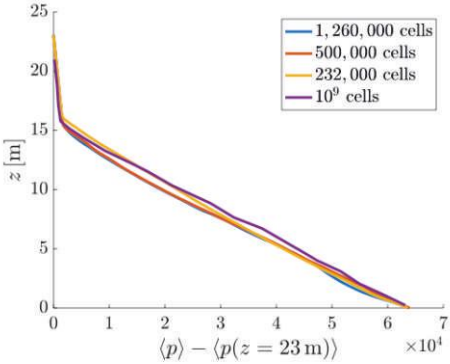


Fig.2: Time averaged pressure as a function of height for different grid resolutions.

Fig.3: Snapshot of the particle volume fraction for a gas-phase polypropylene reactor with a height of 28 meters. A corresponding animation of the simulation can be accessed by using the QR-code.

MACRO | HEAT TRANSFER PREDICTION IN INDUSTRIAL SCALE GAS-PARTICLE REACTORS

Gas-particle reactors are used in a variety of processes and operated under various conditions. Simulations play a crucial part in the design and optimization of these reactors, however, fully resolved simulations of large-scale reactors, whose elongations are several orders of magnitude larger than the single particle diameters is still unfeasible due to computational limitations. Therefore, coarse computational grids need to be employed. These coarse grids do not resolve meso-scale flow properties, such as particles clusters, bubbles or streamers, which have a large influence on the macro-scale flow properties. In order to be able to model these unresolved contributions in coarse-grid simulations, we developed the Spatially-Averaged Two-Fluid Model approach (SATFM), which is a multi-phase turbulence model based on the spatial filtering of the Two-Fluid Model (TFM) balance equations.

In an a priori study, we were able to show that the correction to the heat transfer between the phases can be expressed by a drift temperature, the gas-phase temperature fluctuations seen by the particles. This year, we focused on the validation of our models for the temperature balance equations. Therefore, we considered unbounded sedimentation of Geldart type A particles and compared the predictions of simulations using our models on a coarse computational grid to the results of fine-grid TFM simulations. As can be seen in Figure 1, the evolution of the normalized temperature difference between the phases is correctly captured by the SATFM on computational grids, which are up to 32 times coarser than the fine grid. Furthermore, the dynamic approach, which incorporates the local correlations between temperature and solid volume fraction, yields results, which are grid-size independent. Finally, the instantaneous heat transfer between the phases, which is depicted in Figure 2, is correctly predicted by our models, while it is overpredicted if no corrections due to the meso-scale structures are applied to the TFM.

Finally, after the successful validation of the SATFM for heat transfer, we will focus on mass-transfer corrections as a last step to be fully able to simulate multi-phase flow reactors on the large-scale.

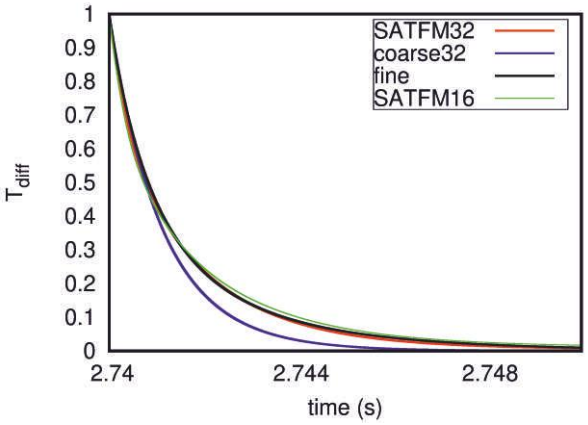


Fig.1: Temporal evolution of the domain averaged normalized temperature difference between the gas- and solid phase after setting the gas-phase temperature 500 K while keeping the solid-phase temperature at 300 K. The SATFM model prediction coincides with the fine-grid simulation data even for coarse-graining ratios of 16 and 32, while the TFM coarse-grid simulation overestimates the decline in temperature difference.

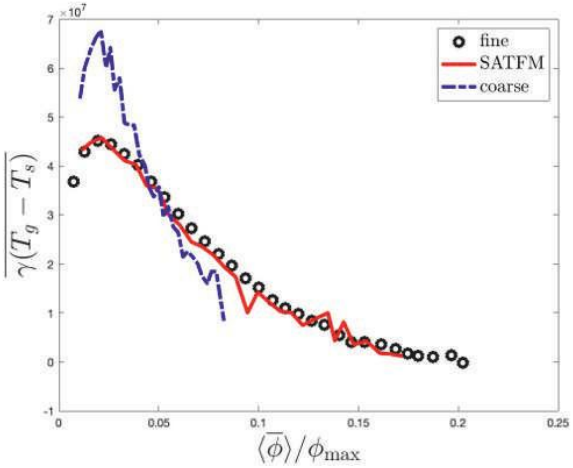


Fig.2: Instantaneous heat transfer predictions.

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MACRO | NUMERICAL SIMULATION OF LARGE-SCALE GAS-PARTICLE REACTORS

Fluidized bed and moving bed reactors are one of the most important technologies in several branches of process industry (steel making, polymer production, carbon capture, fluid catalytic cracking (FCC), biomass reactors). Especially, it is known since decades that iron can be reduced rapidly and efficiently from iron carrier materials using such devices.

However, due to computational limitations a highly resolved simulation of industrial scale reactors is still unfeasible. It is, therefore, common to use coarse grids to reduce the demand on computational resources, which inevitably neglects small (unresolved) scales. These usually are of the form of clusters, streamers and bubbles.

Furthermore, in the case of small particles (especially Geldart C type particles) the formation of agglomerates makes the situation even more complex. For the numerical analysis of the HYFOR process (**hy**drogen **f**ine **o**re **r**eduction) we augmented the Eulerian-Lagrangian MPPIC method with a simple agglomeration model and a sophisticated heterogeneous drag model. Results of cold model simulations show (figures 1 and 2) that this allows the correct estimation of the entrainment rate of fine particles from the bed. The strength of cohesion (determined by the Hamaker constant H) considerably affects the behaviour of the fluidized bed and its expansion.

Finally, we were able to efficiently simulate the hydrodynamics of an industrial-scale gas-phase polypropylene reactor (figure 3) with a height of 28 meters by using our **`twoPhaseEulerTurbFoam`** solver, which assembles our developments on coarse grid simulations of gas-particle flows from the last ten years.

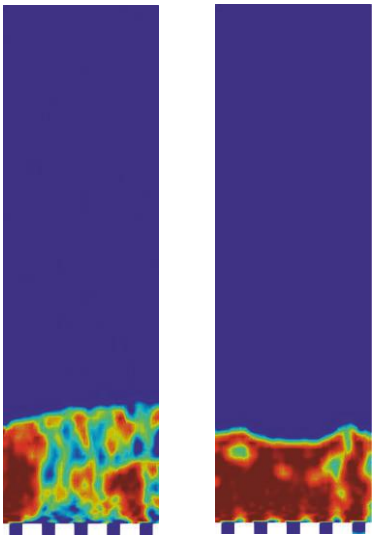

Fig.1: MPPIC simulation including sub-grid drag model for the HYFOR process using different strengths of cohesion; left: low cohesion; right: high cohesion.

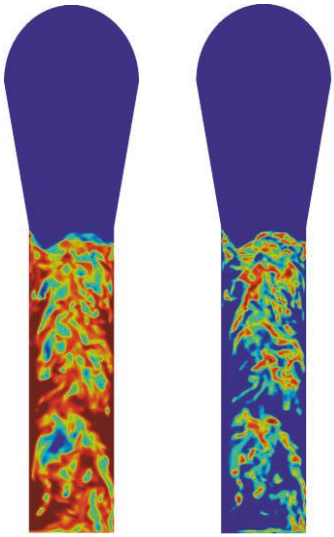

Fig.3: Snapshot of the particle volume fraction (left) and its unresolved heterogeneities (right) for a gas-phase polypropylene reactor with a height of 28 meters.

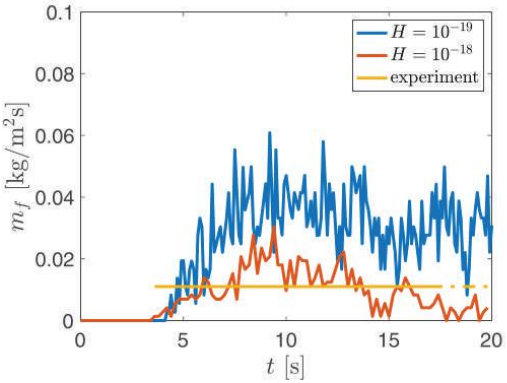

Fig.2: Entrainment rate extracted from MPPIC simulations including sub-grid drag model for the HYFOR process using different strengths of cohesion.

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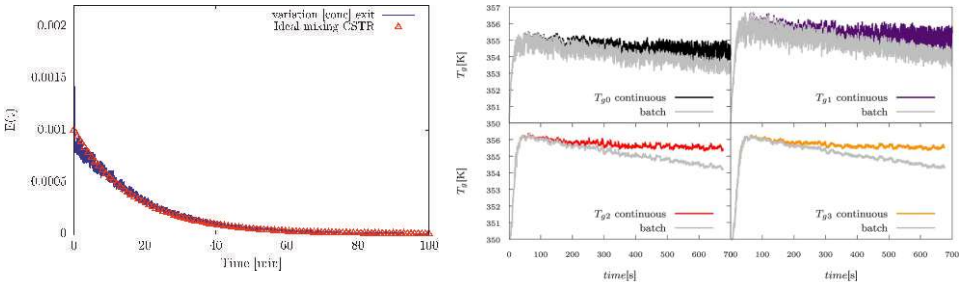
MACRO | TOWARDS A FAST FLUIDIZED BED SIMULATION USING RECURRENCE CFD

Since recurrence CFD (rCFD) is a fast modeling tool that simulates **(efficiently)** slow processes in pseudo-periodic plant-size systems, it can be used as an *a priori* control for the continuous operation plant in order to enhance the quality of product. In this scope, we first employed the transport-based rCFD model to predict the polymerization process in a batch mode industrial-scale Olefin polymerization fluidized bed reactor [1]. Recently, rCFD algorithm is applied on the reactive plant with a continuous solid feed of polymer powder (red source) and solid withdrawing (blue sink) as depicted in Fig.2(b). The reaction starts heating up the system until reaching a thermal equilibrium state after 50s. In the batch mode, the reaction is decreased after 200s, cooling down the reactor towards the inlet gas temperature. While in the continuous mode the thermal balance is maintained because of the incoming feed of solid, as demonstrated in our rCFD results Figs.1(b) , 2(c) and 2(d).

On the other hand, rCFD modeling is applied to predict the residence time distribution (RTD) that is usually compared with the time necessary to complete the reaction. Or how long a pulse solid injection (a red source step) stays in the reactor until it diminishes at the outlet response (blue sink). Our RTD function (Fig.1(a)) fits very well with the ideal mixing state of a continuously stirred tank reactor (CSTR).

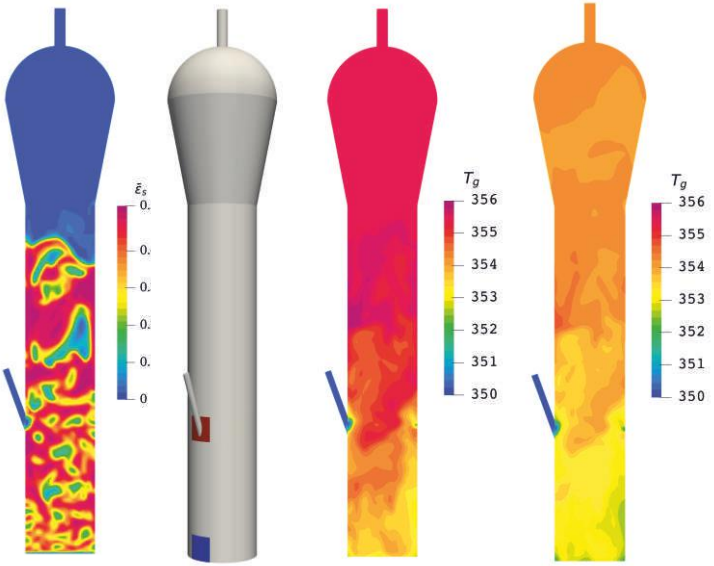
Future tasks will tackle the global assessment of rCFD modeling in the real-scale plant available in Borealis company.

[1] F. Dabbagh, S. Pirker & S. Schneiderbauer, AIChE, 67:e17161 (2021).



(a) (b)

Fig.1: (a) RTD function computed using rCFD in comparison with an ideal mixer. (b) rCFD evolution temperature at different probs in reactor.



(a) (b) (c) (d)

Fig.2: (a) an instantaneous field (t = 6s) of the solid volume fraction outcomes using cgTFM. (b) schematic graph rendering the continuous feed (red) and withdrawing (blue) of solid. (c) and (d) show rCFD gas thermal contours at (t = 700s) in continuous (c) and batch (d) modes.

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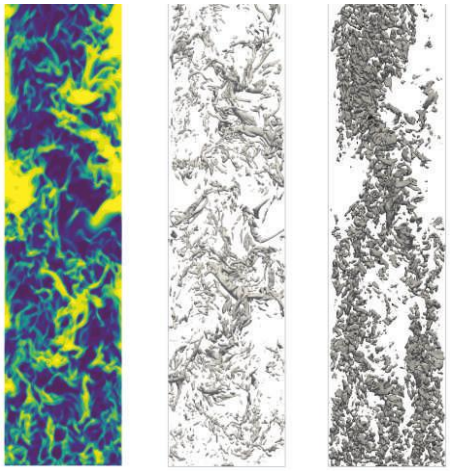
MACRO | SMALL-SCALE FLOW TOPOLOGIES IN TURBULENT FLUIDIZATION

Small-scale topologies are the spirit of turbulence physics. Studying their qualitative aspects, which are invariants in some sense, can improve our understanding of turbulence and help us to develop better modeling. All turbulent perspectives get highly complicated when merging into multiphase flows. For instance, when a turbulent flow pulls small inertia particles in a particle-laden turbulence, the particles at low mass loading drain kinetic energy from the carrier fluid and produce a kind of relaminarization. Whereas, at significantly large mass loading, the particles get self-organized into dense clusters triggering a drag production and momentum feedback on the carrier-fluid and enhance its turbulent kinetic energy **[cluster-induced turbulence (CIT)]**.

Recently and as pioneering work, we have studied the small-scale structures of moderately dense turbulent fluidization using a highly-resolved Two-Fluid model simulations [1]. As a main feature, the invariants of traceless and phase-weighted velocity gradient tensors are computed on gas and solid phases (Fig.1). Plotting the joint probability density functions (JPDF) of Q and R invariants (Fig.2), the small-scale topologies indicate a dominate tube-like vortical structures (clusters) and sheet-like strain slots on the solid phase. The gas phase, nonetheless, reveals a strong tendency to the boundary-layer turbulence with a balanced stretching and contracting enstrophy. Because of this nature, the **CIT** and the subgrid-scale (SGS) drift velocity models which are linearly associated with the solids gradient fail in this kind of fluidization. While, the tensorial nonlinear models arises to be more valid (Fig.3) and lead us to derive a new SGS drift velocity closure based on regularized gas phase rate-of-strain tensor and solids gradient. This research has especially explored new frontiers for better SGS drag models.

*[1] F. Dabbagh & S. Schneiderbauer, Phy. Review Fluids, **6**,074301 (2021).*



(a) (b) (c)

Fig.1: Instantaneous solid phase (a) and high-Q isosurfaces on solid (b) and gas (c).

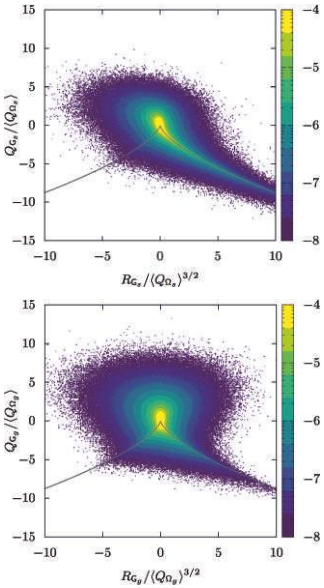


Fig.2: JPDF plots of Q-R invariants on solid (up) and gas (bottom).

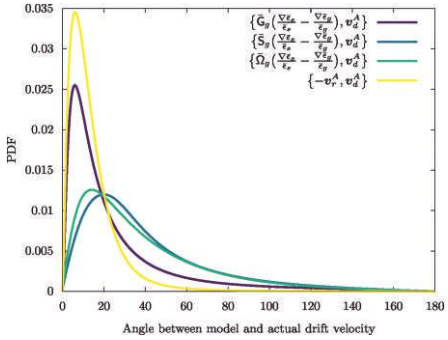


Fig.2: PDF alignments between the actual drift velocity and its nonlinear models.

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MACRO | DEFLAGRATION

Deflagration describes the very fast and typically uncontrolled as well as undesired combustion of dust particles levitated in gas flows. Consequently, any deflagration event is closely coupled to the characteristics of the fluid-dynamical behaviour of dust particles. Deflagration is particularly important for the safety of different industrial processes including fine dusts.

With joint efforts of theoretical, numerical and experimental investigations (page xx), we thoroughly study deflagration events of organic dusts. . However, we have to accept that we at PFM are missing an essential perspective. In this case we don't have the capacities to perform real post-ignition experiments. Thus, we joined forces with Christoph Spijker from the Montan University Leoben for this project.

From an experimental perspective, we want to see the real-world particle distribution inside a visibly accessible chamber (modified Hartmann tube; figure 2). The subsequent particle combustion triggered by an electric spark will be recorded by high speed cameras. Appropriate postprocessing will yield the flame propagation and the form of the flame. Additionally, sensitive measuring devices will be developed to get an accurately determine the temperature distribution.

From theoretical considerations, we can deduce essential model requirements from these real-world observations.

Finally, from a practical perspective, we should try to tackle these phenomena by an efficient and robust numerical simulation environment. Here, we learnt a lot from our developments in the realm of recurrence CFD. We can combine (coarse-grained) Lagrangian predictions with an (imperfect) Eulerian interpolation, only to correct the results by a physics-based balancing correction. Figure 1 shows first results of deflagration modelling in a vertical channel.

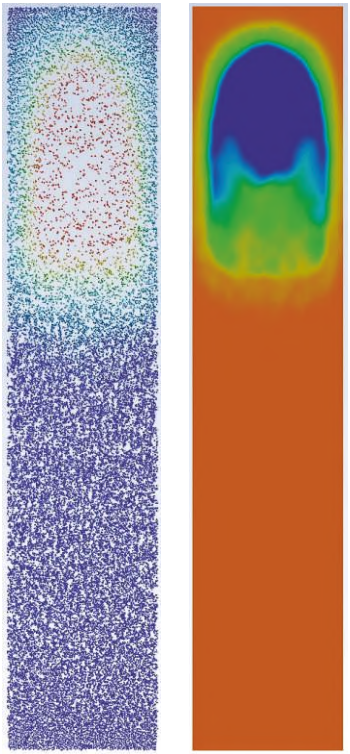

Fig. 1: Particle temperature (blue: 300 K; red: 2000 K) and oxygen concentration (red: 20 %) for a deflagration event of maze starch particles-gas mixture in a vertical channel.

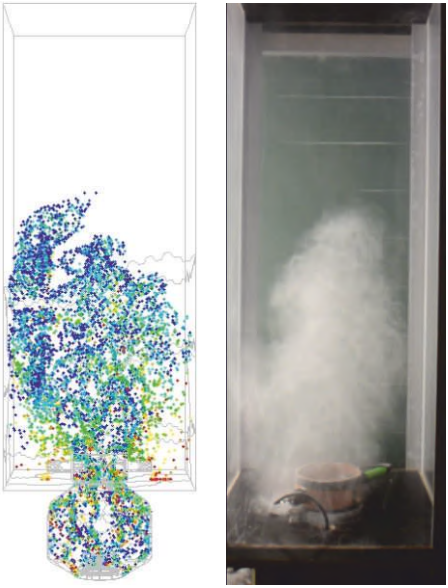

Fig. 2: Simulation of particle entrainment in modified Hartmann tube.

Stefan Puttinger | Simon Schneiderbauer | Stefan Pirker | Christoph Spijker




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MACRO | COVID SPREADING

The potential risk of aerosol-based Covid spreading depends on both – human behavior and ambient flow.

Within a research project organized by Bert Blocken from TU/Eindhoven, we try to address potential Covid spreading modes by combining pedestrian simulations (done by Roland Gaertes from Utrecht Univ.) with three-dimensional flow simulations of air-born aerosols.

As a first test case, we consider a cubic building in ambient air flow (figure 1). We assume that people have to go to this building, where they eventually line up to buy a ticket before they leave to another place. In our simulations, we furthermore consider to positions of the ticket counter with corresponding queues formed either sheltered in the wake of the building (red framed figure 2) or exposed to cross-wind (blue framed figure 2).

In the framework of CFD simulations, we model a potential Covid spreader as a moving aerosol source, while potential 'victims' act as moving sinks. Obviously, addressing such air-borne aerosol transmission by means full CFD simulations would be limited to only a small number of spreader-to-victim(s) scenarios. In contrast, using recurrence CFD enables the calculation of hundreds different scenarios, which, in turn, allows for a statistical evaluation of the Covid spreading probability.

Figure 3 depicts a first evaluation of relative spreading pattern based on 200 rCFD simulations (covering in total more than two days of real-world time). Obviously, there is significantly more risk of Covid infections in case of a sheltered queue, which can be explained by longer residence times of the aerosol in the recirculating wake. In both cases, pedestrians, who line up after the spreader are more at risk as those who line up in front of the spreader.

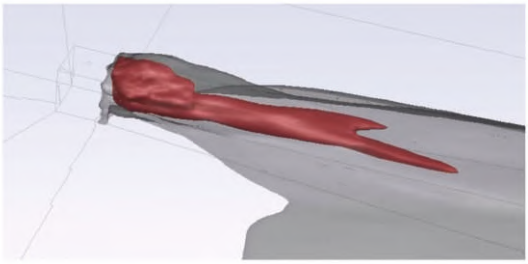

Fig.1: Aerosol accumulation in the building's wake.

Fig.2: Two queuing scenarios, in both cases air flow is from left to right.

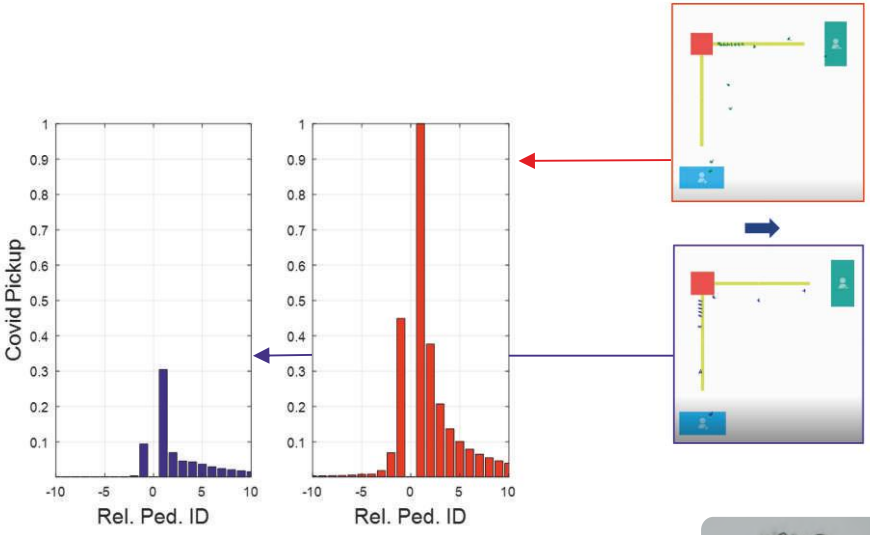

Fig.3: Average risk of aerosol-based Covid transmission from a spreader to potential victims.

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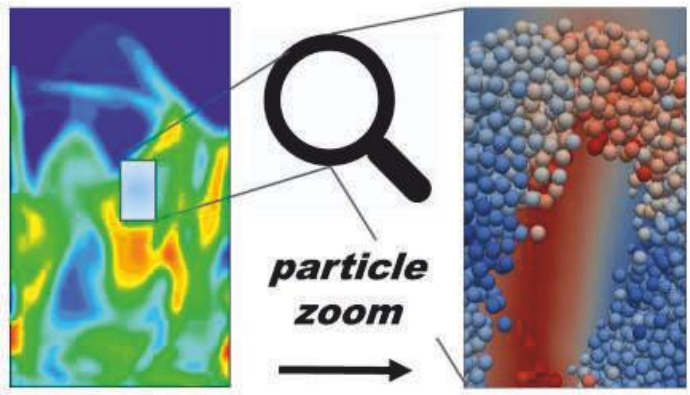
TUSAIL | TRAINING NETWORK

TUSAIL is an Innovative Training Network funded by Horizon 2020 which comprises 16 academic and industrial partners in total, led by the University of Edinburgh. TUSAIL stands for "**T**raining in **U**pscaling particle **S**ystems: **A**dvancing **I**ndustry across **L**ength-scales". Over the course of four years, TUSAIL will train 15 early-career researchers (ESR) to meet industry's requirements for highly skilled staff in the multi-disciplinary field of upscaling industrial particle processes (see https://tusail.eu/). The Particulate Flow Modeling Department currently hosts two ESRs.

ESR14 – Behrad Esgandari: Discrete particle zoom in continuum Two Fluid Model (TFM) simulations of spout fluidized beds

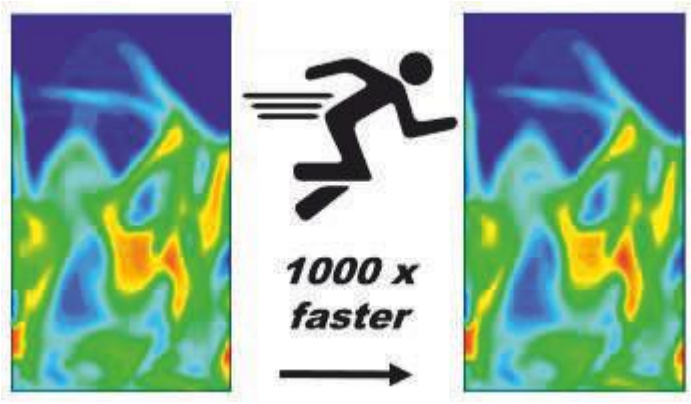
Both, the continuous two-fluid model (TFM) approach, and the discrete element method (CFD-DEM) approach, have been widely applied for simulation of gas–solid systems. In this project we will establish a coupling methodology between a TFM simulation and an embedded discrete particle simulation, which can be placed as a magnification lense into an arbitrary sub-region of the computational domain. ESR14 also has secondments with DCS computing and BASF.



ESR14: Discrete particle magnification lens for a continuum multiphase simulation.

ESR15 – Varun Dongre: Time-Extrapolation of continuum Two Fluid Model (TFM) simulations on spout fluidized beds

The main aim will be to make the simulations run as faster as possible to reduce time dependency. The recurrence CFD (rCFD) method will replace convection with cell-to-cell shifts and conduction by face swaps. Two-Fluid Model (TFM) simulations will be carried out in Ansys Fluent for a fluidized bed in order to generate a database for rCFD. Finally, we aim to explore a potential coupling between real-time rCFD and flow-sheet models. The project will be carried out at JKU|PFM for 24 months and Hamburg University of Technology (TUHH) for 12 months. ESR15 also has secondments with Procter & Gamble.



ESR 15: Solid mixing in a fluidized bed, the (right) data-based rCFD simulation is more than 1000 times faster than the (left) derivation based TFM simulation.

Behrad Esgandari | Varun Dongre

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EDITORIAL IV
EXPERIMENTS & DATA ANALYSIS

Dear Readers,

after a very calm year in the laboratory in 2020 because of the boundary conditions the Covid-19 pandemic imposed, we were ramping up our experimental activities again in 2021. In fact, the discussion about future research projects for the new proposal for the K1Met competence center resulted in many new ideas for validation experiments and data based processing strategies.

PFM now also tackles topics that have long been avoided but need to be addressed to better understand certain classes of real life problems. First, PFM has left the save world of inert fluid mechanics and started a cooperation with Hörbiger AG to investigate dust deflagration. Last year we started deflagration experiments together with Montanuniversität Leoben (**Fig.1**). Second, we reactivated our fluidized bed test rigs and made several test series with non-spherical particles, since fiber-shaped materials like the straw particles shown in **Fig.2** are still challenging to find proper material parameters for DEM simulations.

We also started a cooperation with LCM (Linz center of mechatronics) to build a showcase test rig for rCFD applications in the process industry. In the near future this test rig shall be used at trade fairs and exhibitions as a hands-on experiment so that people can experience the capabilities of rCFD.

Sincerely,

Stefan Puttinger | stefan.puttinger@jku.at

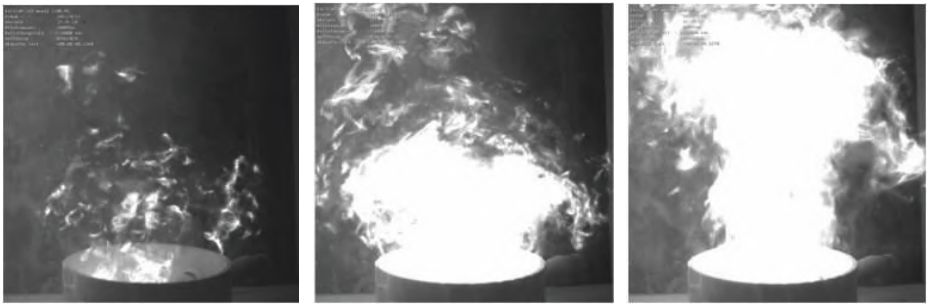

Fig.1: Dust explosion of corn starch initiated by electric arc discharge.

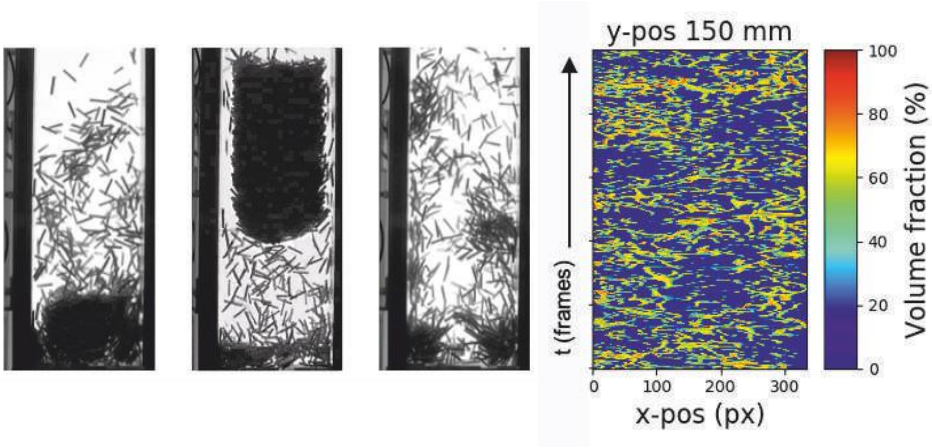

Fig.2: Fluidized bed experiments with 25mm straw fibers. The straw material shows an unpredictable shift between a riser mode and the formation of blocks that can hover at any position in the bed. However, it is still possible to extract relative volume concentrations as depicted on the right. This data can be used for CFD validation as explained on one of the following pages.

EXPERIMENTS & DATA ANALYSIS
DUST DEFLAGRATION

Dust explosions are a severe security risk during transport and handling of fine powders. Such deflagration events are not restricted to organic materials but can also happen in metallic powders.

To support numerical modelling activities we have set up a test rig that is run in cooperation with the Institute of Thermal Processing Technology (TPT) at the Montanuniversität Leoben (MUL). A first series of high-speed recordings delivered promising results. We are able to capture the initial particle cloud as well as the flame expansion accurately. Hence, we can calculate the particle velocities and the flame front velocities from the images.

The more difficult parts will be to (i) extract an estimated volume concentration in the dust cloud, and (ii) have a reliable temperature measurement in the flame front. These values are important factors for the validation of numerical models. CFD simulations have shown that the ignition phase is not easy to predict and it is currently not clear if the initial flame propagation is dominated by convective or radiative heat transfer.

Since it is the first time that PFM is involved in experimental activities including exothermic reactions we are still climbing the learning curve and iteratively improving the experimental setup and post-processing procedures. However, based on the very good results of the first test series we agreed with Hörbiger AG and MUL/TPT to prolongated our cooperation for four more years. The major goal of the upcoming project period is to answer the question how metallic powders behave in comparison with organic materials.

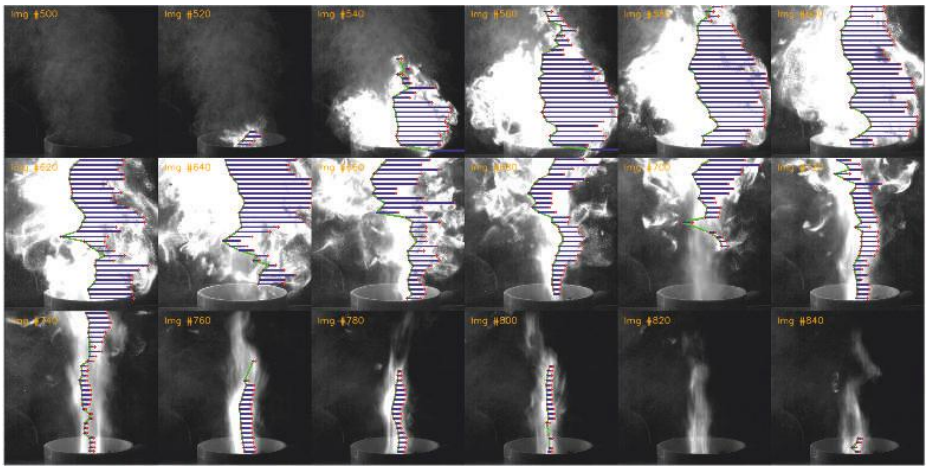

Fig.1: Image series of a dust deflagration experiment. To extract the geometry of the flame it is sliced into a sequence of equally spaced layers and for each of these layers the center location and extension of the flame is calculated.

Fig.2: Color snapshot of a corn starch dust explosion. The dust cloud is ignited by electric arc discharge from the electrodes at the bottom of the test rig.

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EXPERIMENTS & DATA ANALYSIS

VORTEX FORMATION AND ENTRAINMENT EFFECTS

The entrainment of non-metallic inclusions is of high interest in secondary metallurgy. Since such inclusions can lead to material defects in the final product any kind of inclusion should be avoided.

In the 1:1 water model of the tundish at voestalpine we observed vortices in the proximity of the stopper rod (**Fig.1**). These vortices only occur if a globally circulating flow around the rod is present. Plastic particles were used as tracer particles to calculate the vector field at the surface. In literature various vortex identification methods are proposed since the vorticity of the flow field does not provide reliable results to identify vortices in vector fields. The results shown in Fig.1 are based on the so-called λ_{ci} criterion which is a suitable approach for this kind of problems.

Figure 2 shows a comparison of a simplified benchmark experiment for a water/air and a water/oil system. The experiment is based on the forced vortex formation in a cylindrical tank with tangential inlet. It clearly shows that the deformation of the interface and the entrainment of droplets occur much earlier for the liquid-liquid problem compared to the liquid-air case. The physical explanation for this behaviour is the fact, that in the latter case the dominating material parameter is the surface tension of water while for liquid-liquid systems it is the interfacial tension between the two liquids. This an important factor when trying to scale such experimental findings to the real case of liquid steel and slag via non-dimensional numbers and correlations. The surface tension of liquids can usually be found in literature, however, the interfacial tension between pairings of different liquids need to be measured for every system. Recently, we built a pendant drop experiment for that purpose and are now working on an analytic description of droplet entrainment in liquid-liquid systems that allows to better understand the scaling of lab-scale water experiments to real steel/slag systems.

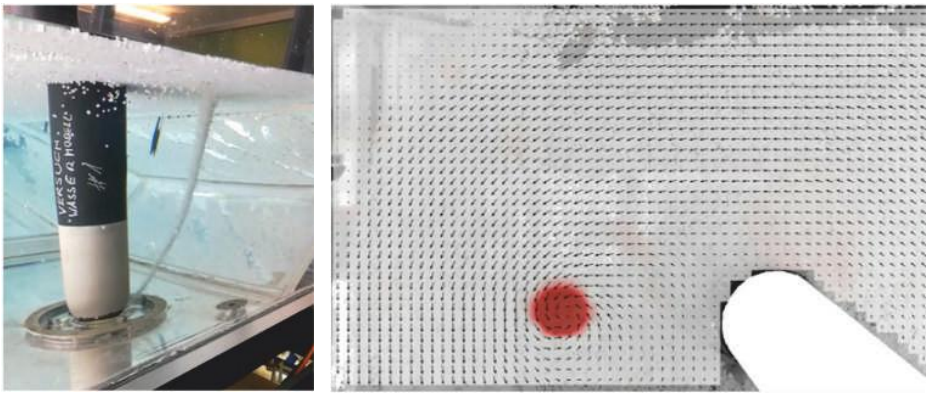

Fig.1: Vortex formation close to the stopper-rod in a 1:1 water model of a steel tundish. Plastic particles serve to visualize the flow and calculate the flow field around the stopper rod. The colormap overlay serves to indicate vortex dominated regions (in this case based on the λ_{ci} criterion).

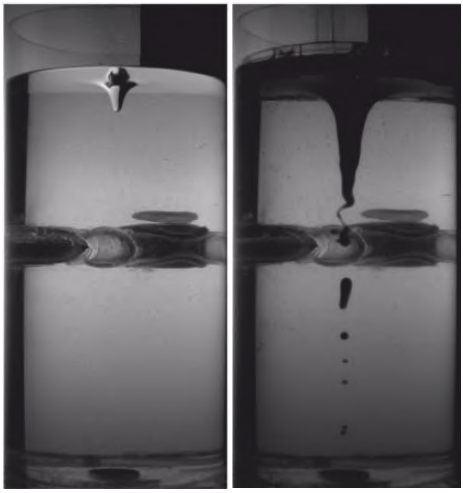

Fig.2: Vortex formation in a cylindrical tank with tangential flow inlet for water/air (left) and water/oil (right). The outlet is at the bottom of the tank. The two images are snapshots taken at the same circular flow rate of 0.06 l/s. This comparison makes clear that the entrainment of droplets occurs much earlier in liquid/liquid systems than for liquid/air systems.

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EXPERIMENTS & DATA ANALYSIS | NON-SPHERICAL PARTICLES IN FLUIDIZED BEDS

Most real life particles are not spherical, and thus, calibration parameters need to be found for DEM simulations using multi-sphere or super-quadric based particle models.

For this purpose we have redesigned and reactivated our fluidized bed test rig. Since rapid prototyping via 3D printing now allows to quickly adapt an experimental setup, the redesign of the test rig followed the strategy to have a modular setup for fast and easy change of the distributor plate.

Based on the new test rig we ran several test series with wheat grain and straw fibers. The gained data was used for the parameter calibration in DEM simulations at DCS Computing and John Deere Inc.

Although it is not possible to extract local volume fractions in kg/m^3 from the visual information of an experiment as shown on the right page, there are still possibilities for pseudo-calibrations that can deliver data that can directly be compared to numerical results. Since we know the gray-level value of the bed in rest (maximum volume concentration) and the freeboard above the bed (0% volume concentration) we assume a simplified linear relation of the volume fraction between these two values. Doing so we can calculate a relative particle concentration. If the numerical results are run through the same processing steps we obtain a fair comparison of experimental and numerical results.

Such pseudo-quantitative validation strategies once again proved to be a useful approach in this project. PFM currently supports John Deere Inc. to build its own validation test rig for the calibration of DEM parameters.

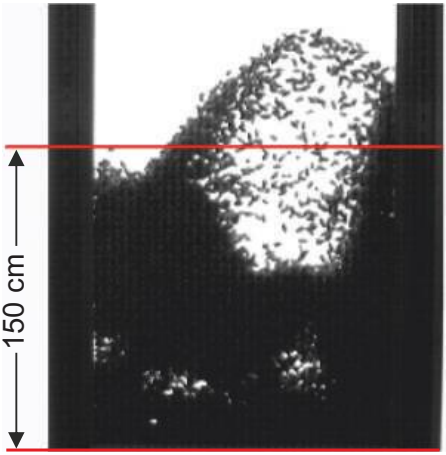


Fig.1:

Example of a fluidized bed experiment with non-spherical particles (wheat grain). The images were obtained in rectangular test rig with LED background illumination (**Fig.1**). A gray-level calibration can deliver time-resolved volume fractions (**Fig.2**) at certain positions in the bed (e.g. the red line in Fig.1), or averaged volume fractions across the bed (**Fig.3**). A Fourier transform of the pressure signals can capture the typical bubble eruption frequency in a certain bed regime (**Fig.4**).

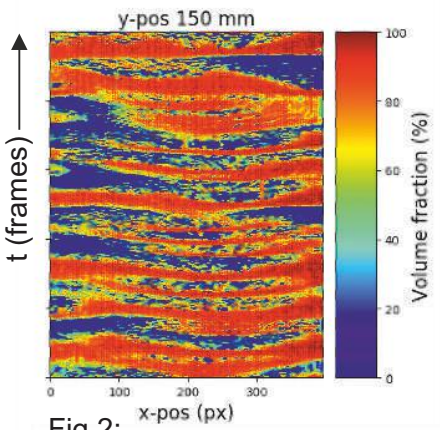


Fig.2:

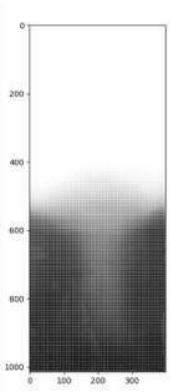
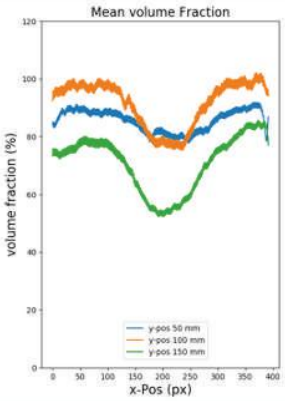


Fig.3:



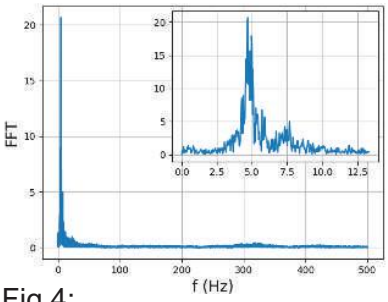


Fig.4:

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SEMINAR | TEARS OF WINE-INTRODUCTION TO MARANGONI-DRIVEN FLUID FLOWS

The Marangoni effect is a complex interfacial phenomenon that occurs due to the gradient in surface tension. A well-known example of the Marangoni effect in nature is the tears of wine, where a gradient in alcohol concentration induced by evaporation results in surface tension gradient and upward Marangoni flow at the glass walls which is gradually counteracted by gravity until tear-like droplets form (Figure 1). Further to this classic example, Marangoni-driven flows have many environmental and industrial applications such as casting, welding, liquid transport, and microfluidics. Therefore, we dedicated this year's seminar in fluid mechanics to this topic. Students contributed to this seminar within three groups: **analytic**, **simulation**, and **experiment**.

The **analytic** group approached this physical phenomenon by exploring the underlying concepts, governing equations, possible analytical solutions, and different physical mechanisms in tears of wine problem as well as several thermo- and solute-capillary systems.

The **simulation** group started its activities by literature review on the state-of-the-art CFD models for Marangoni flow. They focused on solute capillary systems (e.g. surfactant-laden flows), and developed a volume of fluid-based solver in OpenFOAM. They studied a buoyancy-driven bubble rising problem at clean and partially-contaminated environments.Their initial results reveal the impact of Marangoni on the rising path of the bubble as depicted in Figure 2.

The **experiment** group worked on the characterization of the Marangoni effect in a couple of lab experiments. One of their experiments is depositing alcohol-water droplets on the different oil layers. As shown in Figure 3, the water-alcohol solution reduces the local interfacial tension upon deposition and derives a spreading front until smaller droplets are being fragmented. They employed the PIV technique to measure the velocity of the spreading front at different alcohol concentrations.

These activities have deepened our understanding of such a complex phenomenon, and we hope we could stimulate further applied research on this topic in near future.

Fig.1: Schematic description of the Tears of Wine problem. Evaporation (red arrow) induces a gradient in alcohol concentration near the glass walls, Marangoni flow (yellow arrow) causes the upward motion which is gradually counteracted by gravity (green arrow).

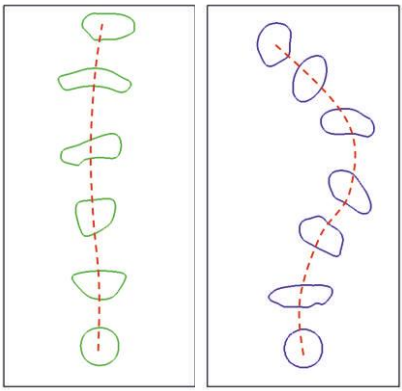

Fig. 2: The trajectories of a 10 mm air bubble rising in pure water (left) and partially-contaminated water (right). The snapshots are taken at similar steps of the two simulations. These initial results are reported by the simulation group (S.Mahmoudi, V. Dongre & M. Saeedipour)ounteracted by gravity (green arrow).

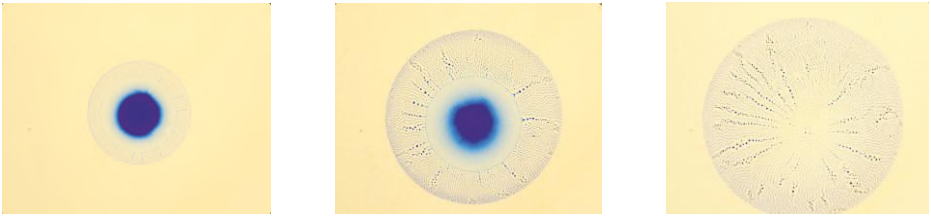

Fig. 3: Different stages of an alcohol-water droplet (45% concertation) spreading on sunflower oil layer. Snapshots display formation of a spreading front limited to a certain diameter (left) at the tip of which droplets are being expelled (middle) until the whole solution is fully fragmented (right). These snapshots are provided by the experiment group (B. Esgandari, T. Kronlachner & S.
Puttinger).

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SCIENTIFIC FRIENDS | TIM M.J. NIJSSEN, KAY A. BUIST, AND HANS A.M. KUIPERS EINDHOVEN UNIVERSITY OF TECHNOLOGY

The blast furnace is one of the most essential reactors in modern-day industry, responsible for 70% of the global crude steel production. Yet, its inner workings remain largely unknown due to the extreme conditions. In this project, we used CFD-DEM simulations to gain insight into the bottom section of this important equipment.

The vast majority of CFD-DEM studies focus on gas-solid systems. In order to include the dense and viscous liquid iron, we have extended the momentum coupling with lift, virtual mass and Basset history forces. Our study on liquid-solid fluidised beds has shown the importance and accuracy of this extended coupling.

Blast furnace hearth simulations were set up with a VOF/CFD-DEM solver, allowing us the represent the solid coke particles, the liquid iron phase, and the gas phase above it. Simulations were conducted on progressively larger scales:

First, a lab-scale set-up was used, allowing us to compare the results with a cold-flow experimental model. Next, an intermediate-scale hearth of 5 m diameter was used to study the dynamics of the floating coke bed and the flowing metal under various conditions and situations. Lastly, a large-scale, 10 m diameter hearth containing 4,000,000 particles was simulated, in which heat and mass transfer calculations were included. This has provided us with a promising outlook on the future of multiphase reactor modelling.

All our simulations were conducted with the CFDEMCoupling code from JKU. After the project, we have reviewed our developments together with the PFM staff, and merged them back into the code base. This way, the open science community can benefit from our developments. We highly recommend this process to any researchers working with open-source codes!

Tim Nijssen | Kay Buist | Hans Kuipers

This work was conducted within the M2i Partnership Programme with financial support from Tata Steel and NWO.

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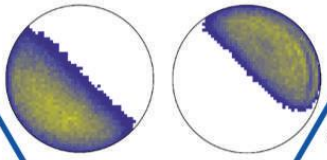
Lab-scale experiments

Experiments in a 3D cold-flow blast furnace hearth model have revealed the migration behaviour of individual coke particles with the bed This provides valuable information on the renewal mechanisms of the deadman.

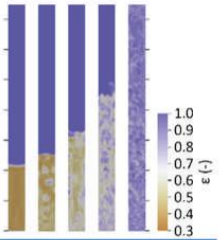
Magnetic Particle Tracking

Analysis of dry and liquid-filled rotating drum systems has shown the applicability of Magnetic Particle Tracking in liquid-solid systems, and demonstrated the importance of the interstitial medium on granular flow behaviour.



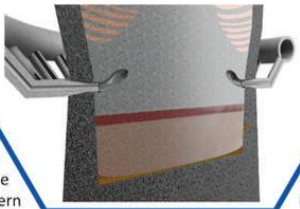
CFD-DEM Modelling

The CFD-DEM model was extended with additional force models to accurately describe the behaviour of liquid-solid systems. A verification and validation study focussed on liquid-solid fluidised beds has shown the accuracy of the extended model, as well as its impact on the bed behaviour.



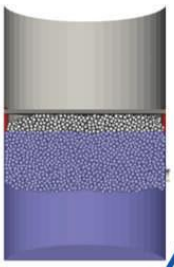
Blast furnace hearth

The hearth section of the blast furnace, where the liquid iron is tapped through the 'deadman' coke bed, is vital to the reactor longevity, but remains largely ill-understood. The dynamic behaviour of the hearth was studied with experimental and numerical methods.



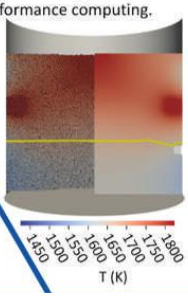
Lab-scale simulations

Lab-scale simulations were compared with experimental results. This has shown that the model accurately captures the force balance acting on the floating bed. Through simulations, the influence of the bed position on the liquid flow pattern could be visualised, which was not possible experimentally.



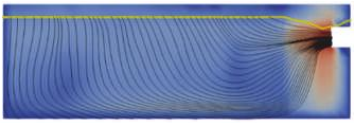
Heat, mass transfer

Heat and dissolved carbon transfer calculations were added to model. This allows for the simulation of the temperature distribution and carbon dissolution processes within the hearth. A full industrial-scale (10m) hearth simulation was used to demonstrate the potential application of such integrated models with high-performance computing.



Large-scale simulations

A series of large-scale (5m) blast furnace hearth simulations was used to investigate the dynamic deadman behaviour under different loading conditions. New insights into the deadman coke movement and liquid iron flow behaviour were obtained, and the complex interaction between them was highlighted.



CHRISTIAN DOPPLER AWARD

In the past twelve years, I had the opportunity to found and shape our new Department of Particulate Flow Modelling. Over the years, we gathered a colorful bunch of more than 40 scientific researchers. Together, we attracted more than 12 M€ of research funds, published more than 200 papers and finished 20 PhD's and three habilitations.

What a ride …

At the same time, I have been starting to feel useless, because all this happens without much of my efforts (like this annual report, I am going to read it only after press). Our PFM group completely relies on a team of high-quality, responsible, self-fueled and independently working senior researchers, who on the one hand, just follow their own interests and who, on the other hand, do see the value of in-group collaborations.

Maybe, this constellation works out so smoothly, because we represent sometimes complementary research characters, looking into different topics in different ways. For instance, while I am really keen on computational algorithms applied to (very) macroscopic flow-based processes, **Mahdi** is really focused into the physics of micro- and meso-scopic interfacial flows (see title image of this report). Mahdi shares his office with **Thomas**, who is also very much physics-based (ok, we are all like physics but maybe at different levels), looking into meso-scale particle models. More than seven years ago, Thomas inherited this topic from Christoph Kloss and Christoph Goniva, who left PFM for their spin-off company DCS Computing. Since then Thomas and **Daniel** could further develop our open-source software platforms LIGGGHTS and CFDEMcoupling (PFM versions). In the meantime, I also commit my rCFD developments to Daniel, and I am very thankful for his ever patient software reviews. Daniel's second name is quality control and he won't let anything approach his software unless it passes his quality checks. Coming back to physics, **Simon** has shown an astonishing performance over the last years. With the modelling of heterogeneous mildly dense gas-solid flows, he found a challenging topic. Gifted by his mathematical

Fig.1: Happy me that I get paid for what I like doing anyway …

abilities and an incredible persistency, Simon could significantly advance continuous two fluid models into a novel multiphase turbulence model for meso-scale heterogeneities. A recent review paper of the Chinese Academy of Science cited no less than 18 papers of Simon. Hats off! Yes, but what are all those theory guys without experimental confirmations. Actually, **Stefan** delivers more than just on-demand experimental validation of our others' models (in most times, it is actually falsification). Stefan found his way into his own research by focusing on advanced methods of digital image and signal analysis. Honestly, Stefan is an indispensable experimental backbone of our group. Finally, another backbone of highest importance is provided by **Andrea** who cares about all financial, juridical and administrative issues. She powerfully protects us researchers from troubles at real-life universities. Even more impressive, Andrea has the ability to listen between the lines – she can detect any miss-feelings among our group before they start to boil up, such that anybody can counteract, even before problems surface.

Dear Mahdi Saeedipour, Thomas Lichtenegger, Daniel Queteschiner, Simon Schneiderbauer, Stefan Puttinger and Andrea Scharinger,

Thank you for all your work !

SELECTED PUBLICATION

Balachandran Nair A., Pirker S., Saeedipour M.: Resolved CFD-DEM simulation of blood flow with a reduced-order RBC model, in: Computational Particle Mechanics, 2021.

Dabbagh F., Pirker S., Schneiderbauer S.: A fast modeling of chemical reactions in industrialscale olefin polymerization fluidized beds using recurrence CFD, in: AIChE Journal, Vol. 67(5), e17161, 2021.

Dabbagh F., Schneiderbauer S.: Small-scale flow topologies, pseudo-turbulence and impact on filtered drag models in turbulent fluidization, in: Physical Review Fluids, Vol. 6(7), 074301, 2021.

Du Y., Blocken B., Abbasi S., Pirker S.: Efficient and high-resolution simulation of pollutants dispersion in complex urban environments by island-based recurrence CFD, in: Environmental Modelling and Software, Vol. 145, 2021.

Puttinger S., Saeedipour M.: Time-resolved PIV measurements of a deflected submerged jet interacting with liquid- gas and liquid-liquid interfaces, in: Experimental and Computational Multiphase Flow, 2021.

Saeedipour M., Vincent S., Estivalezes J.: Toward a fully resolved volume of fluid simulation of the phase inversion problem, in: Acta Mechanica, 2021.

Stefanie Rauchenzauner, Simon Schneiderbauer: A dynamic multiphase turbulence model for coarse-grid simulations of fluidized gas-particle suspensions, in *Chemical Engineering Science*, Vol. 247, Elsevier, 117104, 1-2022.

Soltanbeigi B., Podlozhnyuk A., Kloss C., Pirker S., Ooi J., Papanicolopulos S.: Influence of various DEM shape representation methods on packing and shearing of granular assemblies, in: Granular Matter, Vol. 23, 2021.

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