Simulation of pollutant dispersion in urban environment (Linz, Wissensturm) on a 10M high-resolution grid; classical LES based CFD is opposed to new rCFD simulation, which are more than five thousand times faster; this work earned us an invitation to an international research consortium on the modelling of Covid aerosol dispersion.

© Y. Du & S. Pirker
Dear Readers,

‘Nobody has asked me – I don’t want this.’ At some point, my always patient secretary erupted about how corona influences her life.

On a first glance, we withstood this year’s crisis really good – with a record number of publications and a balanced budget. However, I do feel the loss of informal, between the lines communication. Somehow, individual research islands are drifting apart. While these distributed research efforts are excellent by themselves, we somehow lack a streamlined research vision. I now realize that I essentially managed my research group by chatting with colleagues during lunch and café breaks…

I really hope that these ‘we don’t want this’ times will past soon. Subsequently, we will have a chance to restart as a group based on a team of very experienced senior researchers and a portfolio of advanced models on topics like data-driven and real-time simulations, multi-phase turbulence modelling as well as interfacial and particulate flows.

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

All the best,

Stefan Pirker | stefan.pirker@jku.at
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

### MICRO
- Microfluidics and Blood flow ................................................................. 6
- Hysteretic Regime Transition in Co-Current Liquid-Gas Flows ........ 8
- Inclusion Removal – Focus on its Behavior at Steel-Slag Interface .... 10
- Two-Phase LES with Eddy Viscosity-Based Subgrid Models ......... 12
- Liquid Trickling .................................................................................. 14

### MESO
- Including Heat Transfer and Chemistry in the Multi-Level Coarse-Grain Model of the DEM ................................................................. 18
- Efficiency of Revision Method for the Simulation of Poly-Disperse Granular Materials ................................................................. 20
- Modelling of Fine Cohesive Powders .................................................. 22
- A Recurrence CFD Study on a Turbulent Jet ..................................... 24
- Heat Transfer in a Moving Particle Bed with Variable Melting Zone ................................................................. 26
- Extension of Transport Based Recurrence CFD Method to Granular Media ................................................................. 28

### MACRO
- Spatially-Averaged Two-Fluid Models for Momentum and Heat Transfer ................................................................. 32
- Chemical Reactions and Cluster Induced Turbulence ..................... 34
- Towards a Fast Fluidized Bed Simulation Using Recurrence CFD... 36
- Recurrence CFD Simulation of Pollutant Dispersion in Built Environment ................................................................. 38
- Recurrence CFD .................................................................................. 40

### EXPERIMENTS & DATA ANALYSIS
- Liquid-Liquid Interfaces ................................................................... 44
- Optical Flow VS. PIV/PTV ................................................................. 46
- Raceway Monitoring of Blast Furnaces ............................................ 48

### SEMINAR
- Aerosol Measurements ....................................................................... 50

### SELECTED PUBLICATION

---

2020 | Particulate Flow Modelling
Dear Readers,

In the past year, we further continued our research on fully-resolved description of complex multiphase flows to cover a wide range of industrial and environmental applications.

We have further expanded our research on simulation and analysis of micron-sized particles’ behavior in different environments. Within the last phase of Achuth B. Nair’s PhD, he has achieved a reasonable computational efficiency in resolved CFD-DEM simulation of blood flow with our reduced-order model for red blood cell mechanics. This allows us to simulate blood flow with hundreds of deformable red blood cells suspended in the surrounding plasma (Figure 1). Besides, Xiaomeng Zhang has started her PhD research on fully-resolved simulation of the small particles’ behavior in the vicinity of fluid-fluid interfaces (Figure 2). Her research has a direct industrial application into the inclusion removal during the continuous casting process.

Our research focus on turbulent interfacial flows has further evolved by performing fully-resolved simulations for well-known benchmarks (Figure 3) as well as a-posteriori evaluation of our functional approach based on the revisited eddy-viscosity concept. We succeeded in the implementation of new models into OpenFOAM with the promising improvement compared to standard models. As another interesting topic, the interfacial flow instability and regime transition during the co-current liquid-gas flows were also explored by numerical simulations. We pictured the transition from bubbly to annular flow with a hysteretic behavior. The findings have a direct implication on the continuous casting process.

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

Mahdi Saeedipour | mahdi.saeedipour@jku.at
Fig.1: Micro-channel with large number of red blood cell using resolved CFD-DEM technique. The algorithm is modified to allow using hundreds of RBCs for blood flow simulation at high haematocrits.

Fig.2: Buoyancy-driven upward motion of micron-sized particle in the vicinity of a liquid-liquid interface. This fundamental study provides insight into the interaction of steel-slag interface with particles of different shape and wetting properties.

Fig.3: A fully-resolved turbulent interfacial flow based on the decaying homogeneous isotropic turbulence (HIT). These DNS results are obtained by the VOF method and are used for validation of our new two-phase LES models.
Blood flow is a complex physiological problem which requires a deep understanding of the behavior of biological cells as well as blood plasma, and the interplay between their dynamics. The deformability of red blood cells and their influence on the whole blood rheology is well studied and documented. Simulation tools have been developed to study and understand their characteristics and aid in exploring their behavior in various scenarios.

Several mathematical models have been proposed for simulating blood flow. Some model blood as a homogenous fluid medium and the biological cells as species which have an impact on the rheological behavior of the whole blood. In others, blood cells are modelled as membranes with an enclosed fluid medium. The membranes are made of point masses connected by spring networks to represent deformable red blood cells. These are highly accurate models, however, they require large computational resources. To this end, reduced-order models have been proposed in recent times to improve the computational efficiency of simulations without compromising the accuracy of the results to a great extent.

In the present study, a deformable cell is modelled as a cluster of overlapping spheres connected employing bonds (as in Fig.1). These bonds can translate and rotate based on the velocities of the spheres. The fluid flow is modelled utilizing the classical Navier-Stokes equations which is solved on a computational domain based on the finite volume method. The particle presence is mapped on the fluid domain through a level-set function named as voidfraction. The particle is considered as a porous region with very low permeability (~).

Initially, blood flow in micro-channels ranging from $D = 20 \mu m$ to $40 \mu m$ has been simulated to verify the capability of the model predict the rheological properties of blood such as the cell-free layer thickness, the discharge hematocrit and the relative apparent viscosity. Fig 3. shows the time-average concentration profile $p_{as}$ predicted by the model in our study. The red blood cell concentration can be seen to be more profound at the centre of the micro-channel indicating RBC migration towards the centre.
Finally, the blood flow across constrictions of varying lengths and widths have been studied. Fig. 3 shows the distribution of red blood cells upstream and downstream of the constriction. The ratio between the widths of the red blood cells in these regions have been compared with those observed in the literature and shows excellent agreement. This shows that the model is capable of producing excellent results for real-life industrial applications as well.

**Fig.1:** Red blood cell model (top). Bonds between spheres (bottom).

**Fig.3:** Cell-laden flow across a constriction (top). Ratio of upstream and downstream blood core width as a function of constriction length (bottom).

**Fig.3:** Red blood cell distribution contour (top) and cell-layer thickness (bottom).
**MICRO | HYSTERERTIC REGIME TRANSITION IN CO-CURRENT LIQUID-GAS FLOWS**

The co-current liquid-gas flows are the core of many industrial processes. One example with direct application to the steel industry is the injection of argon gas into the submerged entry nozzle (SEN) during the continuous casting. It is observed in the literature that the flow pattern and phase distribution in SEN are flow-dependent. Thus, the physics of the unsteady two-phase flow experiences different regimes from bubbly flow to annular flow. It is believed that the strong interaction between flow turbulence and fluid-fluid interfaces plays an important role in this regime transition. While argon bubbles help with removing impurities, an annular flow in the SEN could have a negative impact on the quality of steel. Thus, the two-phase flow regime characterization in the SEN is important for quality control.

Besides, the regime characterization maps based on the flow parameters have revealed a hysteresis during the transition from slug flow to annular flow. Using the volume of fluid (VOF) method, we have investigated the regime transition in a downward co-current water-air system by varying the gas content in the pipe. A gradual increase to the maximum gas volume is shown in Figure 1 (top). We have characterized the bubbly flow transition to slug flow (large bubble regimes) by a gradual increase of gas volume in the domain as shown in Figure 1 (left). This transition can be pictured as a change in the size distribution of dispersed bubbles. By further increasing the gas volume the annular flow is established as shown in Figure 1 (right).

At this point, when we start to decrease the gas content back to its initial value, the transition from annular flow to slug flow happens but at a different operation point. A hysteresis phenomenon is observed in our numerical simulations as shown in Figure 2. This interesting phenomenon can be justified by the generation of turbulent vortical structures (corresponding to enstrophy) in such inhomogeneous flow (i.e. density and viscosity contrast with the surface tension force which is dependent on the flow topology). Modelling and analysis of such a hysteresis phenomenon are currently under investigation in this project.
Fig. 1: The gas injection with varying flow rate (ramp-up and ramp-down) generates the co-current gas-liquid flow in a pipe (top). The 3D snapshots of different regimes: bubble/slug flow (left) and annular flow (right).

Fig. 2: The transition of bubbly flow to annular flow during the increase and decrease of the gas content with a clear hysteresis.

Mahdi Saeedipour | mahdi.saeedipour@jku.at
The existence of non-metallic inclusions (NMIs) in steel is detrimental for both the casting process and the mechanical properties of final products. As the last metallurgical vessel before steel solidification, tundish is particularly expected to further remove inclusions and improve steel cleanliness. Among the three stages for inclusion removal, (i) transport in molten steel; (ii) separation at the interface, and (iii) dissolution in slag phase, the intermediate step which is characterized by three-phase interactions is comparatively less studied and is the least understood.

To study the behavior of particle at the steel-slag interface, the numerical model employs moving-grid technique based on overlapped mesh system (Fig. 1) and the six degree of freedom (6DOF) solver along with the volume of fluid (VOF) method for interface tracking. By simulations, the meniscus (Fig. 2) arising from the thermodynamic requirement and its continuous evolution as the particle moves upward are observed. Meanwhile, it is possible to quantitatively analyze the separation process according to parameters related to particle motion such as particle’s force, velocity, and displacement (Fig. 3). This approach has been applied to investigate particles with varying properties, and the current results show that particles tend to be trapped at the interface.

For the next steps, conditions more relevant for the industry will be considered. For instance, the Marangoni effect due to the gradient of interfacial tension arising from accompanying dissolution phenomena is of interest.
**Fig. 1:** Illustration of the computational grid – overlapped mesh.

**Fig. 2:** Meniscus formation under the action of a slagophilic particle at steel-slag interface.

**Fig. 3:** Changes in particle’s (a) force; (b) velocity; (c) displacement during particle motion across the interface (contact angle $\theta=120^\circ$).
Developing fully-functional closure models for all the subgrid scale (SGS) physics in two-phase large eddy simulation (two-phase LES) is yet a challenging task due to the complicated turbulence-interface interactions. We have revisited the classical eddy-viscosity concept for the two-phase flows and proposed a new approach to include surface tension into the description of turbulent energy cascade. It has revealed an a-priori competence for the accurate simulation of the interfacial turbulence using the volume of fluid (VOF) method.

Recently, we further extended this line of research to exploit the potentials of our new approach in an a-posteriori manner, which could be an important step towards the fully-functional two-phase LES. On the basis of the Favre-filtered governing equations, the corrected eddy viscosity model is adopted to close the convective, surface tension, and continuity SGS terms and establishes a functional LES-VOF approach. The models are implemented into an OpenFOAM-based geometric VOF solver.

We studied a freely-decaying, homogenous isotropic turbulent flow (HIT) which is interacting with a thin liquid sheet initially at rest (Figure 1). First, fully-resolved simulations on a 512³ computational grid were carried out for different We numbers and density ratios between the phases. Then, the a-posteriori evaluation on coarser grids of 64³ and 128³ was performed. The results show that our functional two-phase LES approach predicts the energy cascade on the coarser grid more accurate than the classical Smagorinsky model (Figure 2). Also, a quantitative analysis of the interfacial structures such as size distribution of droplets and ligaments show a significant improvement.

The current research will be further continued by proposing new functional SGS closure models for the surface tension effects in the momentum equations.
**Fig.1:** A 3D snapshot of a fully-resolved interfacial HIT problem on a $512^3$ computational grid. The box is fully periodic, and the iso-contours of 50% of volume fraction are colored in green showing the interfacial structures. The velocity at the middle plane is also visualized. This case is used as the reference for comparison between the coarse-grid simulations.

**Fig.2:** The domain-integrated energy spectra at the same time step. The red and green lines denote the coarse-grid simulation results with the presented Favre-filtered LES method and the standard Smagorinsky, respectively. The light blue line is the fully-resolved data. The markers denote the energy spectra of a single-phase HIT problem. The energy rise due to the capillary forces is clearly shown. The Favre-filtered functional approach predicts the energy with a good agreement with fully-resolved data.

M. Saeedipour | S. Schneiderbauer

mahdi.saeedipour@jku.at | simon.schneiderbauer@jku.at
The drainage of liquid metal and liquid slag through the coke bed considerably contributes to the overall heat and mass transfer in blast furnaces (BF) and melter gasifiers (MG).

Thus, we focus on the trickling (dripping) of slag and liquid steel flow around the carbon particles before reaching the bottom of the furnace. While the trickling of the liquid phases across a few coke / char particles can be evaluated by a detailed simulation of the droplets finding their path (figure 1). In particular, figure 1 unveils that trickling behavior considerably depends on the properties of slag (e.g. viscosity, surface tension, surface contact angle). However, such a detailed approach becomes prohibitive in the case of a large-scale coke bed in BFs and MGs.

Thus, we generalized the findings from the detailed simulations and formulated a sub-grid trickling model for the coarse grid simulations of the BF and the MG (Figure 2). First coarse grid simulations show that such a drag model can be used to account for the unresolved liquid dripping in the coke bed.

We further expect to obtain new insights to the role of liquid trickling to the overall conversion of iron ore to liquid metal in BFs and MGs. However, the future modelling efforts should include the analysis of the static hold-up of the liquid slag and metal.
**Fig.1:** Detailed simulations of liquid trickling of liquid slag through a coke bed; left: large contact angle; right: low contact angle.

**Fig.2:** Measured drag coefficient for different fine grid configurations; blue: measured from fine grid; orange: model predictions.

\[ K = aK_{WY}Ca^{0.4}Ga^{-0.22} \]
Dear Readers,

Research on mesoscopic processes constitutes an important link in the chain of multiscale problems which are an almost daily challenge in the projects about multiphase flows we are working on. When we make progress on our understanding of the physics taking place on the mesoscale, we continue to build a bridge that spans the realm of microscopic problems governed by well-known equations with the domain of large-scale flows encountered in many industrial applications. Our goal is to extend our knowledge and understanding of the mesoscopic structures formed by microscopic processes, because they ultimately determine the large-scale behavior.

In this sense, mesoscale modeling can often be regarded as a data-assisted approach. We gather high-fidelity data from detailed, small-scale simulations and try to figure out what processes are taking place if regarded on a coarser resolution. In his Master thesis, Thomas Miethlinger addressed the fundamental question how to best quantify such microscopic information in particulate flows when we need to assess their overall (dis)similarity, and if the choice of approach impacts subsequent simulations. Sanaz Abbasi investigated how we can build reduced order models for transport in turbulent flows by extracting the most dominant features from a recorded time series, and which (hidden) properties beyond the leading modes play an important role. In contrast to these well-separated tasks of data analysis and simulation, Daniel Queteschner created a coupled framework of fine- and coarse-grained particle representations exchanging information on the fly.

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: A turbulent jet with POD modal reconstruction. Snapshot of the instantaneous velocity field (left) and a five-mode reconstruction (right). While the leading modes contain the dominant spatial structures, higher-order modes give rise to fine-scale features.

Fig. 2: Packed particle bed in a MIDREX shaft. While the volume fraction (left) is rather uniform, the granular pressure (right) shows clear heterogeneities. It is significantly higher above the burden feeders than immediately below them, which underlines their importance for a steady operation.
Several of our target applications are to be found in the iron- and steel-making industry, i.e. industrial plants such as blast furnaces and direct reduction shaft furnaces. To make the investigation of these large-scale systems computationally feasible using the discrete element method (DEM), it is necessary to introduce certain model simplifications. One of our favorite candidates 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.

We have previously introduced the multi-level coarse-grain (MLCG) model of the DEM to alleviate the deficiencies and increase the applicability of DEM coarse-graining. In this model we concurrently couple multiple coarse-grain levels to adjust the resolution of the simulation as required. We have also demonstrated in the past that the MLCG model can be extended to fluid-particle systems using CFD-DEM. What was missing so far from the MLCG model to fully picture our target systems, was the ability to consider heat transfer and chemical processes, e.g. the reduction of iron ore. In the latest iteration of the MLCG model we have added and verified these missing capabilities.

To demonstrate this new functionality we used – inter alia – the setup shown in Fig. 1, which mimics one of the experiments conducted in our laboratory. The bin has inner dimensions of 40 mm x 40 mm x 1500 mm. The outflow orifice at the bottom right is 40 mm x 10 mm. The bin was filled up to an initial bed height of about 500 mm. In the corresponding simulation we additionally assumed that the particles are initially heated to 1120 K and the left wall acts as a heat source with a constant temperature of 1220 K. Furthermore, a steady supply of reduction gas was prescribed. Heat transfer and reaction rates have been artificially increased to emphasize the effects in short-term simulations. Particle temperature as well as chemical reduction state of the embedded fine-scale simulation at the bottom were deduced from the overall coarse-grain simulation in the transition zone (i.e. the topmost cell layer).
Figure 2 shows the average particle temperature below the orifice during 2 seconds of outflow. Due to the information transfer from the coarse-grained particles to the original-sized particles, the temperature evolution is in good agreement for both representations of the system. Similarly, the reduction process progressed synchronously as illustrated in Fig. 3.

**Fig. 1:** (a) setup with the outflow orifice at the bottom right of the bin, (b) velocity, (c) temperature, and (d) overall chemical reduction after 0.65 s in a 2-level coupled simulation with coarse-grain ratios 2:1.

**Fig. 2:** Average temperature of the original-sized (red) and coarse-grained (blue) particles at the outlet.

**Fig. 3:** Overall reduction of the original-sized (red) and coarse-grained (blue) particles at the outlet.

Daniel Queteschiner | daniel.queteschiner@jku.at
Discrete element method (DEM) is one of the popular Lagrangian methods used for modelling the dynamics of granular flow in several scientific and engineering fields. However, this method has certain shortcomings in terms of computational cost when used for the simulation of large number of particles. Mixing, separation and blending process of particles are highly influenced by the particle size ratio which as a result, includes even higher number of particles. Therefore, simulating dynamics of highly poly dispersed granular materials are a challenging task for many industrial and scientific application. Therefore, we implement a improvised coarse grain method in contrast with the traditional coarse graining method by using a variable coarse grain ratio instead of a uniform one. This approach although reduces computational cost by significantly reducing particle numbers, it violates geometrical size distribution of particles and hence influence the original particle dynamics. This violation is shown in the simulation of flow of a sand column through a static packed bed of glass beads (Fig. 1b). Here the flow of sand particles through the packed bed are hindered due to inadequate pore space as soon as the original sized particles are lumped into coarse grain parcels with non uniform coarse grain ratio. We apply a revised coarse-graining approach using a corrected parameter for the overlap distance during collisions of parcel containing small particles and the large DEM particles to get the correct segregation of particles (Fig 1a). Following a volume fraction (VoF) comparison, a quantitative error analysis is provided (Fig. 2) w.r.t different coarse grain ratios. Also, the velocity comparison w.r.t an experimental study [W. Sui et al. Nature Sci. Reports, 7, 8, 2017] gives quite a good agreement (Fig. 3). For a particle size ratio up to 1:4, using this approach we are able to reduce the computational time by 94% of the time required for reference fine grain DEM simulation.

Our goal is to get the detail insight of the effect of size ratio and the corresponding coarse grain ratio on the overall dynamics of particle mixture in order to get a better understanding of customized optimization of computational cost associated with its corresponding simulation.
Fig. 1: (a) Left: Parcels of sand grains can percolate (revision method) and (b) Right: Coarse grained sand grain parcels can not percolate through the packed bed of glass beads parcels (without revision).

Fig. 2: Relative error profile of volume fraction of particle mix under different size ratio and coarse grain ratio.

Fig. 3: Velocity profile of sand column for different coarse grain ratio $\alpha = [20 \ 23 \ 25]$ with revision model along with the velocity obtained for the coarse grain model without revision and the experimental data.

Suranita Kanjilal | suranita.kanjilal@jku.at
Powders with small particle size often show cohesive behavior. This makes modeling of the flow properties a challenge and reliable tools are hardly available. We use the discrete element method (DEM) to model the flow behavior of strong cohesive metal powders used for powder metallurgy. To represent the real properties of the powders with the numerical model, the ability to show the relevant macroscopic behavior by means of experiments is necessary.

For this purpose, we developed an experimental setup, consisting of a rotating cylinder, which is partly filled with powder. During rotation, the block-like movement characteristic of cohesive powders can be observed. For this setup, a new evaluation routine based on image analysis was created.

This routine uses a neuronal network-based optical flow estimation to determine a two-dimensional velocity field. This is necessary since the powder shows the property of forming big homogeneous areas, which cause problems with classical PIV algorithms. From the velocity field, the block-like movement is characterized in size, direction, etc. Based on this analysis method the DEM model material parameter should be calibrated. Due to the small particle size of the powders, additional strategies have to be used in the case of DEM simulations, to reduce the computational costs to a reasonable amount, especially with the focus to do industrial-scale simulations. Since the parameters of the bigger DEM particles differ from the original powder properties, additional difficulties arise, and the same macroscopic behavior is hard to guarantee.

Additionally, there is also a focus on the relation of humidity in the environment and moisture content in the powder as well as the influence on flow behavior. Therefore, additional experiments were done to evaluate in which cases significant influence can be observed.
**Fig.1:** Schematic sketch of the experimental setup.

**Fig.2:** Digital image analysis for experimental setup (a) visual image, (b) calculated displacements.

**Fig.3:** DEM simulation of experimental setup.

*Tobias Kronlachner | tobias.kronlachner_1@jku.at*
The “recurrence CFD” (rCFD) method time-extrapolates a system’s behavior based on its reappearing patterns and reduces the computational costs considerably. However, in some cases there is no apparent periodicity in the system. Therefore, we first need to identify the characteristic coherent structures and then study their temporal evolution. Yet it is essential to know whether they provide enough information on the flow field to study the species transport.

For this purpose, we created a computational domain with 650000 cells and studied a confined turbulent jet at Reynolds number of 16400 for 250 seconds after the flow is fully developed. We used the method of snapshots in order to extract the most energetic modes and considered the remained ones as incoherent contributions. In the interest of analyzing the effect of these small-scale, short-term fluctuations, we considered two cases: first, we created a database comprised of reconstructed velocity fields with the first 10 modes for the case “rCFD-1” and for the second case “rCFD-2” we added a sub-database including a specific number of incoherent velocities. These incoherent fields were allotted to a group of coherent flow fields which were similar to each other according to a specific threshold. Consequently, we could reduce the size of this sub-database to 5% of the main one. Figure 1 compares the time-averaged velocity resulted from large eddy simulations (LES) with the ones resulted from rCFD-1 and rCFD-2. We could see slight deviations in rCFD-2 since we used a small database for incoherent fluctuations. On the other hand, Fig. 2 depicts the importance of retaining the turbulent fluctuations to get acceptable accuracy in modeling variance of velocity. As the next step, we studied the distribution of mean species in Fig. 3. One can observe the underestimation of rCFD-1 which could be improved significantly in rCFD-2 by a small number of incoherent snapshots.

In summary, we reduced the computational time by a factor of 15 since we just solved one passive scalar equation in rCFD. Additionally, We could reduce the required memory by only storing the first required modes and a small number of incoherent fields (5% of original database).
**Fig.1:** Mean velocity contour plot resulted from LES (left), rCFD-1 (center) and rCFD-2 (right). Although incoherent velocities added some noise, the results agreed very well with LES.

**Fig.2:** Contour plot of root mean square of velocity resulted from LES (left), rCFD-1 (center) and rCFD-2 (right). The incoherent structures are important in recovering the temporal variations.

**Fig.3:** Mean species distribution contour plot resulted from LES (left), rCFD-1 (center) and rCFD-2 (right). Coherent structures alone were not sufficient in transporting the species.
Dense granular systems such as packed, moving beds found e.g. in blast and shaft furnaces pose a serious challenge for computer simulations. If one wants to picture the complicated contact mechanics especially relevant in the dense regime correctly, the discrete element method (DEM) offers a very detailed approach. However, small time steps limit this strategy to at most a few minutes of process time so that long-term investigations appropriate to study slow heat transfer are out of reach.

Over the last few years, our group has developed the novel method rCFD for systems with strongly separated time scales applicable both to recurrent (fluidized beds, turbulent flows) and pseudo-steady (moving beds) cases. Using previously recorded data from short, detailed simulations, the future time evolution of the dynamics is extrapolated while slow, long-term processes are simulated on top of this approximate, future flow fields. For pseudo-steady motion as found in a moving bed, one simply needs to obtain the static particle velocity and volume fraction fields once as they hardly change over time. This saves a huge amount of numerical costs and allows to solve the fluid equations of motion together with heat transfer in both phases over process durations of many hours (“CFD with tracers”).

However, the thermal properties of a particle bed may very well affect its dynamics. In a blast furnace, layers of coke and ore move slowly downwards through the furnace. While coke is burnt at the raceways to produce carbon monoxide which reduces the ore to iron, the latter melts in the cohesive zone (CZ). Clearly, this region highlighted in Fig. 1 is determined by the temperature range where iron first softens and trickles down through the coke beds as liquid iron droplets. On the other hand, the removal of iron from the particle bed influences the granular flow behavior which therefore changes slowly over time along with the temperature field.
To account for this coupling between particle dynamics and the thermal properties of the reactor, we introduced flow field updates during the long-term simulation as sketched in Fig. 2. After a couple of hours, an intermittent, short DEM simulation with an updated CZ produces more realistic grain trajectories until finally, a steady state for both the temperature field and the location of the CZ is reached.

Fig.1: Particle temperature field over time. The CZ (black lines) changes from 0 h to 10 h before it finally converges after 20 h (left to right).

Fig.2: Particle volume fraction field. The predefined cohesive zone and deadman manifest with higher packing fractions while the raceways are almost void.

Thomas Lichtenegger | thomas.lichtenegger@jku.at
A wide range of applications in industrial processes involve the flow of granular media. Examples include powder flow in the pharmaceutical industry, fluidized beds in the iron- and steel-making industry as well as hopper flow in various industrial branches.

The DEM, by now a wide-spread simulation method for granular flow, uses Newton’s equation of motions for time propagation while resolving every single particle-particle contact. Although this approach provides accurate predictions of granular flows, it suffers from high computational demands. This prevents the use of the DEM in industrial-size processes which potentially involve millions of particles and several hours of process times.

Recurrence CFD (rCFD) provides a convenient time-extrapolation for long-term quasi-periodic processes, based on short-term simulations performed via established methods. Sequences of short-term simulations get stitched together to reach process time scales. Based on this extrapolation method, rCFD allows to simulate long-term transport phenomena. A variation of rCFD, namely transport-based rCFD (trCFD), provides a possible speed up by four order of magnitudes in comparison to standard methods.

However, for granular flows, trCFD suffers from several issues. For instance, trCFD requires proper selection of propagation time step size to ensure accurate information propagation. Typically, a wide range of velocity ratios in granular systems leads to problems. Furthermore, trCFD may introduce severe numerical diffusion. While in some cases like e.g. granular heat conduction, this effect can be adopted to physical diffusion phenomena, in other cases, diffusion must be avoided.

The goal of this study is to make trCFD suitable for granular media flow simulations. To this end, we introduce a multi-time-stepping approach and apply techniques to reduce numerical diffusion. To demonstrate the feasibility of this approach, we have applied these enhancements of rCFD for granular flow to a simple hopper flow problem with alternating layers of two different materials.
Fig.1: Standard trCFD method for Hopper flow.

Fig.2: Relative cell crossing time per cell in Hopper flow. Optimum value for standard trCFD -~2.

Fig.3: Comparison DEM reference simulation of Hopper flow (left side) with novel granular transport based rCFD (right side).

David Haider | david.haider@k1-met.com
Dear Readers,

The last year’s focus was laid on further bring our models nearer to feasible, cheap and reliable industrial scale simulations. For example, we extended the rCFD method to reactive gas-particle flows and subsequently applied this approach to a pilot scale polymerization fluidized bed reactor (Firas Dabbagh). rCFD has also been successfully applied to the pollutant dispersion in urban environments (Yaxing Du). Additionally, we further developed heat and mass transfer models for coarse grid simulations, which are based on the concept of multiphase turbulence (Stefanie Rauchenzauner). Here, our multiphase solver was further validated (Figure 2). We further investigated the liquid dripping of liquid steel and slag through a coke bed, which resulted in an effective drag model. This can be used for coarse grid simulations of a blast furnace. Furthermore, the effect of cohesion shows a considerable impact on the fluidization behavior of fine particles. Finally, we studied dust deflagration (figure 3), which can lead to severe damages in industry.

Scientifically, we closer explored the turbulent structure in fluidized gas-particle flows (figure 1) and particularly, to generalize these findings to different kinds of multiphase flows.

Finally, I want to thank my team members for their encouragement and their excellent work, which has been honoured by high impact Journal such as Physics of Fluids and the International Journal of Multiphase Flow.

Sincerely,

Simon Schneiderbauer | simon.schneiderbauer@jku.at
Fig. 1: Particle volume fraction (left) and vorticity including turbulent structure (right) in a turbulent fluidized bed.

Fig. 2: Numerical prediction of pressure gradient in a gas-particle riser.

Fig. 3: Particle temperature during dust deflagration in a modified Hartmann tube (blue: 300 K; red: 2000 K).
In industrial scale gas-solid flows, like fluidized beds or risers, clusters are observed to form due to the momentum coupling between the gas- and particle phase in the presence of a mean body force, such as gravity. In applications, coarse numerical grids are used in order to render simulation of industrial sized reactors feasible. These coarse grids do not resolve the particle clusters, which can only be a few particle diameters wide. As we showed in a-priori analyses, the unresolved mesoscale structures have a large influence on the macro-scale flow properties, such as bed expansion and temperature distribution. Therefore, we developed Spatially-Averaged Two-Fluid Models for momentum and heat transfer in moderately-dense gas-particle flows.

An a-posteriori validation of the developed models for momentum transfer showed that the macro-scale flow properties can be correctly estimated in coarse-grid simulations. In Figure 1, a comparison of coarse-grid simulations with different grid-sizes to the fine-grid simulation of the same Geldart A-type, homogeneously bubbling fluidized bed is shown. The bed expansion and volume fraction distribution over the height of the bed could be correctly reproduced by our models.

Furthermore, in order to visualize the importance of the clusters on the heat transfer, we started an initially isothermal simulation of unbound fluidization of Geldart type A particles with a domain averaged solid volume fraction of 0.05. After the system reached a statistically steady state, the gas-phase temperature was set to 500 K, while the solid-phase temperature was set to 300 K and heat transfer between the phases was enabled. After only a few time-steps, the thermal equilibrium in the system was restored. Figure 2 shows a snapshot of the system with the iso-surfaces of the volume fraction at 0.05 depicted in white colour. One can clearly observe that temperature differences between the phases only prevail in regions which are devoid of clusters.

Our next steps will be not only a qualitative but also quantitative analysis of the heat transfer reduction in coarse grid simulations using and validating the models which we developed in our a-priori study.
Fig. 1: Snapshots of the solid volume fraction of a wall-bounded 3-dim fluidized bed of Geldart type A particles. a) Fine-grid simulation, b) fine-grid simulation smoothed with a filter of size 8, and coarse-grid simulations with c) a coarse-graining ratio of 6, d) a coarse-graining ratio of 8, and e) a coarse-graining ratio of 12.

Fig. 2: Normalized temperature difference between the gas- and the solid phase. Iso-surfaces of the domain average of the solid volume fraction at 0.05 are shown in white colour. It can be observed that temperature differences between the phases only prevail in regions devoid of clusters.
MACRO | CHEMICAL REACTIONS AND CLUSTER INDUCED TURBULENCE

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.

Especially, clusters and bubbles reduce the overall heat and mass transfer compared to homogenous suspensions. In particular, figure 2 shows that the reaction rate is reduced to up 80% when using coarse grids, which is stemming from the unresolved small scale distribution of the reactant species concentrations (figure 1).

In future, we will develop closure models accounting for the impact of the unresolved scales on the reaction rate, which are based on the concept of cluster induced turbulence (CIT). This will considerably improve the numerical predictions of reactive industrial scale gas-particle flows.
Fig. 1: Impact of filtering on the spatial distribution of reactants. I.e. small scale features are lost.

Fig. 2: Reduction of the reaction rate as a function of the filter length (-- filtered fine grid, -- model).

Simon Schneiderbauer | simon.schneiderbauer@jku.at
The major efficiency of recurrence CFD (rCFD) lies in opening new frontiers in unattainable plant-scale systems within a moderate cost.

In this regard, we develop our rCFD algorithm to include the transfer of exothermic chemical reaction kinetics in the framework of transport-based rCFD model [1]. Tackling a big problem, we consider an industrial-scale Olefin polymerization fluidized bed reactor, where a non-reactive recurrent hydrodynamics is obtained using a coarse-grained Two-Fluid-Model (Fig. 1b). It constitutes the rCFD database that delivers the chemical species conversion and heat propagation much longer in time. Following a temperature-pressure driven reactivity, the polymerization process determined by the consumption/production of gas/solid species is applied within rCFD modeling. It implicates the particle growth of polymer solid, the destruction of monomer gas, and the produced heat by reaction, applied locally in cells. Doing so, the rCFD outcomes are compared against the hybrid model [2] (Fig. 2) to show a very reliable agreement with a computational cost reduction from 150 h to 15 min.

Futural work will constitute the extension of rCFD capability to enable treating with continuous plant operation including feeds of solids.

Fig. 1: rCFD gas temperature evolutions averaged over the powder polymer material classes, and taken inside bed, at the freeboard and the outlet of the reactor (ref is [2]).

Fig. 2: (a) rCFD snap-shots of gas temperature at different moments revealing the heating up by reaction. (b) an instantaneous field \( t = 6\ s \) of the solid volume fraction outcomes using cgTFM.
Rapid and accurate prediction of near-field hazardous pollutants in complex urban environment remains an important issue for individual health and city planning. In our previous work, we have successfully applied rCFD in simulating pollutant dispersion around a benchmark case of an isolated building [1]. The rCFD method relies on a prominent recurrent nature of the flow. While this was possible for the simple benchmark case, this might be impossible for more complex topologies. To overcome this existing limitation of rCFD, a domain decomposition approach such that we organize the global domain into smaller recurrence islands is proposed.

In this approach, sub-domains of prominent recurrent flow features (such as wakes of buildings) have to be first identified. Once identified, the databases for those recurrence island are built up which then is exploited for the simulation of local dispersion.

In the case of a two side-by-side building, the result of spatial decomposition can be seen in Fig. 1, together with recurrence matrix of the ‘background sea’ and recurrence island. Two individual per-building islands are established. A significantly higher recurrence prominence than the global ‘background sea’ can be identified.

Fig. 2 is a contour plot of mean concentration in a horizontal observation plan (half building height). While both versions of rCFD once again successfully reproduce the main features of the reference solution, we can detect specific prediction errors in case of the global-domain based rCFD (existing rCFD). Specifically, the two middle streaks are strongly asymmetric for existing rCFD approach. As for this evaluation, our island-based version of rCFD obviously achieves better agreement with the reference solution.

While full LES-based CFD simulation took 393 hours of wall-clock time on a 32-core computer, rCFD took only 61 hours, including the time needed for building the databases (see Fig. 3). Once the database was established, rCFD simulations account to 14 minutes in comparison to 368 hours of corresponding full LES simulations, resulting in a speed-up of more than three orders of magnitude (i.e. 1500 times faster).

**Fig. 1:** Recurrence matrix and recurrence vector plots for two side-by-side cubical building case.

**Fig. 2:** Comparison of mean concentration coefficient between full LES and rCFD in horizontal plane at z/H=0.5.

**Fig. 3:** CPU time consumption.
Typically, numerical predictions of CFD could be easily illustrated by colorful figures. It is a common saying that every conference presentation on CFD must contain at least one movie of unsteady simulation results. However, in developing data-based CFD methods we sometimes have to dig deep into the algorithmic structure of the underlying software. While this can be documented by flowsheets and lines of code, these are not as handy as typical CFD results.

Figure 1, for instance, depicts the algorithmic flow sheet for island-based rCFD. In case of large computational domains featuring complex topologies, it will be impossible to find similar states globally. Or in other words, we would need excessively large databases in order to cover the extremely long return times. As a obvious remedy, we partitioned the domain into a set of prominent recurrence islands which are embedded into a background sea of low recurrence prominence. While this is easy to say, the implementation of this required a complete re-design of the underlying software for rCFD simulations. Along with this domain decomposition we re-designed our parallel MPI communication concept such that we could reduce memory usage by one order of magnitude.

Personally, for me this hands-on working on the code is an essential source for the development of new algorithmic concepts. Directly experiencing the limitation of the existing approach paves the way towards new algorithm. While the current versions of rCFD are field-based (in a sense that the database contains field data), I anticipate that our next generation of data-based will work more locally, thus providing greater flexibility.

As a first eye catcher, I tried to picture fluid flow by interconnected neurons of different size (Fig. 2). Once trained by conventional CFD, these neurons could reproduce local fluid flow surprisingly well (Fig. 3) – even if only a part of this data has been used for training: Interesting stuff to look into in future …
**Fig. 1:** Flowsheet of island-based rCFD.

**Fig. 2:** Conventional CFD simulation with a couple of inter-connected Neurons watching the flow.

**Fig. 3:** Conventional CFD monitors of point velocity together with predictions by trained Neurons of different size.

Stefan Pirker | stefan.pirker@jku.at
Dear Readers,

due to the Covid-10 pandemic we were forced to reduce our lab activities for quite a long time. However, there are still plenty of results to report. The shut-down period gave us the opportunity to focus on academic aspects of previously conducted lab projects and document the results in the form of several journal papers. Hence, we were focussing more on data analysis over the last month and this will also be the case for the near future, since the rapid development of machine learning techniques has also swapped into the fluid mechanics community. So there are lots of exciting new techniques to be tested within our activities in the field of multiphase flows.

PFM has ever since emphasized the importance of know-how transfer to our industrial partners. RHI-Magnesita now has taken a pioneering task in the know-how transfer of validation experiments as it is the first company partner that has directly taken over a complete test rig from PFM. Michael Weiß has successfully moved and rebuilt the particle centrifuge that was designed to investigate the flowability of cohesive powders to the technology center of RHI-Magnesita in Leoben. We would like to thank the Christian Doppler Association for supporting this project with a student internship.

Sincerely,

Stefan Puttinger | stefan.puttinger@jku.at
**Fig.1: Example of detailed PIV data analysis:** Strain and vortex dominated regions based on the so-called $Q$-criterion for a submerged jet beneath a free surface (left) and the same setup covered with an additional layer of a lighter liquid that is deformed due to the inertia of the deflected jet (right). This situation is simplified setup of a continuous casting mold to mimic the behavior of liquid steel and slag. Blue colored areas are strain dominated, while red areas indicate high vorticity. The black line marks the current position of the interface.

**Fig.2: Centrifuge for flowability experiments under increased gravity conditions up to 100G.** Test rig assembly at the technology center of RHI-Magnesita in Leoben.
I took some time during the lock-down period in spring 2020 to revisit the high resolution PIV data of our mold flow benchmark experiment (Fig.1). Beside the time resolved fluctuations of the jet we can extract the detailed distribution of energy in the mold and provide useful information for the validation of our LES modelling activities.

The analysis of a small layer below the interface (Fig.2) shows that the energy is shifted from horizontal velocity fluctuations to a vertical orientation (Fig.3). Calculation of the gradients allows to visualize strain and vortex dominated regions (c.f. Fig 1 on page 43). In addition proper orthogonal decomposition (POD) shows the differences in energy content of coherent and incoherent turbulent structures.

The results of this in-depth analysis of time-resolved PIV data has recently been published in Experimental and Computational Multiphase Flow.

**Fig.1:** Benchmark experiment for investigating interfacial behavior in stratified two-fluid systems (left). Snapshot of the interface deformation in the side view taken via shadowgraphy (right).
Fig. 2: Snapshots of the water/oil experiment recorded from top of the basin. The images show the deformation of the water-oil interface due to the deflected submerged jet. The area of the so-called “open eye” is then calculated via image processing.

Fig. 3: Power spectral densities snapshots of $u'$ (top) and $v'$ (bottom) for the case with and without oil layer. The results show a shift of energy from horizontal to vertical velocity fluctuations due to the presence of the oil layer and the altered flow direction of the deflected jet.
The term optical flow is widely used in computer vision and describes the extraction of object motions from image data. Since the established algorithms for particle image velocimetry (PIV) and particle tracking velocimetry (PTV) have reached an impressive level of quality and computational speed, optical flow has not received much attention from the fluid mechanics community for many years. However, this is changing rapidly as the algorithms used in optical flow have improved significantly. Likewise, the calculation times have dropped dramatically by the use of massive parallelization on GPUs. Recent developments couple optical flow with deep learning methods. Such enhanced methods – which are usually termed deep flow – can even be applied on PIV raw images to obtain vector fields.

Optical flow is also a quite flexible tool, as it can be used to calculate the movement of every pixel (dense optical flow, c.f. Fig.1) or in combination with feature extraction tools as a sort of Lagrangian object tracking method (although the algorithm only deals with pixels and is not aware of any objects).

Especially for applications that do not fit into the standard scheme of PIV and PTV methods, optical flow is definitely a method to keep an eye on.

Fig.1: Dense optical flow used to extract the motion of particle clusters in a high-speed video. A common approach in optical flow is to use the HSV color space to visualize the magnitude and the direction of the flow in one contour plot.
Fig.1: Shadowgraphy recording of a bubbling fluidized bed. The Lucas-Kanade method was used to extract the motion in the video. In this case the optical flow approach serves a kind of front-tracking method. A quick quantitative comparison of the bubble rise velocities with formerly calculated results based on Lagrangian object tracking of the bubbles shows a good agreement in bubble rise velocities (c.f. figure below, the vector data is completely unfiltered and still shows a realistic range of bubble rise velocities).

Range of rel. bubble rise velocities based on Lucas-Kanade results.

Stefan Puttinger | stefan.puttinger@jku.at
Since May 2019 the process control system of the blast furnaces at voestalpine Donawitz calculates a raceway blockage signal for every tuyere based on our results of project 2.1 in the first funding period of K1Met. A detailed analysis of the collected data was recently published in Steel Research International. The statistical data shows differing results for the two furnaces. While the number of strong blockages is quite similar for both furnaces, the total number of events is significantly larger on BF1 (Fig.1). The differences in the number of short events is currently not fully understood, however, the geometry of the furnaces is not identical and the different volume of the liquid pool of iron in the BF hearth might trigger a different flotation behavior of the dead man.

The data also shows that the frequency of strong blockage events correlates in many cases with a subsequent damage of the tuyere (Fig.2). This is definitely an aspect to be investigated in more detail on the long run, since the blockage signal could serve as a performance indicator for upcoming tuyere damages and the planning of maintenance activities.

**Fig.1:** Long term statistics of raceway blockages on BF1 (left) and BF4 (right) at voestalpine Donawitz (data covers approx. 7500 hours of blast furnace operation). BF4 shows a significantly lower number of blockage events than BF1.
**Fig. 2:** The blockage signal (magenta curve) that is now calculated online in the process control system shows a clear increase of strong raceway blockages starting around 90 minutes ahead of the actual breakdown of the water cooling circuit. Thus, the blockage signal could be used as an indicator for predictive maintenance.

**Fig. 3:** Tuyere nozzle of BF1 with severe damage. Photo courtesy of voestalpine Donawitz.

*Stefan Putttinger | stefan.putttinger@jku.at*
High quality measurement equipment is very expensive, and hence, the density of measurement stations is rather low (e.g. there are ten stations in and around the urban area of Linz). However, to validate locally resolved environmental flow simulations (that typically cover only a few blocks, c.f. this year’s title page) we would need a large number of sensors that could be placed at various locations across that area (like the leeward side of high rise buildings, that can suffer from pollution accumulation due to vortex formation downstream of the building). These sensors in fact do not need a high absolute accuracy, it would be sufficient if the results allow a qualitative comparison between the stations. The absolute results could be referenced to the nearest accurate measurement station. To test this strategy we dedicated our last years seminar to aerosol measurements based on low-budget equipment. Compared to our first attempt in 2014 there is now a wide selection of ready-to-use sensors available and open hardware platforms like Arduino make it possible to build a fully functional sensor network within a few hours.

**Fig.1:** Mobile data logging unit based on the Arduino architecture.
**Fig.2+3:** Image of the setup for the sensitivity tests of moving particle sensors showing all necessary ingredients for students to have fun with aerosol science for several hours. Oil droplets < 1µm are produced by a PIV seeding generator located under the table and are released from the black plastic pipe. The oscillating signals on the right correlate with the circulation period of the train with and without cross-wind.

**Fig.4:** Measured dust concentrations during a walk across the city center of Linz visualized in Google Earth. The two peaks on both sides of the bridge across the Danube (Nibelungenbrücke) show exactly the locations of two intersections with high traffic load (the vertical scaling is arbitrary but linear to show the particle concentration).

*Stefan Puttnger* | stefan.puttnger@jku.at
SELECTED PUBLICATION


Lichtenegger T., Pirker S.: Toward Data-Assisted Particle-Fluid Simulations of Heat Transfer in Blast Furnaces, in Steel Research International, 2020

Puttinger S., Stocker H.: Toward a Better Understanding of Blast Furnace Raceway Blockages, in Steel Research International, 2020

Schneiderbauer S.: Verification and validation of spatially-averaged models for fluidized gas-particle suspensions, in Chemical Engineering & Technology, 2020