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BOOK OF ABSTRACTS

5th Aspherix® & CFDEM® CONFERENCE

26-27 September 2024

Vienna, Austria

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Erratum

In the abstract entitled “Solids Conveying of Polymer Powder in Twin Screw Extruders Investigated by Means of DEM” (p. 33), only Marcel Ratka was incorrectly listed as the author.

However, the following authors were also involved in the creation of the abstract:
Jasmin Kaiser, Alptekin Celik and Christian Bonten.

In the e-book edition, the incorrect pages were replaced, and the missing names were subsequently added to the abstract.

CONTENT

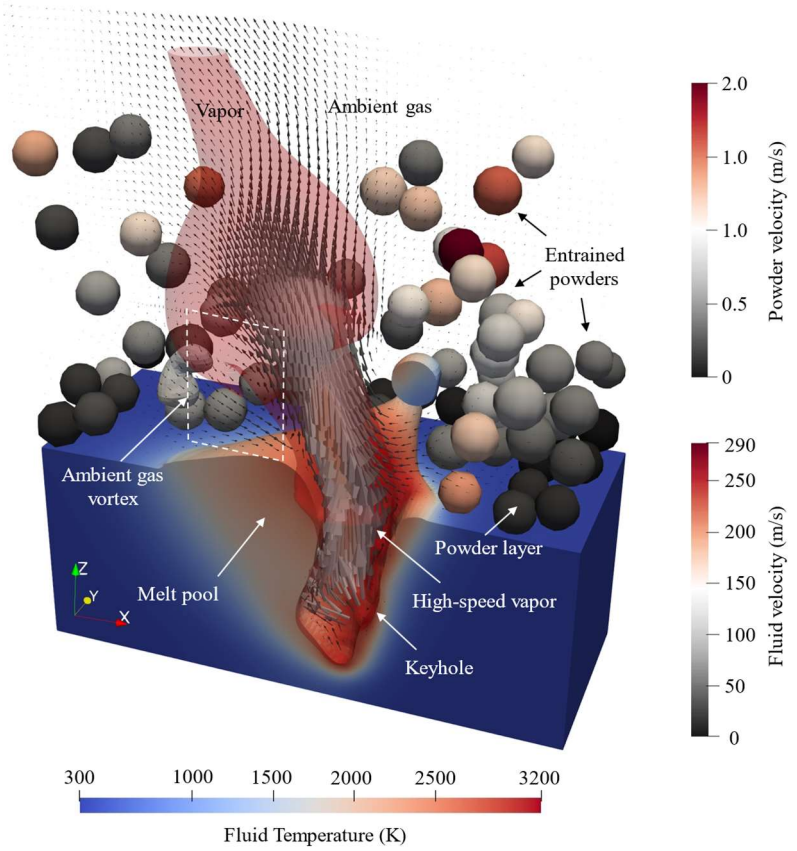
Keynote Abstracts

High-Fidelity Simulations of Complex Particle-Fluid Interactions in Granular Media

Jidong Zhao

The Hong Kong University of Science and Technology

In this talk, we discuss the methodological challenges and latest progresses in developing rigorous coupling schemes for Computational Fluid Dynamics (CFD) and Discrete Element Method (DEM) to tackle a class of engineering and industrial problems involving complex multi-phase, multiway interactions among granular particles with complex shapes, single or multiphase fluids, and structures. We provide an overview of the development and applicability of four coupling schemes: unresolved, semi-resolved, fully resolved, and hybrid coupling schemes of CFD-DEM for practical use. A couple of representative engineering/industrial examples are presented to demonstrate the strengths and pitfalls of these schemes. These include modeling of debris flow and mitigation measures, coastal wave/tsunami sloshing with breakwater and coastal levee structures, and laser powder bed fusion (L-PBF) in additive manufacturing. We highlight the importance and complications of accurate characterization and modeling of particle shapes and possible phase transitions in developing efficient coupling schemes for these challenging processes.

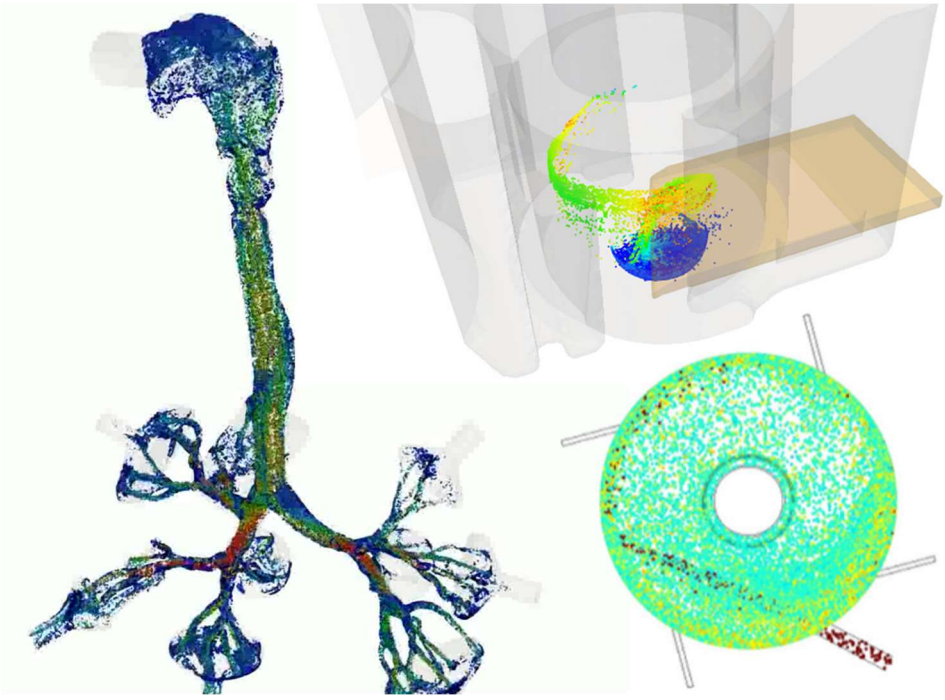


Open Issues in CFD-DEM Simulation of Orally Inhaled Drug Products

Andrea Benassi

Chiesi Farmaceutici s.p.a.

Orally inhaled drug products (OIDP) are designed to deliver the active pharmaceutical molecule through the formation of a poly-disperse aerosol of particles/droplets, its subsequent inhalation by patients, and its landing on the inner walls of the deeper airways/alveoli. The physics governing the behavior of such products is thus intrinsically multi-phase and multi-scale, as well as highly non-linear, ideal to be described through coupled CFD-DEM simulations. Many applications of CFD-DEM simulations will be illustrated encompassing different phases of OIDP design and manufacturing, e.g. synthesis and particle engineering of the powder to be aerosolized, drug dose aerosolization inside inhalers during administration, journey of the airborne particles inside the patient bronchial tree. For each application insights and advantages obtained by employing simulations will be illustrated as well as the current numerical, computational or practical limitations preventing us from exploiting further their potential.



Multiscale Modeling: From Macroscopic to Atoms – and Back …

Erich Wimmer

Materials Design, Inc.

The predictive power of macroscopic simulations hinges on the completeness and accuracy of the materials properties used as input. When such data are not available from experiment, computations provide a solution. This leads us from the macroscopic scale via the mesoscale to the level of atoms and electrons. The main challenges in connecting these scales are (i) the daunting span of time scales, namely from years to femtoseconds, and (ii) the required accuracy in predicting properties such as temperatures of phase transitions. This talk will illustrate the current capabilities in predicting physical and chemical properties of solids, fluids, and their interfaces. For example, using state-of-the-art forcefields, density, viscosity, liquid-vapor equilibria, diffusion coefficients, heat capacity, and thermal conductivity as a function of temperature can be predicted at a level of accuracy close to experiment. High-throughput first-principles quantum mechanical computations, now possible with highly efficient and robust programs in convenient modeling environments, enable the generation of large and systematic data sets for training machine-learned interatomic potentials. This exciting capability has opened unprecedented opportunities for multiscale modeling, as will be illustrated by examples such as the prediction of phase transitions, oxidation, and plastic deformations of metals. Of particular value are property calculations of solid/solid and solid/liquid interfaces including chemical reactions. An assessment of these capabilities and opportunities for their improvements will conclude this talk.

Enhancing Simulation-Driven Development at Grundfos: Leveraging Aspherix® & CFDEM®

Mark Herskind

Senior Fluid Mechanics Specialist at Grundfos, Bjerringbro, DNK

As a world-leading pump manufacturer, Grundfos continually seeks to pioneer innovative new solutions to global water challenges and enhance our existing product portfolio. Simulation-Driven Development has long been a core aspiration at Grundfos as it is scalable and provides strong insights into the problems at hand. To realize this vision, we aim to stay informed and to explore new tools to maintain and expand our simulation capabilities.

Given the nature of our products, fluid simulation plays a pivotal role. CFD is a stable in our simulation portfolio and is widely used in solution development and maintenance.

In many applications, we encounter solids in various forms—particulates, packed/fluidized beds, fibers, pellets, and flocculates, among others. Some solids may have specific properties, which can be a challenge to standard CFD approaches. We see the coupled Discrete Element Method (CFDEM) approach as a powerful tool which may expand our capabilities in these areas.

In this speech, I will delve into our ongoing journey - which we have only just begun - highlighting specific cases and commenting on challenges faced. I will explore how we see the Aspherix and CFDEM and their place in our simulation portfolio, and how we are planning to move forward.

Mechanistic Modeling of Fluidized Bed Granulation: A CFDEM Approach for Equipment Transfer and Scale-Up

Martin Lubej

Novartis AG, Fabrikstrasse 2, 4056 Basel, CH

In the pursuit of operational excellence within pharmaceutical manufacturing, the application of Computational Fluid Dynamics and Discrete Element Method (CFDEM) modeling for fluidized bed granulation (see Figure 1) presents a transformative approach to equipment transfer and scale-ups. This study leverages the combination of thermodynamic and CFDEM model to critically assess the operational variances across equipment from different vendors and their subsequent impact on product quality. The model serves as a cornerstone for the development of a comprehensive transfer guideline, initially focusing on equipment in a laboratory setting, with the potential for future scale-up applications.

The primary objectives of this research include the establishment of a modeling framework that incorporates multiple impact factors, and the assessment of process transferability across different manufacturers' equipment. The success of the model is measured by its ability to identify equipment-independent parameters and validate the model's predictions through experimental trials with placebo and active compounds.

By identifying scale- and equipment-independent factors, the CFDEM model aids in the development of a modeling-informed transfer guideline. This approach not only enhances process understanding but also aims to reduce the number of technical batches required for scale-up or transfer at scale, leading to cost and time savings.

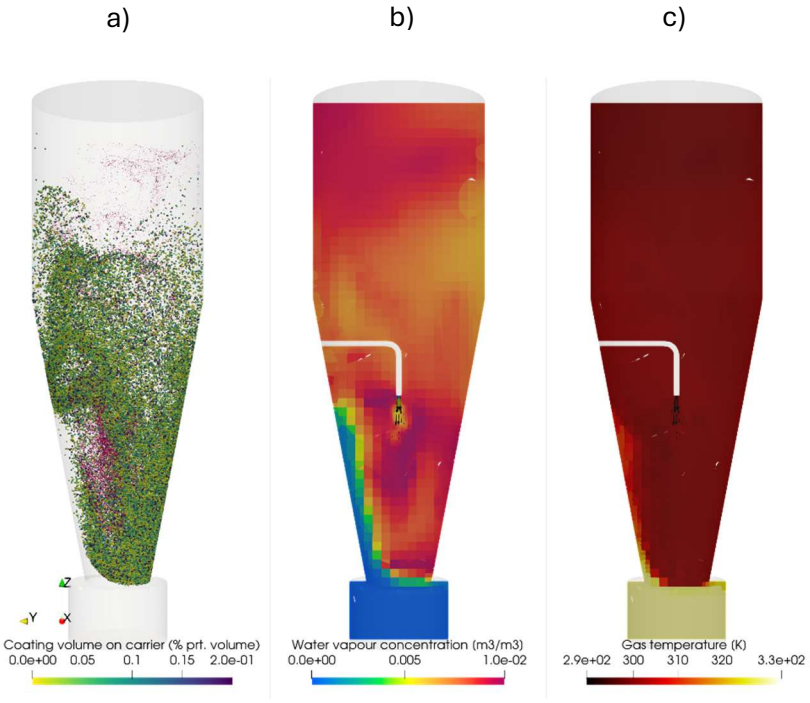


Figure 1: CFDEM simulation of lab-scale fluidized bed granulator. a) carrier particles colored by the percentage coating volume and spray droplets (magenta points), b) water vapor concentration and c) gas temperature fields in vertical section crossing the center of the vessel.

Keywords: CFDEM modeling, fluidized bed granulation, scale-independent factors, equipment-independent factors, pharmaceutical manufacturing, product quality

Challenges in Modelling and Understanding of Particle Formulation by Spray Granulation

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Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Hamburg Germany

E-Mail: Stefan.heinrich@tuhh.de

Fluidized bed spray granulation is the process of choice for producing highly functional, high-value granular products. The interactions between the spray liquid and particles are complex and depend on the drying or thermal conditions as well as the properties of the spray and the material system itself. The simultaneous high demands on the quality of granular products require highly precise measurements and educated modelling of the particles in the fluidized bed. In this work, recent developments in both fields are presented.

Advanced measurement techniques allow the collection of process data at an unprecedented resolution and accuracy, ranging from locally resolved inline measurements of particle water content and particle size distribution to 3D volume tomography and lagrangian sensors that follow the movement of particles in the fluidized bed. This data is crucial for the understanding of the spray granulation but also for the validation of numerical methods which benefit from higher spatio-temporal resolutions of reference data. Among others, recent advances in numerical modelling include the usage of CFD-DEM for the investigation of the liquid distribution in various fluidized bed geometries and the validation of scaleup rules as well as the successful validation of machine learning models for soft sensing and forecasting of key particle properties. However, the increase in complexity of numerical models has not only led to higher accuracies in simulations but also gave rise to computational costs. Current research thus addresses the computational efficiency by the development of surrogate models and data-assisted methods such as recurrent CFD and machine learning. Other approaches rely on the efficient modelling of whole process chains through our in-house dynamic flowsheet simulation tool Dyssol. Based on the presented breakthroughs in measurement techniques and numerical methods, the path for the development of intelligent digital twins for fluidized bed spray granulation is outlined.

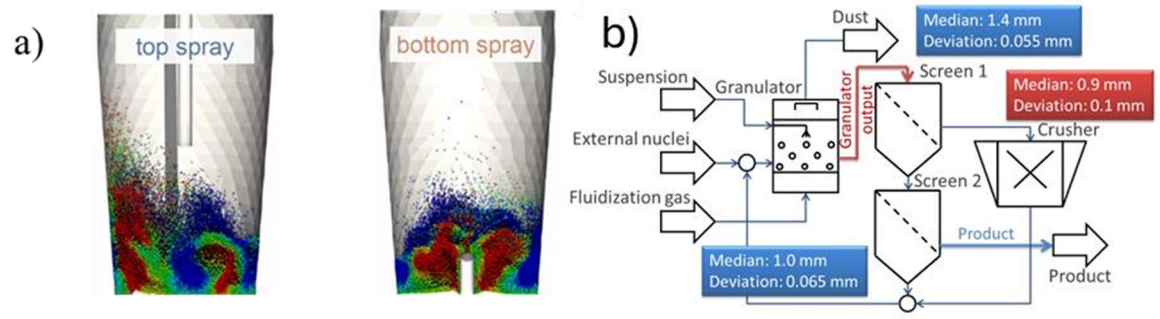

Figure: a) CFD-DEM simulation of different fluidized bed setups with liquid injection and
b) Flowsheet simulation setup for a granulation process.

The Uncertainty Inherent to Granular Flows

Lukas Maier, Michael Mitterlindner, and Stefan Radl

TU GRAZ

Uncertainty quantification (UQ) is well established in areas like fluid flow prediction, or stress analysis [1]. This uncertainty is caused by small variations in the initial or boundary conditions, as well as the parameters of a, e.g., CFD model. However, in the area of granular flows, applications of UQ are relatively sparse [2],[3]. The reason for this fact is that discrete particle simulations are computationally expensive, and always transient. Also, there are additional uncertainty parameters compared to fluid flow predictions, which are (i) the initial particle positions and (ii) particle orientations. With respect to the particles' initial orientation, literature [4], [5] suggests that there is a strong effect in flows involving non-spherical particles: their shape anisotropy leads to different stresses in steady-state shear flows. Especially for flows that may never approach a (quasi) steady state, e.g., discharge from a silo, UQ data is extremely scarce, and one may expect significant uncertainty connected to experimental and simulated data.

Our current contribution systematically investigates the effect of particle shape on the uncertainty introduced by two factors: (i) the initial particle configuration, and (ii) the variability of contact properties (e.g., the particle-particle friction coefficient). Our analysis includes flow properties (e.g., the discharge profile of a draw down tester), as well as thermal properties of particle packings (e.g., the heat conductivity). We find clear indications that particle shape and the particles' interlocking tendency is a key factor causing uncertainty in experiments and particle simulations. Also, we will highlight consequences of these uncertainties for applications like automated calibration of model parameters.

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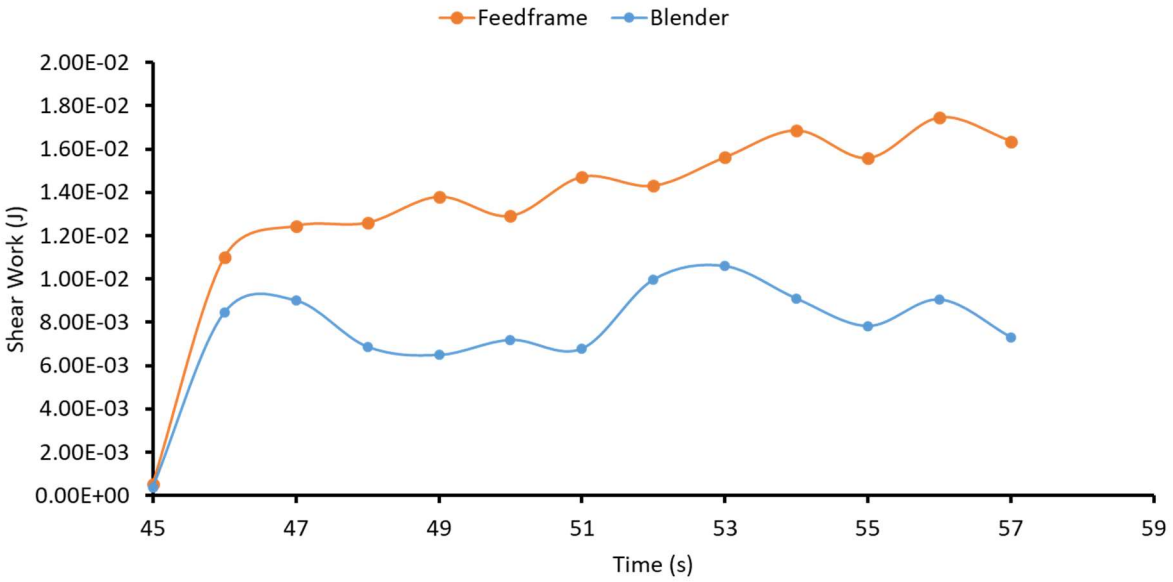
[5] Y. Guo, C. Wassgren, W. Ketterhagen, B. Hancock, B. James, and J. Curtis, "A numerical study of granular shear flows of rod-like particles using the discrete element method," *J Fluid Mech*, vol. 713, pp. 1–26, Dec. 2012, doi: 10.1017/jfm.2012.423.

Investigating Particle Attrition and Overlubrication Propensity in a Feedframe Compared to a Blender using Discrete Element Method

Karthik Salish*, Prajwal Thool, Chen Mao

Genentech Inc.

This study utilizes Discrete Element Method (DEM) simulations to analyze particle behavior within a tablet press feed frame, a crucial component impacting tablet quality. DEM tracks individual particle interactions and motion, providing insights into the influence of residence time, shear work, and forces on overlubrication and particle attrition. While tablet production involves multiple unit operations, the feed frame meters and forces powder into dies, potentially leading to issues due to extended residence time. This research addresses this gap by comparing the propensity for overlubrication and particle attrition within the feed frame compared to a blender. Results indicate a significantly higher shear work value (0.174 J) within the feed frame compared to the blender (0.099 J), suggesting a greater risk of overlubrication. Additionally, the study reveals a higher potential for particle attrition during feeding compared to mixing, highlighting the unique challenges within the feed frame. These findings demonstrate the value of DEM simulations in optimizing tablet production processes by understanding particle behavior at the individual level.



Comparing the overlubrication inside a feedframe with that of a blender

Keywords: Blending, feedframe, overlubrication, particle attrition, DEM

3 Axis of a Modelling Coordinate System
From Model Fidelity to Fast Results, from Open Source to Proprietary, from Development to Deployment

Christoph Kloss & Christoph Goniva

DCS Computing GmbH, Linz, Austria

We would like to share our experience of 14,5 years of developing modelling projects and products to serve the CAE community – most notably, LIGGGHTS®, CFDEM®coupling, ParScale, CFDEMworkbench, Aspherix®, and most recently Engicloud.

The starting point of our journey is about (monetary and non-monetary) motivation for developing software and tools and the baseline situation that creates within the M&S community and market.
As a modelling group, we've had many learnings over these 14,5 years, and we'd like to share and discuss these along 3 axis:

- For someone with a PhD in modelling, it's not always easy to build a good model. But even harder is the question: How do I build the *right* model (from 1D python to 3D CFD-DEM)?
- (commercial) exploitation: How do I choose the right license? How do I tell "right from wrong" ?
- Once you've created an amazing tool, how can you make sure it survives until it hits the users? How do I make sure my tool is still relevant in 5yrs?

Also, we would like to highlight the needs of different user personas and how their coordinates can be located with respect to these 3 axis.

Of course, we also share some recent highlights of new functionalities within the Aspherix® DEM and CFDEM®coupling CFD-DEM software and the road for our new Engicloud platform that may lie ahead.

Geo-Technical Applications

Numerical Simulation of One-Dimensional Compression in Geotechnical Engineering using Computed Tomography

Mohamed Abdennadher

Hamburg University of Technology

Understanding soil compression behavior is a fundamental aspect in geotechnical engineering. Traditionally, constitutive models have been employed to represent the collective behavior of soil particles, rather than focusing on individual grains. These models require specific parameters, which are usually determined through laboratory experiments. This paper presents a workflow for simulating one-dimensional soil compression using a digital twin approach. Computed tomography (CT) is utilized to capture the morphology of individual soil particles. Advanced image processing techniques are then employed to generate three-dimensional models of these particles, facilitating the assembly of a digital representation of the soil structure (Figure 1). Subsequently, numerical simulations of compression tests are conducted on the digital soil. To optimize computational efficiency, a multi-layer meshing strategy is implemented, employing a fine mesh at the inter-particle contact zones, crucial for capturing particle interactions, and a coarser mesh within the particle interiors. This approach enables the inclusion of a larger number of particles in the simulations, leading to a more comprehensive analysis of soil compression behavior. Furthermore, the study investigates the optimal particle distribution and minimum number of particles required to achieve an accurate representation of real soil. Comparing the simulation results with laboratory data reveals a strong correlation, validating the effectiveness of this method. This opens up opportunities to extend numerical simulations to more complex laboratory experiments in soil mechanics. Eventually, the approach may enable engineers to entirely replace physical laboratory experiments with virtual experiments, saving time and resources while still producing reliable and accurate data.

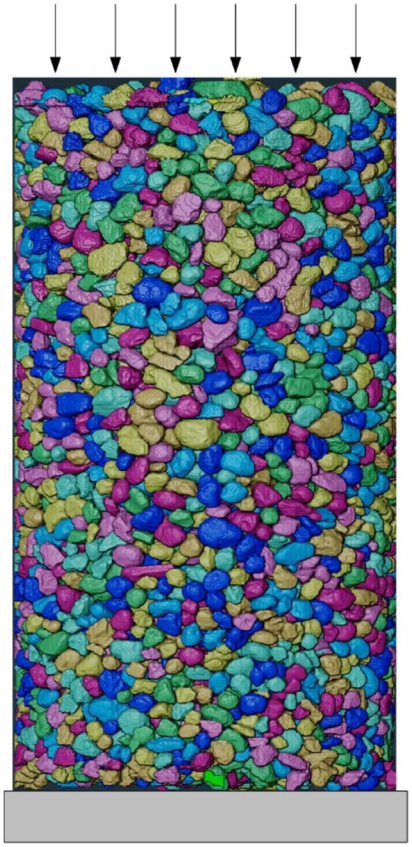


Figure 1: Assembled soil structure from 3D models of individual soil particles.

Enhanced Simulation of Triaxial Tests by a Coupled DEM-FEM Method

Olzhas Sayakov

Nazarbayev University

Accurate simulation of soil behavior under triaxial tests is crucial in geotechnical engineering. This study introduces an advanced simulation approach, coupling the Discrete Element Method (DEM) with the Finite Element Method (FEM), and employs a coarse graining (CG) method to enhance the representation of soil-particle interactions and membrane effects. Our methodology systematically includes sample preparation, application of confining pressure, vertical loading, and detailed post-processing analysis. We explore the impact of the CG coefficient, which adjusts the particle radius to reduce computational demands while preserving detailed behavior, and the role of confining pressure in influencing the simulation results. The particle interactions are modeled using the Hertz-Mindlin contact model, and the particles are scaled according to a CG coefficient of 2, maintaining the original particle size distribution but increasing the radius size proportionally. This modification is pivotal as it directly affects the simulation's computational efficiency and accuracy. Figure 1 represents the sample before and after the simulation. Figure 2 presents the relationship between axial strain and normalized stress, highlighting the simulation's capability to accurately depict stress responses under diverse conditions. Despite utilizing a combined approach of DEM for detailed particle-level simulations and FEM for overall continuum mechanics, the results indicate a need for further refinement. Adjustments to the material parameters could enhance the model's accuracy, thereby improving the realism and applicability of geotechnical simulations. These enhancements are critical for advancing the design and precision of geotechnical experiments and broader engineering applications, offering a more reliable and scalable tool for predicting soil behavior.

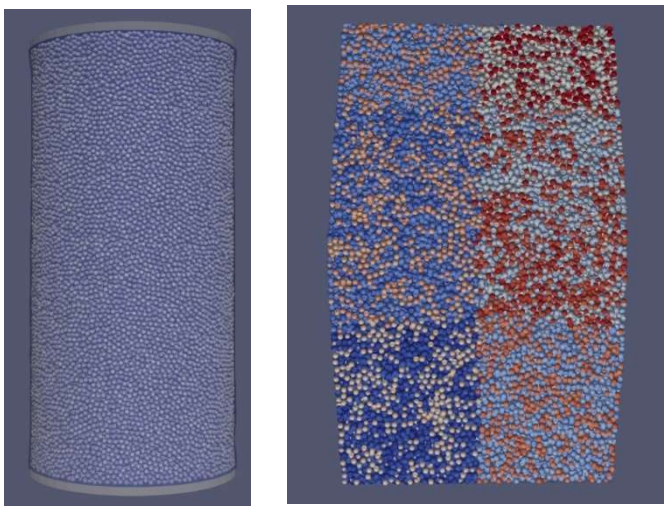


Figure 1. Simulated Triaxial Test Sample Before and After (Cross Sectional View) Vertical Loading

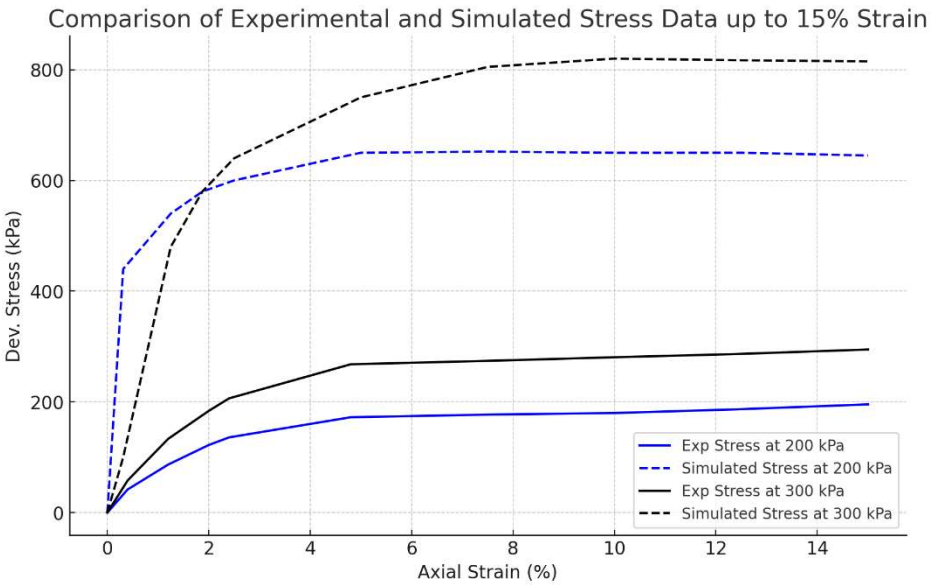


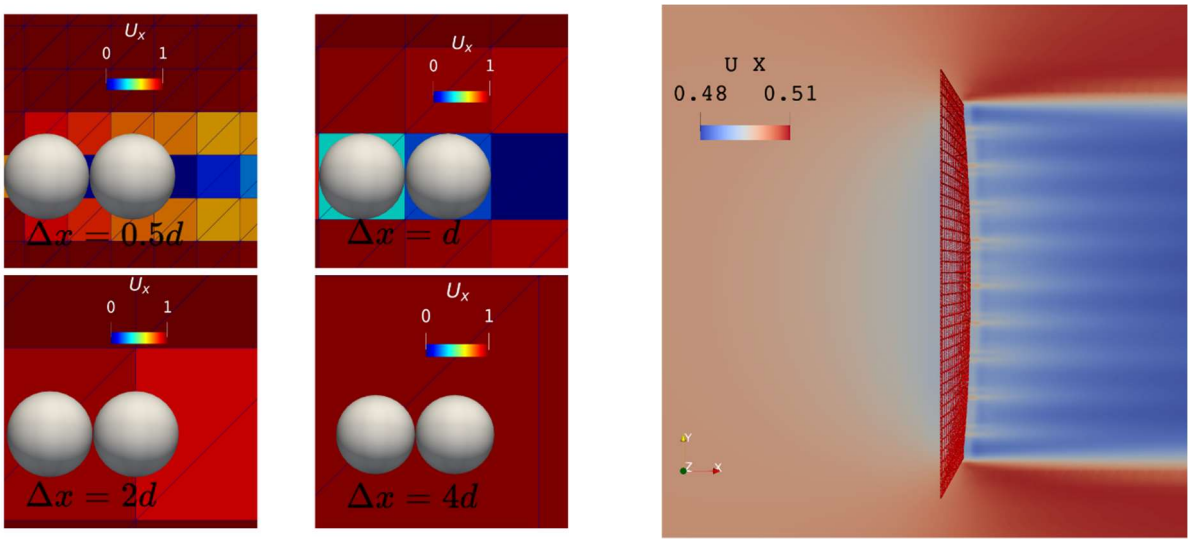
Figure 2. Experimental and Simulated Stress-Strain Relationship in Triaxial Test

An Unresolved CFD-DEM Approach for the Simulation of The Ocean Cleanup Systems

Andriarimina Daniel Rakotonirina

The Ocean Cleanup, Rotterdam, The Netherlands

The Ocean Cleanup is a non-profit organization determined to rid the oceans of plastic. We target both existing plastic and future influxes. For the Great Pacific Garbage Patch (GPGP), we have developed and deployed a floating barriers aiming at capturing plastic marine debris. The main component of such a system is fishing net that is repurposed for our mission. The current barrier *System 03* is a 2.2 km long system supporting a porous screen crafted from repurposed fishing nets, reaching 4 meters beneath the water surface which is towed between two slow-moving vessels. This makes the drag force one of our most crucial Key Performances Indicators (KPIs). Therefore, we built an accurate model to support our decisions stemming from the response of our systems to the ocean environment. Notably, we borrowed the well-known CFD-DEM approach [1] to model the nets of our systems. The twines of the net consist of identical spherical particles in a straight line and virtually bonded [2] using relatively simple contact models allowing the net to bend, stretch, and twist under realistic loads. The momentum transfer between the two phases is estimated by using Eulerian cells ranging from one twine diameter up to four twine diameters (hence particle diameters) requiring the modification of the classical closure laws due to the shedding of the bonded particles on one another, i.e. the quantification of the shielding effect created by a leading particle onto the drag correlation of a following one at various relative angles. Our results are compared to experiments to ensure for the validity of the application of the method on netted screen.



References

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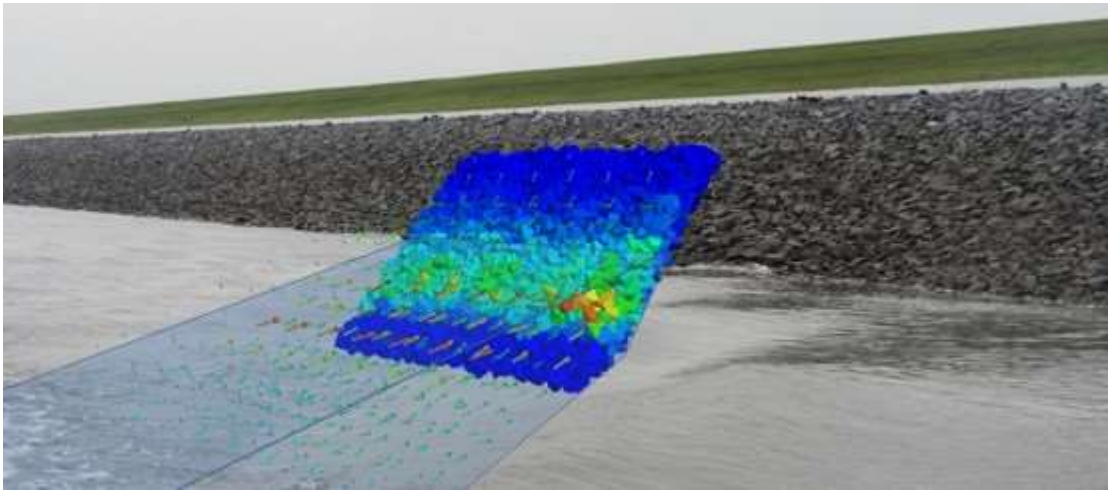
Towards a Resolved CFD-DEM Model for the Analysis of Stability of Loose Armor Stone Revetments in Maritime Waterways

***Marica Broseghini*, Martin Pohl**

Federal Waterways Engineering and Research Institute (BAW), Hamburg, Germany

Loose armor stone revetments are widely used to protect costal structures and river banks from the erosion produced by natural and ship-induced waves and currents. However, construction rules tailored on the peculiar hydraulic load conditions of estuary areas and maritime waterways (e.g. large tidal water level changes, waves and currents produced by seagoing vessels with continuously increasing size and velocity) are currently not satisfactory. This leads to inefficient design of the revetments and, in turn, to non-negligible maintenance costs.

For a safer and more sustainable design of the revetments in maritime waterways, the present work exploits coupled CFD-DEM simulations for investigating the stability of loose armor stone revetments subjected to hydraulic loads typical of these areas. In particular, within the CFDEM coupling framework, a resolved CFD-DEM model will be developed to simulate the interaction between the irregularly shaped revetment stones and natural as well as ship-induced waves and currents. Results of hydraulic flume tests will be used for the calibration of model parameters while field measurements will be exploited for defining the hydraulic loads and for the model validation. The displacement of individual armor units as well as the pressure distribution and the flow velocity will be investigated in order to understand the failure process of the structure under wave impacts. Gained knowledge could lead to improved design rules for the revetments, aiming at increasing their stability, durability and safety and at reducing building and maintenance costs.



Membrane Particle Interaction in Triaxial Testing: FEM-DEM Coupling and CT Imaging Insights

Dennis Heinrich[1], Martin Niemann[2], Christoph Goniva[2], Christoph Kloss[2], Jürgen Grabe[1]

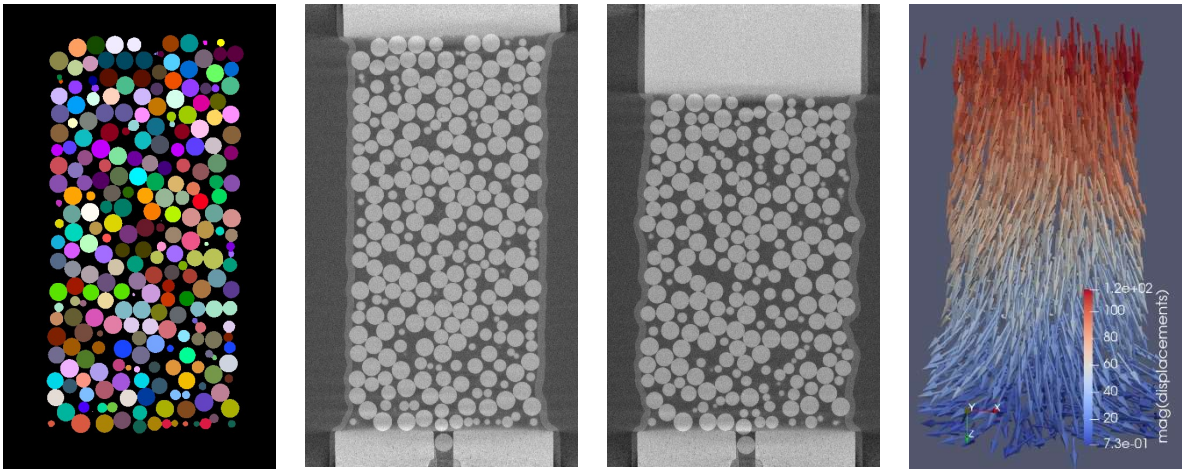
[1]Hamburg University of Technology
[2]DCS Computing GmbH

This conference contribution presents recent advances in implementing a FEM-DEM solver into Aspherix. Implementing this FEM-DEM coupling aims to account for membrane particle interaction in numerical simulations, i.e., encountered in triaxial testing, a standard test in soil mechanics, where the DEM accounts for particle motion and the FEM for the membrane deformation. Furthermore, we showcase specific image processing techniques based on 4D (3D+time) *in situ* X-ray computed tomography (CT) experiments to set up and validate such numerical simulations.

Miniaturized triaxial experiments have been performed on a cylindrical (height 20 mm; diameter 11 mm) dry granular particle assembly. Here, a specimen made of 1 mm glass beads is examined. Axial deformation is exerted onto the specimen, leading to a consecutive shear deformation. At each 1 % of axial strain (*here*: engineering strain with $\varepsilon = \Delta l / l_0$) the experiment is halted to acquire a tomography of the current state. A total of 15 % of strain is applied.

On the one hand, the acquired image data of the initial particle configuration is processed to act as input for the numerical simulation. On the other hand, sophisticated image analysis based on an image correlation procedure tracks individual particles throughout the experiment solely based on the acquired image data, giving displacement vectors for each particle (see figure below). This data is complemented by externally measured axial force, which describes the examined specimen's shear resistance. Both force measurements and displacement vectors act as a validation for the numerical simulation.

Finally, current limitations of the implementation are discussed, such as available element types for modelling the membrane, and an outlook for further improvements is given.



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

Image analysis based on CT image data using a Discrete Digital Image Correlation (DDIC) algorithm. Here, the label image (a) of the initial particle configuration (b) is used as a mask to track each particle. The correlation is computed based on the present image texture on the grayscale level. Image (c) shows the sample after ca. 3.5 mm of vertical compression was applied. a) to c) show a vertical slice of the 3D image data. The resulting displacements are shown in (d), where the vectors and their corresponding coloring show the direction and magnitude of displacements for each particle.

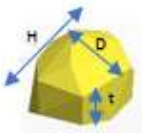
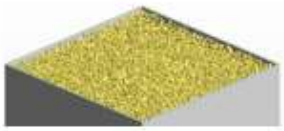
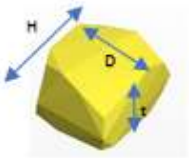
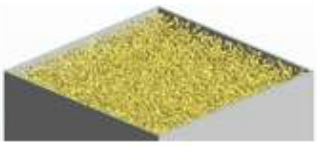
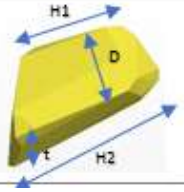
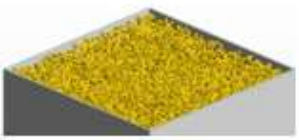
This contribution is based on a research cooperation between Hamburg University of Technology (TUHH) and DCS Computing GmbH funded by the German Research Foundation (DFG; Project 461859082) and the Austrian Fund for the Promotion of Scientific Research (FWF; Project I 5374-N) covered by the D-A-CH agreement.

Evaluation of the Pull-Out Capacity of Dynamic Anchors Considering Different Shape and Size of Particles using DEM Model

***Amirali Zad*, Hamidreza Mohammadkhani Fard**

Islamic Azad University, Central Tehran Branch

Capturing the real behavior of anchors has always posed challenges in geotechnical engineering due to the involvement of various uncontrollable parameters that involve and the cost of controlling all of them in experimental tests. To address this issue, numerical modeling methods such as Finite Element Method (FEM), Discrete Element Method (DEM), and coupled Eulerian element (CEL) method have been utilized by different researchers. Among these methods, DEM is particularly noteworthy for its ability to model the interaction between anchors and surrounding soil particles, providing valuable insights into anchor performance across different soil types and conditions. However, DEM has limitations, such as the influence of particle shape and size on results. While researchers have proposed various sizes and shapes for geotechnical problems, there is a research gap regarding the interaction between the soil of particles and dynamic anchors that has not been extensively explored. This study introduces the use of diverse shapes and sizes of soil particles to assess the pull-out capacity of dynamic anchors. The numerical results suggest that incorporating realistic particle shapes can enhance the accuracy of anchor behavior evaluation. Additionally, various particle mixing scenarios were proposed, and the numerical outcomes showed good agreement with experimental test results. Furthermore, a novel numerical method was introduced to simulate the sand pluviation technique in the laboratory, enabling particles to settle at different angles.

Name of particle	Dimensions	Shape of particle	Shape of the model
Soil 1	H=.002m D=.001m t=.009m		
Soil 2	H=.003m D=.002m t=.001m		
Soil 3	H1=.002m H2=.003m D=.001m t=.009m		

Details of soil particles

DEM Based Erosion Simulation of a Lunar Landing Pad

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Current space programs, such as NASA's Artemis and ESA's Argonaut missions, share the goal of returning humans and cargo to the lunar surface. The plume of the rocket swirl up regolith particles, which can destroy infrastructure on the lunar surface. Fur future missions, it is necessary to reduce the dust emissions caused by rocket plumes interacting with the lunar surface. This can be achieved by using an in situ manufactured lunar landing pad (LLP). Due to the extreme conditions on the lunar surface and the limited amount of data available, a simulation model and experiments are beneficial for characterizing the erosion of the lunar landing pad.

This study utilizes a simulation model based on the Discrete Element Method (DEM) to describe the erosion caused by the rocket plume. The model uses particles ranging from 55 to 550 µm. The sintered material structure of the landing pad is modelled with bonds between particles based on an elastic beam. Additionally, a heat transfer model is applied to describe the fracture behavior of the bonds due to the thermal influence of the rocket plume. The rocket plume is modelled using a shear force and heat flux applied to the top of the landing pad. This causes the pad to heat up and erode, as shown in Figure 1. The heat flux and shear force data are based on previous Computational Fluid Dynamics (CFD) simulations of the rocket plume. The erosion rate is calculated by evaluating the movement of particles over time. The simulation results show that the erosion rate of the lunar landing pad is influenced by the LLP's porosity, the thermal capacity of the particles, and the thermal conductivity of the bonds. Furthermore, the rate of erosion is affected by the location beneath the rocket, altitude, and heat flux on the LLP.

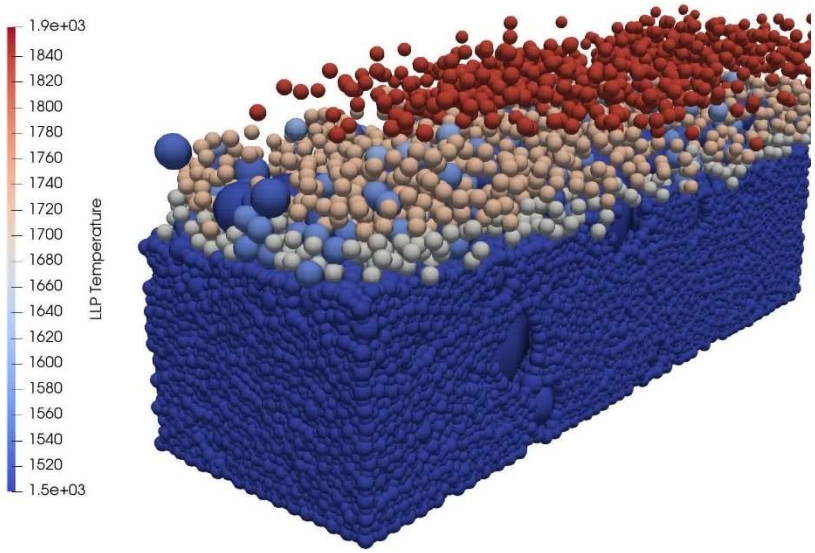


Figure 1: Result of the erosion simulation

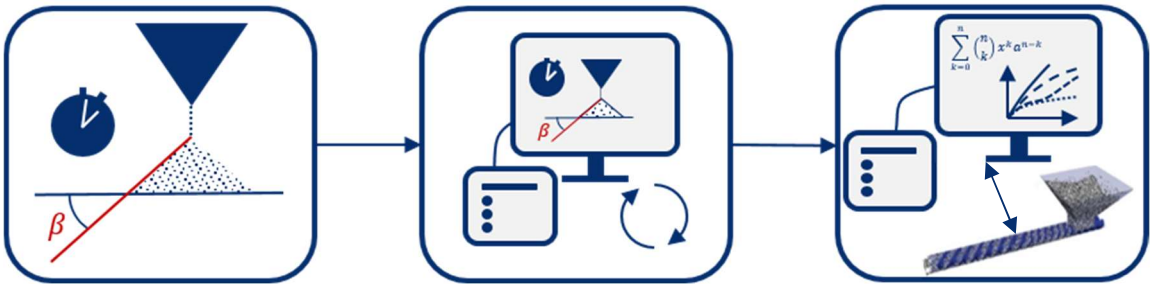
Extrusion

Solids Conveying of Polymer Powder in Twin Screw Extruders Investigated by Means of DEM

Marcel Ratka, Jasmin Kaiser, Alptekin Celik and Christian Bonten

University of Stuttgart, Institut für Kunststofftechnik

In the present work, a plane wedged hopper with adjustable sidewalls is used to characterize different materials. The characterization is reproduced in discrete element (DEM) simulations. In this process, the material parameters of the simulation, in particular rolling friction and cohesion, are varied and adjusted so that the flow time and the angle of repose in the simulation of the hopper match the results of the experimental investigations. When modeling a powder, satisfactory results were obtained with the combination of rolling friction and cohesion in the simulations. For the modeling of granules, rolling friction was used exclusively. The calibrated representative (powder-)particles were used to study for the first time the solids handling properties of an industrially relevant sized twin-screw extruder (TSE) at high speeds above 2m/s with DEM and evaluate its maximum throughput. In order to visually validate the simulation results with the experimental investigations, the trials are carried out on a TSE with PMMA housing (at speeds <1m/s). Further trials with a regular TSE were carried out. The simulation results of the granules show a good agreement with the experimental investigations. The simulations of the TSE with powder delivered promising results with good qualitative agreement to the experiments.



Model Experiment DEM-Simulation

Funded by the Federal Ministry of Economic Affairs and Climate Action based on a resolution of the German Bundestag, within the IGF project 20989 N of the AiF Forschungsvereinigung: Forschungs-Gesellschaft Verfahrens-Technik e.V. (GVT), thanks for the funding, further details are available in the final report of the project.

The Potential of DEM Simulation for the Prediction of Torque Differences in the Melting Zone of Co-rotating Twin-Screw Extruders

Laura Austermeier, Volker Schöppner

Paderborn University

Polymers have been the most important group of materials in terms of volume for many years. Due to decreasing new developments of base polymers and increasing requirements, the demand for modified plastics through additive and blend production is increasing. These are usually produced in twin-screw extruders, which are among the most important plastics processing machines. In contrast to other machines, twin-screw extruders are underfed and metered as the processes are usually limited by the torque of the machine. While the drive power is constantly being increased, the screw diameters are being reduced in order to achieve higher throughput and thus greater profitability. However, this carries the risk of overloading and failure of the screws. In addition, little is known about the torque difference between the screws, which makes design even more difficult.
Thanks to new measuring methods, it is now possible to measure the torque of both screws simultaneously and assign it to the individual process zones. One of the most important zones is the melting zone, as this is where the greatest torque is generated. The figure illustrates examples of operating points at different speeds and throughputs, which show the differences between the screws.

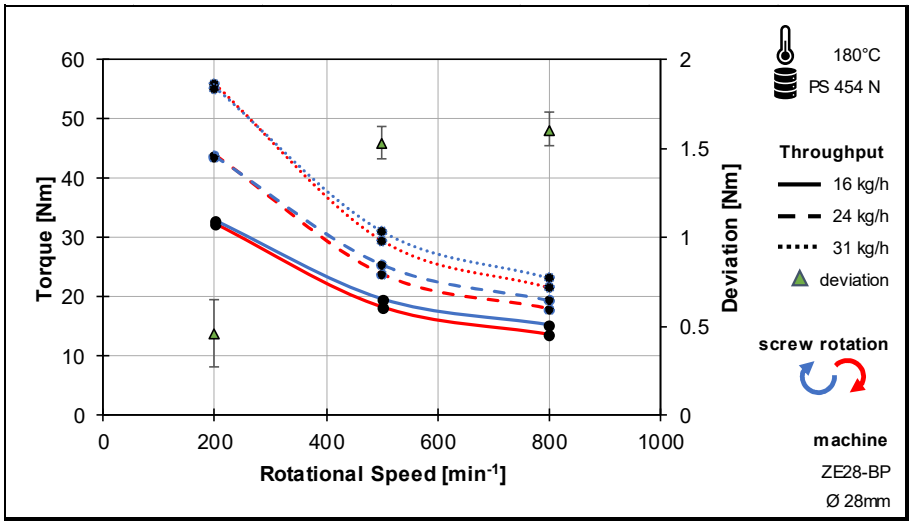


Figure 2: Comparison of the torque measurements of both screws in the melting zone of a ZE28-BluePower

Simulations of the processes could greatly simplify prediction and thus machine design but have so far proved to be a challenge. The melting processes in co-rotating twin-screw extruders are dominated by the plastic deformation of the pellets in the intermeshing zone. While the solids transport up to this area can already be well described by DEM simulation, the challenge of particle deformation appears here, indicating a need for development and research. This research gap shall be closed by a joint research project.

Industrial Applications

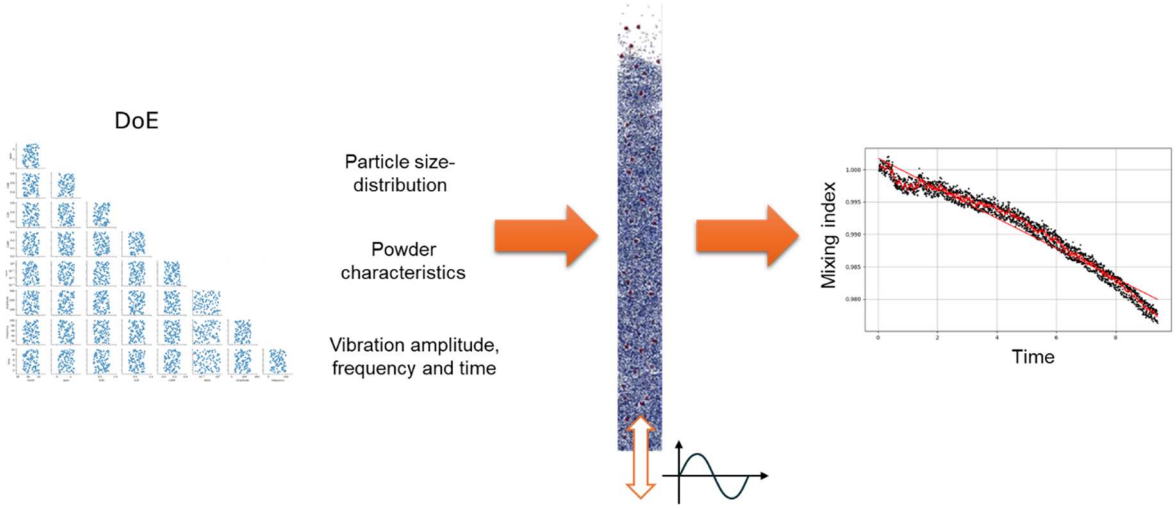
Densification and Segregation in Hot Isostatic Pressing using DEM

***Luigi C. Capozzi*[1], *Daniele Ugues*[2]**

[1]Lancaster University (UK), [2]Politecnico di Torino (Italy)

Hot Isostatic Pressing (HIP) is a net-shape powder metallurgy process that consists of producing dense, high-strength and high-integrity components from the sintering under pressure of fine metal powders. The first step of HIP consists of filling a metal capsule with metal powders. The filling step plays a fundamental role in determining the quality of the final component as it can cause non-uniform shrinkage during the sintering and, finally, result in components with high distortions. Vibration-assisted filling is commonly employed to increase the powder discharge rate, increase the packing fraction of the final powder bed, avoid excessive voids, or, in the case of complex-shaped capsules, avoid the presence of unfilled regions. However, vibration can also cause variations in packing density and segregation.

In this work, we employed Discrete Element Method to investigate the effects of (i) powder size distribution, (ii) powder characteristics, and (iii) filling conditions on powder densification and segregation during vibration-assisted capsule filling. A Design of Simulation Experiments approach was implemented to identify the critical factors influencing the characteristics of the final powder packing. Subsequently, we have analysed the role of cohesion and particle size distribution in a real case scenario using Astroloy powder. The powder was subjected to different conditions by comparing as received and dried powders, alongside fractionated particle size distributions.



The results were partially obtained in the context of project Clean Sky 2 Joint Undertaking under the European Union's Horizon 2020 research and innovation program (Call Reference No: JTI-CS2-2017- CfP07-ENG-03-22) under grant agreement No 821044.

Large Scale 3-Dimensional Numerical Model of an Industrial Biomass Furnace using the Extended Discrete Element Method

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[1&2] Université du Luxembourg, [3&4] LuxEnergie S.A., Luxembourg

The eXtended Discrete Element Method (XDEM) is a novel approach to the modeling of fuel particle combustion. The method uses a coupled model wherein the fuel particles are modelled using DEM while the gas-phase is modelled using CFD. The DEM model includes the necessary thermodynamics for combustion. This method allows the development of high-fidelity models that capture the entire combustion process.

In this study the XDEM approach was used to develop a full 3D numerical model of a large feeder-grate type industrial biomass furnace (44 ton/h, 8 MW capacity). A novel co-located partitioning strategy is used to solve the large 3D numerical model efficiently on a High-Performance Cluster (HPC). The thermal performance of this biomass furnace has been investigated with regards to its fuel and airflow configuration.

The numerical model includes the introduction of wet fuel particles which are subjected to drying due to conductive and radiative heat transfer before they undergo pyrolysis, and finally gasification reactions. The pyrolysis of the particles yields solid coke which is then also gasified. The gaseous products of the particles' solid-state reactions are transferred to the gas-phase model where the reactions complete; thus, yielding the total energy and final products associated with the particles' combustion.

The recirculated flue gas and the secondary air inlets produce a mixing effect within the furnace which increases the gas-phase reactions of the gaseous products. In agreement with empirical observations the burn-out combustion of the biomass particles towards the end of the grate occurs at significantly higher temperatures due to the gasification of the coke created by the initial pyrolysis reactions as shown in Figure 1: Gas & Particle Temperatures inside the Biomass Furnace

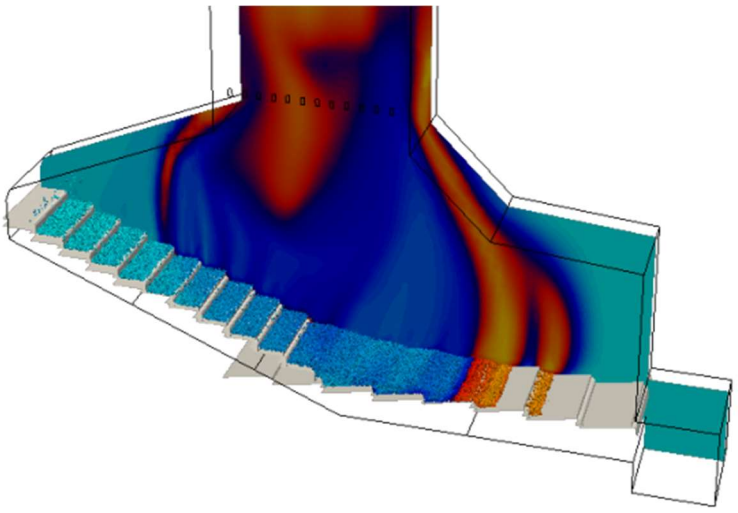

Figure 1: Gas & Particle Temperatures inside the Biomass Furnace

3D Printing of Structures for Chemistry and Energy Applications

Vesna Middelkoop

VITO, Belgium

Innovative 3D printed multi-channel thermo-catalytic and photo-catalytic monoliths as well as multi-layer electrode meshes were developed and evaluated in a laboratory setting for a variety of chemical and energy applications. Emerging 3D printing technologies such as Direct Ink Write (DIW), and Digital Light Processing (DLP) were used to actualise their design and apply functional material layer by layer with excellent reproducibility and fidelity. To provide precise control over mass and heat transfer, flow dynamics, mixing, and active particle accessibility, well specified 3D networks were constructed by tailoring both the macro- and microstructure of the materials. In this manner, a variety of functional materials, mixed metal oxides, non-oxide ceramics, nanocomposites and metals were directly printed and patterned.

This presentation will showcase a number of bespoke reactors for active catalyst particles deposited within 3D printed monoliths. The reactors present a step change in chemical engineering for industrially relevant direct conversion of CO2 and H2 to methane, methanol and DME. In addition, examples will illustrate electrochemical process optimisation with 3D printed metal mesh-like electrode design providing optimum transport across the flow field under the target operating conditions. Relevant experimental data, including modelling were employed to optimise the multi-layered structures in each development cycle. (Figure 1). The physical and chemical evolution of the support material and active nanoparticles was studied using multiscale 3D imaging techniques such as in situ/operando X-ray computed tomography (CT) and scanning transmission electron microscopy (STEM).

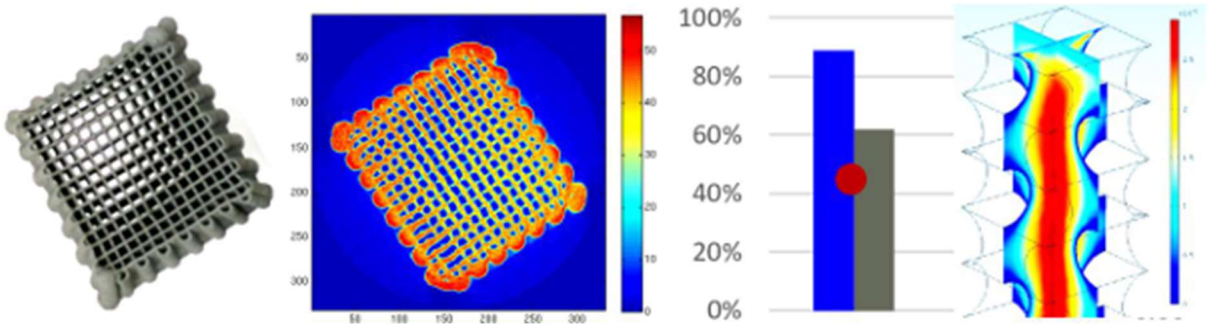

Figure 1. Studies on (from left to right) 3D printed catalysts, XRD-CT images revealing the physico-chemical characteristics of 3D printed catalyst, performance measurements and related flow field modelling.

CFD-DEM Model Development for Large-Scale Reactive Flows: Blast Furnace as an Example

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Power and Flow group, Eindhoven University of Technology (TU/e), NL
Eindhoven Institute for Renewable Energy Systems (EIRES), TU/e, NL

To date, more than 70% of the iron consumed is produced via blast furnace (BF). In modern BFs, the high-speed air injection creates a void region, called "raceway", nearby the injection zone, where the along-injected pulverized coals are combusted to provide heat and reducing agents, complementing the usage of expensive coke. The raceway formation is crucial for the overall furnace performance. Direct measurement is almost impossible due to high temperature and pressure. We resort to numerical modelling to unveil the complex underlying physics in the raceway using CFD-DEM.

Two modelling reduction techniques are employed, making industrial-scale BF simulations feasible. The coarse-graining method replaces groups of particles with representative parcels to ease the computational burden. In this work, we extend the method to polydisperse particle systems with a novel particle-size dependent smoothing scheme [1], which improves the mass/heat exchange between the Euler and Lagrange phases. The computational cost is further reduced by applying the Flamelet Generated Manifold (FGM) method for gas-phase combustion [2]. It employs a pre-computed lookup table and retrieves combustion information in the process of simulation.

The developed coarse-grained CFD-DEM-FGM model is used to simulate raceway formation in a real industrial BF [3]. Large coke particles (mean size of 34mm) and small coal fines (mean size of 110 μm with a coarse factor 8) are simultaneously considered in the simulations. It is shown that the high momentum air blast results in a physical raceway whereas the combustion sustains a chemical raceway. The two raceways clearly do not overlap, indicating that not all crucial reactions occur within the physical raceway which might be the commonly measured ones. Furthermore, the simulation results highlight the significance of enhancing PC-air mixing to improve the PC utilization and provide insights into optimizing BF operations.

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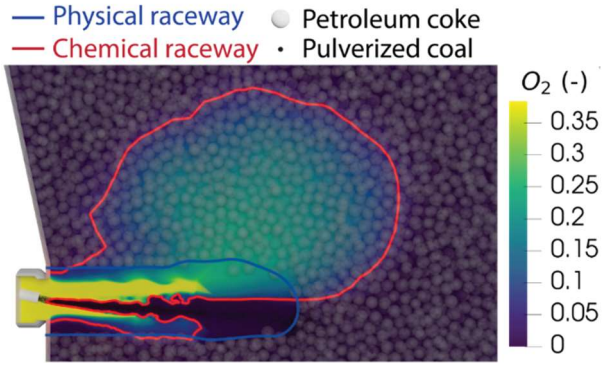

Fluidization and Granulation

CFD-DEM Simulation of the Drying and Solidification Behaviour of Individual Droplets During Spray Drying

Moritz Buchholz[1], Riccardo Togni[2], Dominik Weis[1], Christoph Goniva[2] and Stefan Heinrich[3]

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[3] TU Hamburg, Institut für Feststoffverfahrenstechnik und Partikeltechnologie, Hamburg

The spray drying process enables the efficient production of large quantities of granular material from liquid solutions or suspensions. This process is typically a step in a larger production chain, which includes upstream process operations such as synthesis, and downstream processes for additional drying, sieving, or further processing of the granular material. In addition to their size distribution, the morphology of the spray-dried particles has a significant influence on the resulting quality and handling of the product material. For example, hollow particles are characterized by lower tensile strength, which can lead to an increased fragmentation of the product. The particle morphology can be influenced by the drying conditions experienced in the spray dryer, as well as by the upstream processes that determine the properties of the drying material. Due to the challenges of scaling-up the results obtained from laboratory experiments to larger scales, computer simulations can be used to support the design and optimization of facilities at production scale. This contribution presents a novel unresolved CFD-DEM simulation approach for modelling single suspension droplets undergoing drying and a solidification process in a hot gas. The key mechanisms of the model, which describe the particle-fluid interactions, the energy and mass exchanges with the surrounding gas, are illustrated in Figure 1a. The droplet solidification is accounted for by the formation of solid bonds between the primary particles in the suspension. A sensitivity analysis reveals that the properties of the solid bonds determine the droplet´s drying rate and can thus lead to the formation of particles with different morphologies; see Figure 1b, c.

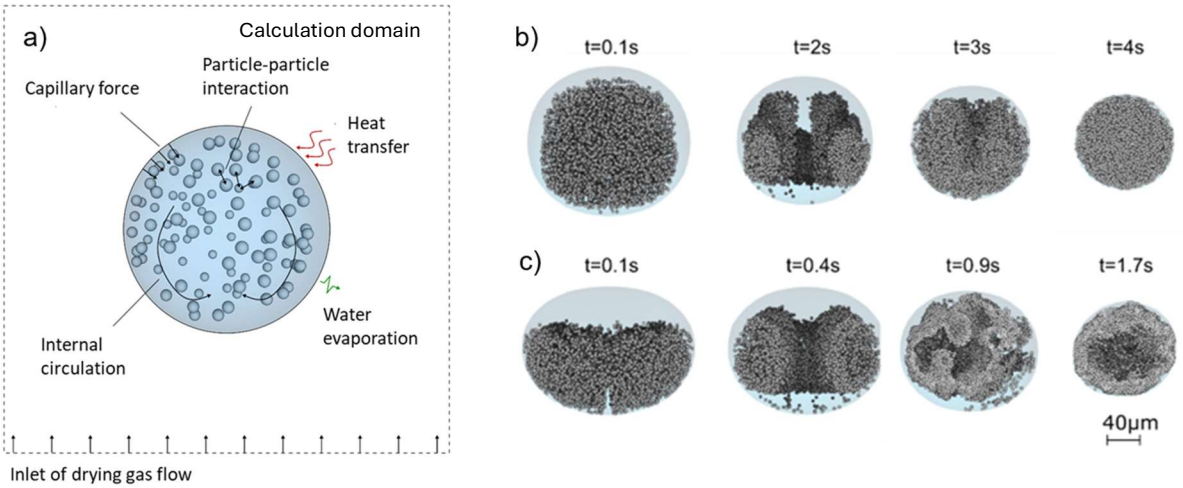

Figure 3: a) Calculation domain of CFD-DEM simulation and interactions between primary particles, the liquid and surrounding gas to describe the drying process of a single suspension droplet in a hot gas environment. Time series of drying and solidification of different suspension droplets leading to the formation of a dense, spherical particle (b) and a hollow particle (c) [1].

Bibliography

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Processes, 12 (2024) 3, DOI: 10.3390/pr12030480

Eulerian-Lagrangian Simulations of Particle Dispersion in Fluidized Bed Heat Exchangers

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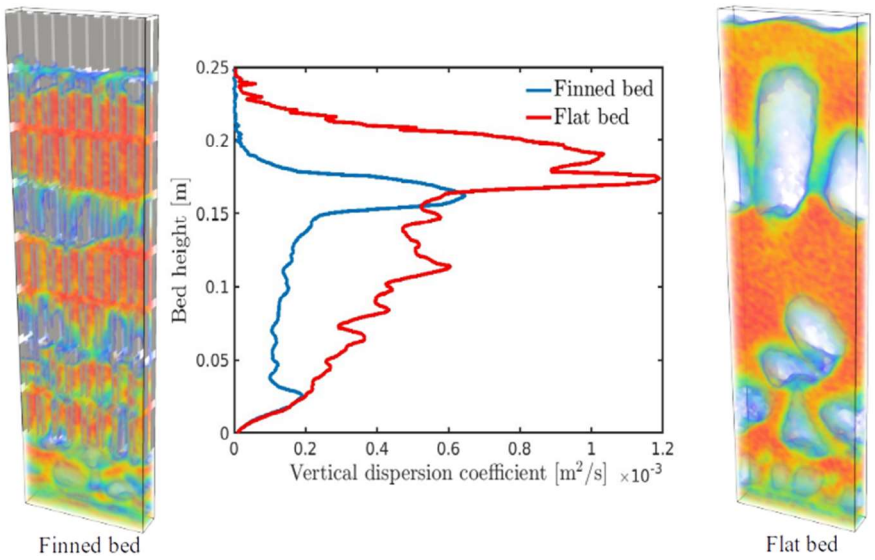
High-temperature particle-based thermal energy storage (TES) systems operating above 700°C are highly effective for providing continuous heat from advanced concentrating solar power (CSP) plants. Narrow-channel counter-flow fluidized bed heat exchangers are a promising technique for extracting heat from hot particles, as fluidization enhances mixing and increases the particle-wall heat transfer coefficient. However, while experiments indicate that particle dispersion across the depth of the bed channel improves particle-wall heat transfer, dispersion along the greater vertical lengths spreads the thermal energy throughout the height of the fluidized bed, evening out the temperature profile. This mixing reduces the effectiveness of the heat exchanger by decreasing the effective logarithmic mean temperature difference between the particles and the power cycle fluid.

Eulerian-Lagrangian simulations are employed to investigate the effects of extended surfaces in narrow-channel fluidized bed heat exchangers as a way to reduce particle dispersion along the vertical direction and mitigating vertical mixing. To demonstrate the effectiveness of extended surfaces, the overall particle-based dispersion coefficient without extended surfaces is compared against aligned and staggered extended surface configurations. We demonstrate the effectiveness of fins in reducing vertical particle dispersion for a range of operating conditions. We also compare Eulerian-Lagrangian simulations against experiments, for which the particle dispersion coefficient can be estimated from the fluctuations of the pressure across the bed. The role of heat transfer and the effects of fins on the heat transfer coefficient is also discussed by comparing different models for the particle-wall heat transfer in Eulerian-Lagrangian simulations.



Wear, Breakage and Erosion

Coupled CFD-DEM Simulation of Flow-Induced Erosion in Cohesive Materials

***DI Dr. mont. Sandra Vollmann*, Mohsen Rahimilarki**

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Erosion is one of the continuous wear mechanisms in cohesive and non-cohesive materials induced by shear forces applied by the fluid flow on the liquid/solid interface. In cohesive materials, the degree of erosion resistance is markedly influenced by the strength of inter-particle bonds, which introduces a layer of complexity to the erosion process. The current understanding of the relationship between inter-particle bond strength, erosion factors, and their respective contributions to the flow-induced erosion process is still not fully understood and remains a topic of ongoing research. The present research establishes a coupled Computational Fluid Dynamics (CFD)-Discrete Element Method (DEM) framework for visualizing and conducting quantitative analyses of flow-induced erosion in cohesive materials. A cohesion model was then employed to describe the strength of the cohesive bond. This model considers the cohesive forces for the grain/matrix of cohesive materials, such as soils and refractory. The simulation results indicated that the current coupled approach can capture the evolution of erosion topography on the meso- and micro-scales. The proposed CFD–DEM approach can effectively estimate the erosion initiation and erosion rate of cohesive materials in different applications and geometries. This work is a proof of concept and a basis for quantification with lab experiments in future studies.

Keywords: CFD–DEM modeling, Cohesive material, Topography evolution, Cohesion model, Erosion modeling

Aggregation and Breakage Dynamics of Alumina Particles under Laminar Shear by CFDEM®coupling

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Controlling aggregation and dispersion of particles is important for mineral processing as particle characteristics affect product grade and process efficiency [1]. For example, aggregation of fine valuable mineral particles enables their collection by froth flotation. Control methods involve adjusting pH, adding polymers, or applying shear forces to suspensions to manipulate interparticle interactions [2]. Despite shear forces being inherent in most operations, their precise effect on aggregate characteristics remains poorly understood due to difficulties in observing aggregate behaviour over microseconds. Computational Fluid Dynamics – Discrete Element Method simulations offer a promising approach for studying aggregate dynamics as they enable direct observation of aggregate formation in suspensions [1].

Here, CFDEM®coupling is applied to investigate the effect of laminar shear on particle aggregation and dispersion, accounting for particle-particle and particle-fluid interactions. The steady state aggregate size distribution closely matches the experimental distribution (Figure 1 [1,3]), validating the employed simulations. The temporal evolution of the aggregate number concentration is in excellent agreement with first-order aggregation theory [4] at low shear rates, while at higher shear, a collision efficiency equation is proposed which can be used to correct the theoretical first-order aggregation theory. Particle dynamics can be described by three distinct regimes depending on the shear rate and aggregate size, including the pure breakage, breakage and restructuring, and restructuring and aggregation regime (Figure 2 [3]). A breakage rate equation is proposed, capturing the transition from the breakage and restructuring regime to the pure breakage limit [3].

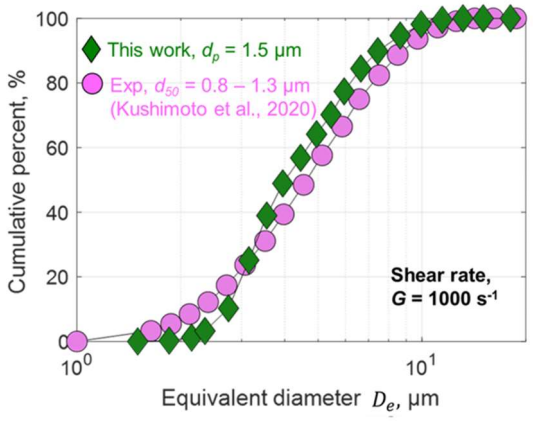

Figure 1. CFDEM-obtained [3] and measured [1] size distribution.

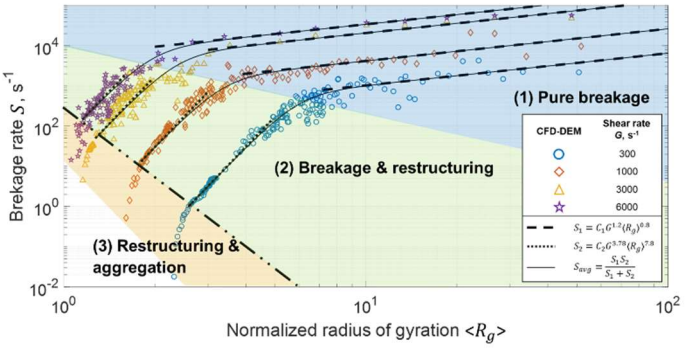

Figure 2. Breakage rate vs. aggregate size.

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Simulation Calibration and Validation of Abrasive Wear in Bulk Material Handling

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Wear is a general problem in the field bulk material handling equipment, where many abrasive materials are handled with a high mass flow rate. Abrasive wear on machine parts like chutes is one of the main maintenance issues not only for handling minerals but also in the "Agribulk" field. DEM simulations became in the past a standard tool for the optimization of bulk material handling. For a qualitative wear prediction such DEM simulations are also used since more than a decade. However, the quantitative prediction of wear and hence, the prediction of wear liners lifetime and maintenance intervals are still a challenge.

The chair of material handling of the university of Magdeburg is working on this problem since a long time. This paper will summaries the obtained results regarding the key problems of this topic:

- What kind of wear models should be used? Several wear models have been published and integrated in LIGGGHTS. The presented work indicates which models give the best results.
- Can a DEM simulation with a short observation time predict the long-time wear behavior?
- How should the wear factors in the DEM model be calibrated to reproduce realistic results?
- How well will the calibrated DEM simulations predict chute wear with different and combined types of flow?

The paper will focus on both mechanisms of abrasive wear: sliding and impact. Two calibration tests including a ring sliding wear tester, and an impact wear tester were used. The experimental results for granite and the wall liner materials aluminum alloy are presented. This combination allowed a relatively fast evaluation of the mass loss of the wear liner and limited the attrition of particles. The validation was carried out on a 15 m belt conveyor test rig which allowed the measurement of the wear in several transfer zones.

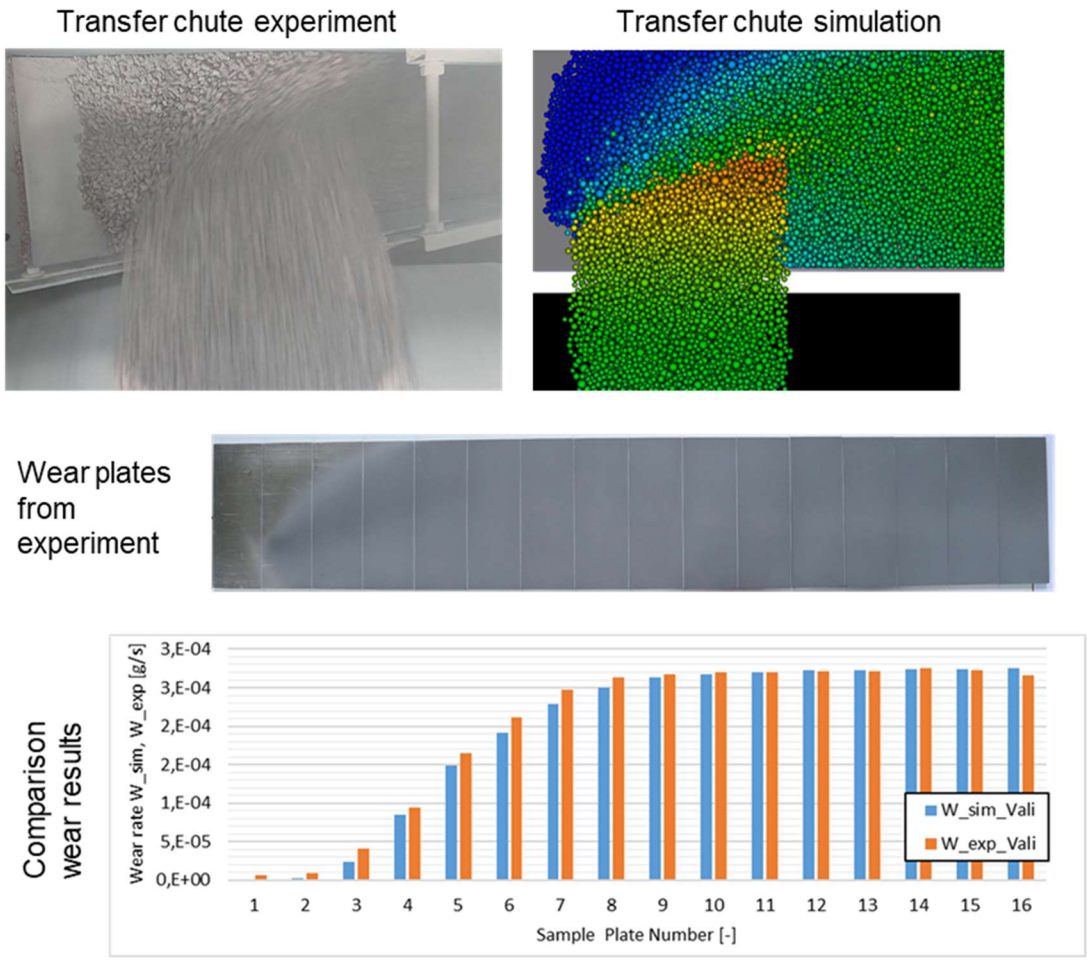


Fig. 1: Validation experiment and simulation, comparison of the wear measurements.

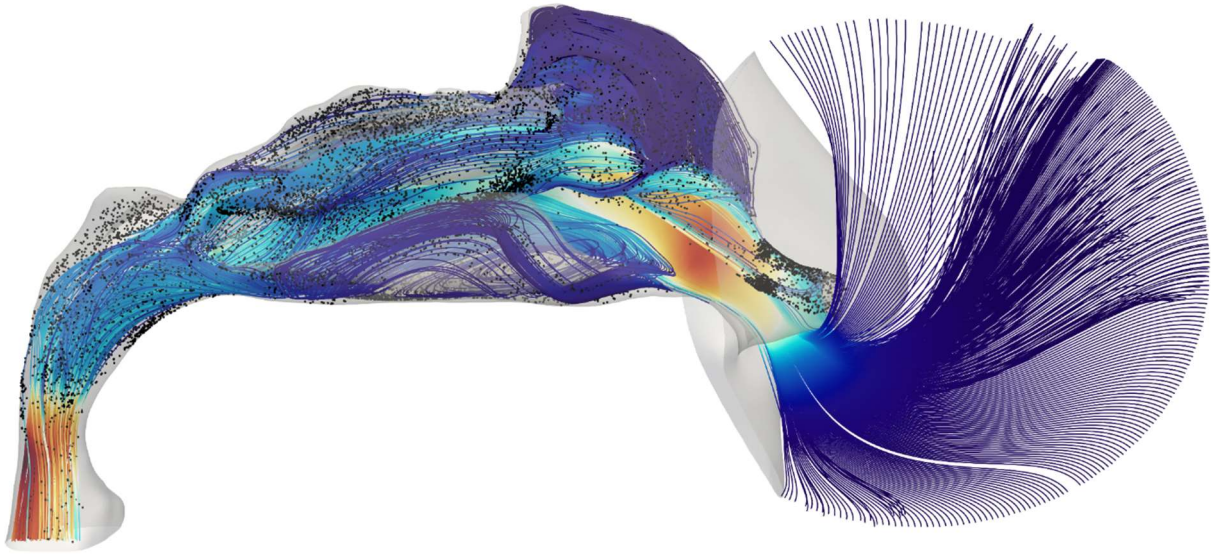
Biomedical Applications

Droplets Inhalation and Deposition in the Human Upper Airways

Alfredo Soldati

Institute of Fluid Mechanics and Heat Transfer, TU Wien

In this work computational fluid dynamics is used to investigate water spray delivery in the human upper airways, with a focus on photodynamic inactivation (PDI) therapies for the treatment of respiratory infections. The airflow in the nasal cavity is studied by means of RANS simulations, while the water droplets inhalation and deposition is described with a Lagrangian approach. Simulations are performed on a patient-specific anatomy, reconstructed from CT scans images, and under steady inspiration. A one-way coupling between the flow and the droplets is assumed, with droplets behaving as rigid spherical particles subjected to gravity and drag forces. For two different breathing intensities, ($Q = 10{,}20\ l/min$), eight different droplets diameters are considered ($dp = 1{,}3{,}5{,}7{,}9{,}10{,}20{,}30\ \mu m$) in order to represent different types of PDI treatments. The results are analysed qualitatively and quantitatively in terms of droplet deposition, in order to assess the effectiveness of the different treatments. In particular, the final droplets deposition is evaluated in terms of deposition fraction, while the droplets transient behaviour is characterized by calculating the deposition flux. The final droplets distribution and clustering on the nasal cavity walls is then observed by computing the deposition density and applying the Voronoi tessellation technique.



Figure

1: Instantaneous visualization of the flow field and droplets on a lateral view of the human nasal cavity, for $dp = 1\ \mu m$ at time $t = 0.34\ s$. The turbulent flow is highlighted by stream traces coloured according to the velocity magnitude, while the droplets are represented by black spheres. The 3D geometry is shown in gray with transparency.

Assessing the Risk of Thrombogenesis in the Left Atrium using Computational Fluid Dynamics

Manuel García-Villalba

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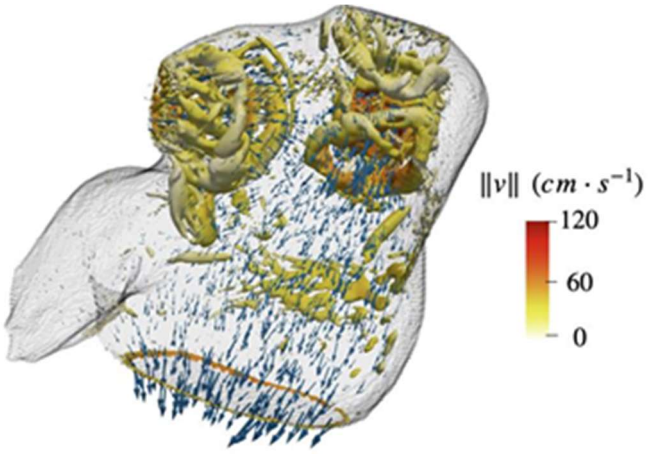
Cardiovascular diseases are the leading cause of mortality worldwide. In particular, ischemic stroke affects over 18 million people each year. It is estimated that 30% of these strokes are caused by thrombi generated in the left atrium (LA) of patients with atrial brillation, the most common arrhythmia. Furthermore, up to an additional 30% of all ischemic strokes are suspected to be atriogenic in patients with subclinical AF or normal cardiac rhythm. Most of these thrombi are formed inside the left atrial appendage, a small saccular protuberance whose anatomy and hemodynamics vary significantly among patients. However, current medical procedures to estimate ischemic stroke risk are based on population demographics and do not consider patient-specific information about LA haemodynamics, a crucial causal thrombosis factor.

Computational fluid dynamics analysis based on patient-specific medical images is a powerful tool for investigating LA flows. Together with our collaborators in Madrid, San Diego and Seattle, we have developed a methodology to perform numerical simulations of the flow in the LA. From the medical images, after a process of segmentation and registration, we obtain a spatio-temporal model of the atrial wall motion that can be imposed as boundary condition. The inlet boundary conditions also require particular attention since there is some uncertainty on how much flow enters the LA from each pulmonary vein. As a result of the simulations, in addition to the velocity fields we determine the residence time of the blood in the LA. We also employ biochemical models of blood coagulation to determine the concentration of relevant substances. CFD-DEM simulations are still not employed in this analysis, but they will certainly be relevant in the near future. By analysing the results of the simulations, we can assess the risk of thrombogenesis. In the presentation, I will discuss the developed methodology, and I will show results from simulations of the flow in the LA of patients with and without impaired atrial function.



Visualization of the flow in a patient-specific left atrium

Computational and Experimental Investigation of Dispersion and Dissolution in Pharmaceutical Powders

***Khizra Abdul Wadood*[1,2], *Dr Andrew Ingram*[1], *Dr Christopher Windows-Yule*[1], *Dr Matthew Molloy*[2]**

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This research addresses the prevalent challenge of lump and aggregate formation during the mixing of pharmaceutical powders with solvents, a critical issue in drug formulation. Conventional experimental approaches often prove impractical for rare or expensive materials, necessitating the development of computational methods that provide efficient, scalable solutions. Employing a combination of computational models and experimental approaches, this study explores and refines the dissolution processes of pharmaceutical powders under varying conditions. The primary objectives are to develop a robust modelling approach for the mixing of these powders, identify key variables that influence the process, and create scalable models applicable to industrial settings. The study introduces sophisticated computational fluid dynamics and discrete element methods (CFDEM) to simulate these processes, focusing on the interactions between particle surface characteristics and fluid dynamics. By analysing dimensionless parameters such as Bond number, Capillary number, and Reynolds number, the study identifies optimal mixing conditions that prevent the formation of dry lumps and enhance dissolution efficiency. The comprehensive approach not only examines the dissolution process through its successive stages—wetting, sinking, swelling, dispersion, and dissolution—but also quantifies the impact of forces like capillary pressure and buoyancy on powder behaviour. The outcomes offer a robust roadmap for improving mixing strategies in pharmaceutical manufacturing, highlighting the potential of computational modelling as a viable alternative to traditional methods. This innovative approach promises substantial benefits for the pharmaceutical industry, including cost reduction, increased efficiency, and enhanced product quality and safety.

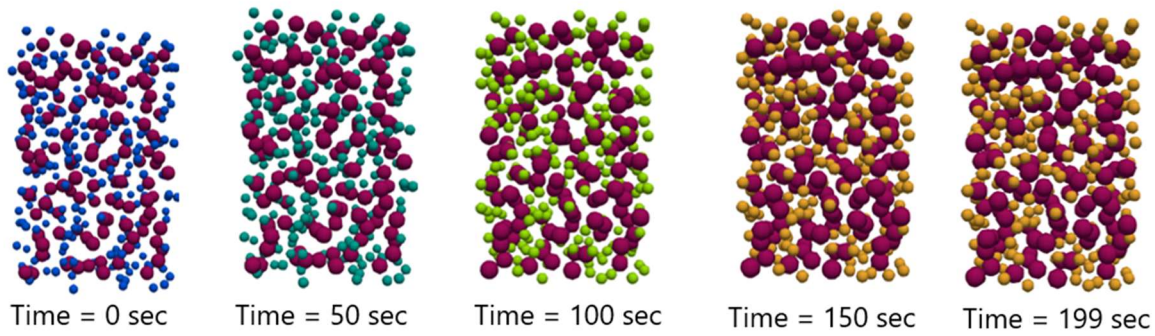

Figure 1: DEM Simulation of Particles Swelling

Immersed Boundary Methods

Liquid-Gas Flow around Resolved Densely-Packed Objects in CFD-DEM

***Martin Niemann*[1], *Dennis Heinrich*[2], *Giovanni Viciconte*[1], *Christoph Goniva*[1], *Jürgen Grabe*[2], *Christoph Kloss*[1]**

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This contribution presents recent solver enhancements in CFDEM®coupling for two-phase liquid-gas flows in the presence of resolved solid objects modelled by the Immersed Boundary Method (IBM). The method is very versatile and allows using all particle shapes as well as triangulated surface meshes. Particular focus is given to solver validation using various validation examples. Ensuring the impermeability of solid objects is crucial in this regard and paramount to mass conservation. Moreover, the handling of contact angles of the liquid-gas interface at the particle surface modelled by the IBM is discussed. A suitable test case to quantify the impact of the contact angle is the force exerted by a liquid bridge between two adjacent particles.

Finally, the imbibition of a packed sand bed is investigated as an application case for the developed set of models. The particle packing is extracted from in-situ X-ray computed tomography data of a corresponding laboratory experiment. The shape of each individual particle is approximated as a purely convex body to reduce computational complexity. The imported and initially dry bed of sand particles is filled with water from the bottom, and simulation results from the presented IBM are compared to those of a similar setup using body-fitted meshes. This contribution, moreover, demonstrates the impact of particle motion that can now be modelled with the presented approach.

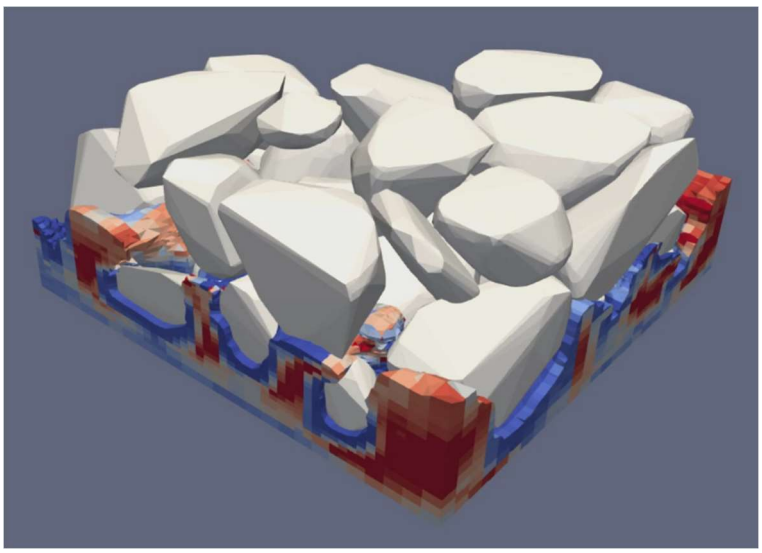

Figure 14: Small imbibition case with few convex particles segmented and extracted from the experimental CT data. Liquid enters from the bottom at a fixed velocity and is coloured by its velocity magnitude.

Small-Scale Investigation of Bubble-Particle Interactions using a Coupled VOF-IB Method

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The three-phase bubble columns are widely used in different chemical industries as a multiphase reactor for petrochemical, biochemical, and metallurgical processes. The design of these columns is still challenging due to the complex nature of hydrodynamics at different spatial and temporal scales. Thus, a fully-resolved picture of bubble-particle interactions is important for design and optimization purposes. In this study, a coupled volume of fluid-immersed boundary method, namely resolved VOF-DEM, is employed to investigate the interactions of a single rising bubble with a solid particle at different physical conditions. The OpenFOAM-based geometric VOF technique of isoAdvector is coupled with LIGGGHTS to track the liquid-gas interface with the one-fluid assumption and treat the particle presence as an immersed body within the computational domain. Simulations were carried out for the air bubble diameters of 3-6 mm in water, and particle sizes of 1-3 mm at different relative velocities and liquid viscosities indicating a wide range of Capillary and Eötvös numbers.

The results reveal that as the bubble approaches the particle, under specific conditions of bubble diameter and liquid viscosity, a strong thin liquid film forms between them preventing their collision as shown in Figure 1. Furthermore, it is observed that reducing the liquid viscosity or the bubble diameter results in the fast disappearance of the said liquid film, leading to the eventual collision of the bubble and particle. When the particle is fixed in space, this observation is aligned with an existing theory known as the Stefan-Reynolds model that describes the liquid film drainage process. Further analysis of particle wettability, smaller particle sizes in the sub-millimeter range, and in-house experimental validation are the subjects of ongoing research. This small-scale investigation is essential for the development of scale-up simulation strategies applicable to real-scale three-phase bubble columns.

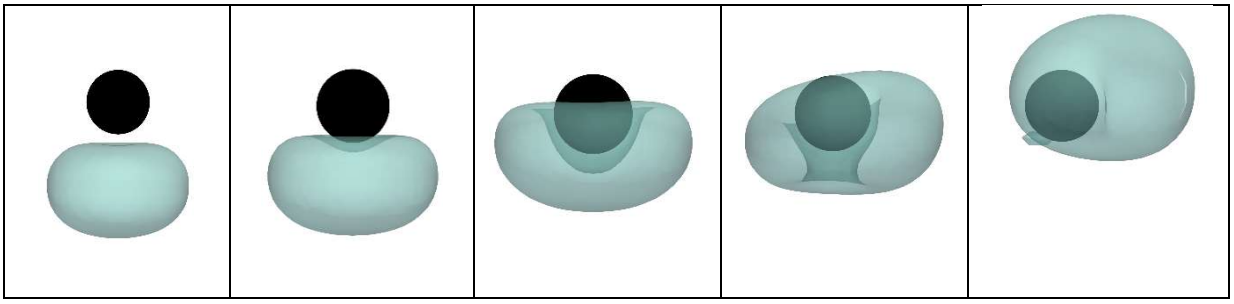

Figure 1:
Time sequences of a rising air bubble with d_b = 6 mm (light blue) approaching a solid particle with d_p = 3 mm (black) in a highly-viscous liquid. The physical conditions correspond to the dimensionless numbers of Ca = 0.35 and Eo = 5. The formation of liquid film is evident and the bubble eventually passes by the particle without collision. The snapshots were captured at intervals of 20 ms.

IBM-DEM Approach to Consider the Suspension Rheology

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The CFD-DEM simulations have gained interest in the simulation of different complex processes. One of the main areas of interest is the simulation of the rheological behavior of the suspensions, it is because increasing the volume fraction of the particles could change the rheological response of the suspension. To gain a deeper understanding of the suspension physics, we conducted a fully resolved CFD-DEM simulation, paying particular attention to the flow field surrounding the particles. For this reason, we developed a variant of the immersed boundary method before coupling it with our in-house DEM code, named XDEM. This model was validated with different test cases to make sure that it could correctly capture the correct forces faced by the particles, ranging from hydrodynamic interaction to collision forces between particles. Then, we implemented our developed CFD-DEM model to consider the behavior of the particles within the suspensions. The Phillips and Krieger-Dougherty models were used to validate the distribution of particles and the suspension relative viscosity, respectively. In this step, different particle sizes and volume fractions were investigated. After this successful validation between the numerical and analytical results, we aimed to visualize the field data over the particles to explain the reason for the shear induced particle migration. This allowed us to better interpret the shear induced particle migration.

Keywords: Immersed Boundary Method, Discrete Element Method, Coupled Simulation, Rheology

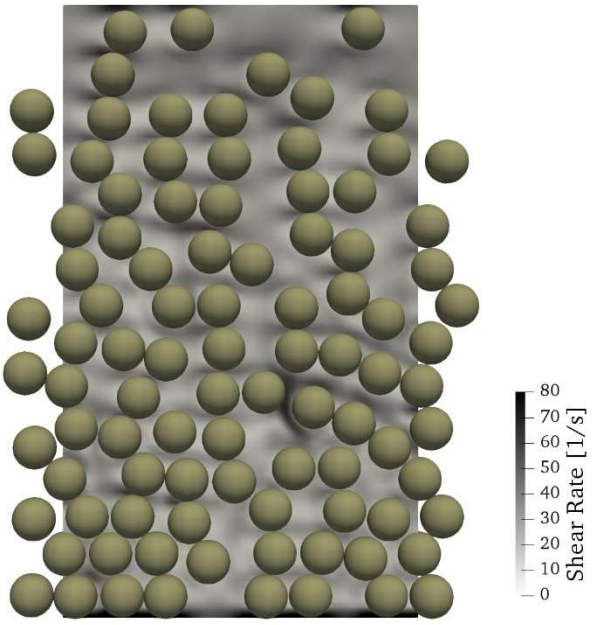


Figure 1. Shear rate distribution over the particles

Innovative Numerical Methods

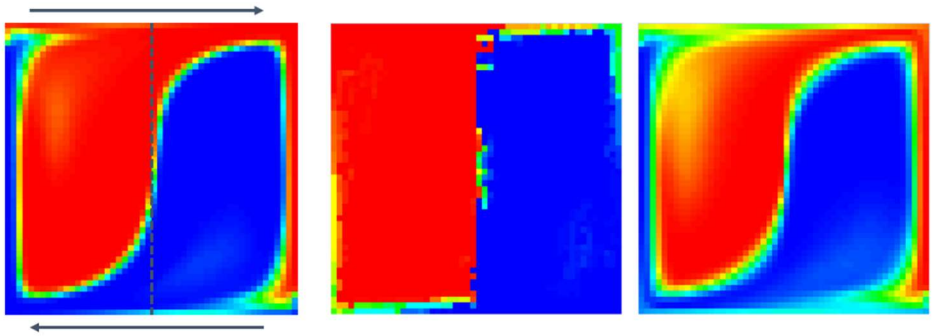
Time-Extrapolation of Pseudo-Periodic Flows by recurrence CFD (rCFD) – Doing the Homework ...

Stefan Pirker, Daniel Queteschiner, Hannes Lumetzberger, Thomas Lichtenegger

Johannes Kepler University Linz

rCFD has been shown to speed up pseudo-periodic flows like fluidized beds by three to four orders of magnitude. While early success stories just focused on the bright side of rCFD by emphasizing on its fascinating computational efficiency, this methodology still suffers from a series of potential pitfalls.

To start with, the existing version of rCFD exhibits significant propagation errors in nearly stagnant flow regions. In order to overcome this problem, an automated calibration procedure for cell-to-cell shifts is introduced, which is based on a new calibration scheme for the Lagrangian propagator of fluid flow. In a first lid-driven cavity test case, we prove that this calibrated version of rCFD reduces propagation errors significantly. Finally, this new method is applied to secondary gas injection in a fluidized bed.



Fifure 1: Lid driven cavity: (left) full CFD, (middle) old and (right) new rCFD

Next, we discuss the case of non-passive propagation of temperature. Obviously, resulting gradients in the temperature field give raise to buoyancy driven natural flow, thus changing the original flow field. Consequently, any isothermal flow database will be violated. Based on a lab-scale demonstrator experiment, we show that in this case multiple databases are needed, and we further discuss ways of how to establish and execute them.

Since multiple databases are prone to excess data requirements, we finally propose a coarse-graining concept for rCFD for the purpose of data reduction. This coarse grained rCFD can be regarded as a spatially filtered representation of a high-resolution Lagrangian propagator. Based on a metallurgical process, we show the functionality of this data-reduction methodology.

While all of these potential pitfalls of rCFD still exist, we introduced conceptual counter-measures. We believe that these under-the-hood improvements will lead to an extended applicability of rCFD in the realm of process modelling.

Simplified Fluid Model for Confined Domains

***Andreas Aigner*, Christoph Goniva, Christoph Kloss**

DCS Computing GmbH, Linz, Austria

One the one hand coupling particle and fluid simulations has proven to be crucial for showing and understanding physical phenomena in a wide range of industrial applications. On the other hand, this coupling can be not only computational expensive but also the setup of complex moving apparatus may be challenging.
In this work we show a simplified modelling approach that can be implemented fully on the particle side and therefore, avoid the setup and computation of a full CFD simulation. Obviously, such a modelling approach always implies restrictions where to use it, but the advantages of a simple and fast setup and low computational overhead outweigh the disadvantages by far.

The method presented in this work uses a 1D-cellular automata to calculate depending on the current particle distribution a flow resistance and distribute the fluid flow accordingly. Thus the fluid flow in the main direction of interested is depicted quite accurately while crossflows are neglected. Particle motion as well as mesh motions may contribute to the introduced fluid flow. (see Fig. 1)

Comparing simulation results of simulations for standard DEM, fully coupled CFD-DEM and the new approach show good agreement with little overhead. (see Fig. 2)

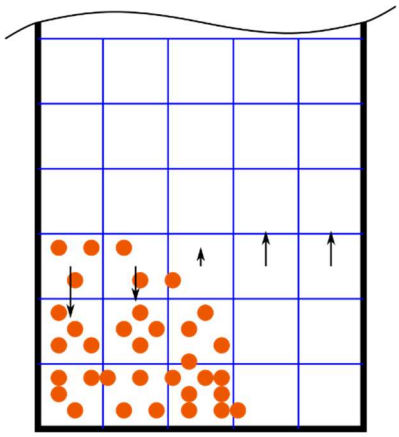
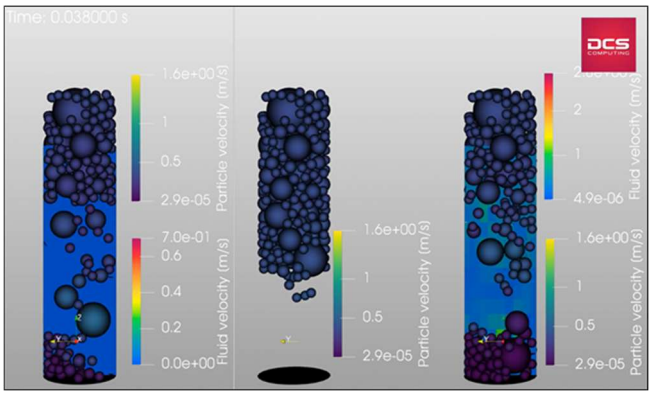


Fig.1: Falling particles (orange) trigger fluid motion and return flow (black arrows)



ASX fluid model (presented model) | ASX no drag (standard DEM) | Full CFD-DEM (reference)

Fig.2: Comparison between standard, fully-coupled and new approach

Comparing Aspherix® against Open-Source DEM Frameworks for Simulations of Common Bulk Processes

Marcel Kwakkel, Augusto Moura, Chris Goniva, Chris Kloss

DCS Computing, Linz

There is a wide range of discrete element method (DEM) based software for modelling the dynamics of granular materials. Their commonality is that they all track the behaviour of particles by iteratively solving the equations of motion via explicit time integration. During each time step all particles in contact are detected, after which the calculated interaction forces and torques are used to integrate their motion. Despite such similarities, there is a significant difference between their efficiency, usability and applicability. These are directly affected by aspects like: data structure selection, parallelization techniques, physical model availability, convenience of (graphical) user interfaces and documentation quality.

A recent benchmark study [1] compared the performance of nine widely-used DEM frameworks: BlazeDEMGPU, ESyS-Particle, GranOO, Kratos Multiphysics, LIGGGHTS, MercuryDPM, MFiX, MUSEN and YADE. Only open-source software packages were considered, since these are freely available and their underlying algorithms can be reviewed and tested. In addition to analysing the simulation results, also the performance of the DEM software was compared. For this, all benchmark cases were run on a personal computer equipped with one CPU and one GPU.

The benchmark consists of three common bulk processes: (i) emptying of a silo, (ii) mixing in a rotating drum and (iii) impact of a particle on a particle bed. In all three cases, the standard formulation of the visco-elastic Hertz-Mindlin model for dry contacts was used and only spherical particles were modelled.

This work will extend these benchmark results by running the same cases with Aspherix, a commercial DEM software package developed by DCS Computing, Austria. An in-depth analysis of differences between Aspherix and LIGGGHTS will be given.

References:

[1] Dosta, M., Andre, D., Angelidakis, V., Caulk, R. A., Celigueta, M. A., Chareyre, B., Dietiker, J. F., Girardot, J., Govender, N., Hubert, C., Kobyłka, R., Moura, A. F., Skorych, V., Weatherley, D. K., & Weinhart, T. (2024). Comparing open-source DEM frameworks for simulations of common bulk processes. Computer physics communications, 296, Article 109066. https://doi.org/10.1016/j.cpc.2023.109066

DEM Surrogate Modelling of Particulate Processes

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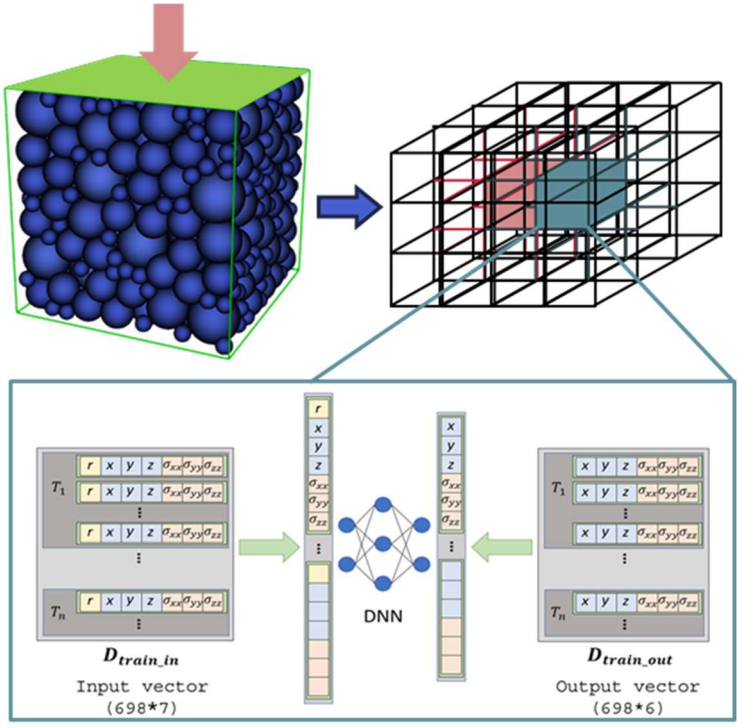
Artificial Intelligence (AI) is currently undergoing a revolution in terms of capabilities and acceptance in science and industry. In recent years, very advanced "narrow AI" methods have been published, such as Alphafold (protein folding) or GNoME (materials science), which act as highly accurate and quick to apply surrogate models that demonstrate the ability to accelerate progress by orders of magnitude. In the context of this work, such a surrogate model is demonstrated for discrete elements method (DEM), dynamically emulating the DEM itself. By training fast-applicable AI models based on neural networks that emulate DEM, significant acceleration and exploration to much larger simulation domains can be achieved, while maintaining the inherent flexibility of simulations compared to custom predictive models of more specific systems. In the specific case, the simulation domain is discretised into a grid of neighbouring cells in which a neural network periodically predicts particle motion, contacts and other properties such as forces over time, followed by periodic grid updates to allow particle migration throughout the investigated domain. High accuracies can be achieved for different application cases, such as the compaction of particle beds or the free flow of particles in a stirred tank. The approach is compared with both classical simulations and specific predictive models of mills. Model scaling, time advantages, accuracy and corresponding properties are presented.

Figure 1: Training and inference of the surrogate DEM model. Particle interaction patterns are captured and trained into a neural network architecture to predict the temporal and spatial interactions in large domains of communicating unit cells.



Fundamentals

Mixing in Coarse-Grained Rotating Drum Simulation

Balázs Füvesi[1,2], Christoph Goniva[2], Vanessa Magnanimo[3], Stefan Luding[1]

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The discrete element method (DEM) is commonly used to simulate granular flows and optimize processes involving particulate materials in various industries. DEM treats granular materials as individual particles, tracking their movement and interactions. However, accurate simulations with DEM often require a large number of particles, leading to high computational demands that can make DEM impractical for industrial-scale applications.

Coarse graining (CG) applied to DEM presents a potential solution. CG involves replacing groups of small real particles with larger virtual particles, significantly reducing the number of simulated particles and computational load. However, applying CG to DEM simulations of mixing and segregation processes presents specific challenges, as the goal is to capture the effects associated with the original, fully resolved particle mixture.

In our study, we explore mixing dynamics within a rotating drum by gradually increasing CG factors across different operational regimes from rolling to cataracting. This approach allows us to observe flows with varying degrees of dynamic behaviour. We evaluate the mixing performance in each drum simulation using different mixing indices. We compare the mixing characteristics and features between CG simulations and the original, unscaled simulations across different CG factors and operational regimes.

Some of our findings are as follows: Firstly, we find that maintaining consistent mixing evaluation with CG is more reliable in the rolling regime but becomes challenging as the dynamic behaviour increases in the drum. Furthermore, we highlight the importance of selecting appropriate mixing indices to measure specific mixing mechanisms, such as diffusive or convective mixing. Additionally, we note that utilizing mixing indices less sensitive to CG allows the usage of higher CG ratios, leading to substantial reductions in simulation costs.

Modeling of Cohesive and Interlocking Bulk Solids using Tetrahedral Multi-Spheres

Michael Mitterlindner, Lukas Maier, Hadie Benabchiasli and Stefan Radl

Institute of Process and Particle Engineering, Graz University of Technology

The recycling process of batteries will play a crucial role in the near future, providing a pathway towards efficient utilization of valuable resources and mitigation of environmental impacts. Our present contribution focusses on simulating the handling of shredded nickel-metal hydride (Ni-MH) batteries during a typical recycling process: after a shredding step, the material must be conveyed and cooled prior to storage. By developing a simulation approach for such materials, we aim to optimize this recycling processes with respect to resource efficiency and environmental impact.

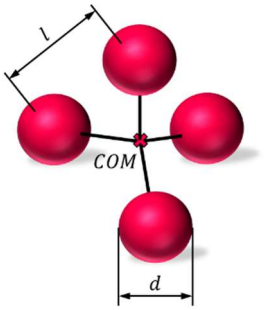


Figure 1: A tetrapod.

Conventional experimental validation is difficult due to the carcinogenic nature of the material, dust generation, and corrosiveness. In addition, the modeling process is challenging due to (i) the cohesive nature of the material (mainly caused by interlocking flakes, fine particles and liquid bridges), (ii) large differences in the material behavior when stress is applied (ranging from low stress flow to high pressure compaction), and (iii) the low effective heat conductivity of the material. To address these challenges, we propose a novel DEM approach using tetrahedral multi-spheres (i.e., “tetrapods”, see Figure 1). Specifically, two key improvements were implemented in the tool LIGGGHTS:

(1) Flexible tetrapods: this feature allows individual spheres within a tetrapod to displace, which is essential to model large tetrapod deformations. While rigid tetrapods (i.e., the vanilla multi-sphere implementation) with a simple cohesion model already perform well in low stress scenarios (e.g., a draw-down test, see Figure 2, a compaction process requires more complex modeling techniques. Flexible tetrapods prove to be an essential component for such a more realistic compaction modeling, as they are able to capture complex material responses. For example, our plastic deformation model of the tetrapods can be used to represent the inherent tendency of the material to remain compacted after the stress has been released.

(2) Finite intra-tetrapod heat conduction: this feature overcomes the unphysical infinite heat rate transfer problem, present in the classical multi-sphere approach. Our "intra multi-sphere thermal conductivity" model predicts the exchanged heat between individual spheres that constitute the tetrapod. By adjusting this conductivity value, heat transfer within a tetrapod can be tuned to better reflect the presence of air gaps and match the effective bulk conductivity of shredded battery material.

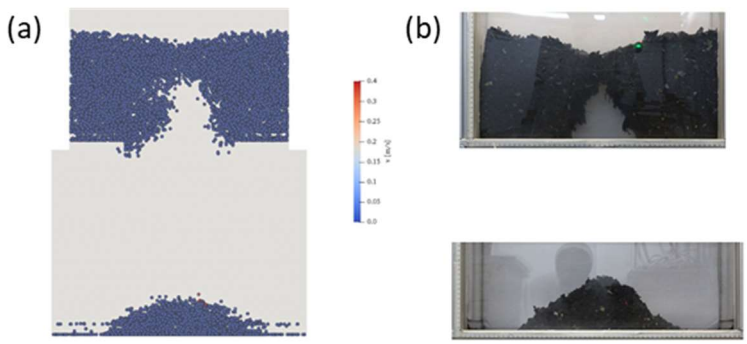


Figure 2: Comparison of the draw-down test results between simulation (a) and experiments (b).

Coupled Methods

DEM-SPH Study of Particles Dispersion in Fluid

Dinesh Adepu, Guoping Lian, Charley Wu

University of Surrey, Guildford, United Kingdom

Mixing powdered substances in tanks using a stirrer is a common occurrence across various industries. Typically, this phenomenon is studied numerically due to the complex nonlinear physics involved. In our current study, we have developed a solver combining Smoothed Particle Hydrodynamics (SPH) and Discrete Element Method (DEM) to investigate the mixing behavior of rigid circular particles within a tank under the influence of a stirrer operating at different speeds. The SPH method governs the fluid phase, while the dynamics and interactions of particles are captured by the DEM. We achieve a fully resolved coupling between solid particles and fluid particles by discretizing solid particles into dummy SPH particles. Our validation process includes verifying the fluid solver's accuracy through a Poiseuille problem and validating the DEM solver by benchmarking interactions between two particles and particle-wall impacts. The coupled model's is validated by simulating single-particle entry in a 2D steady tank and a cube settling in a tank, which is a 3D case. Following validation, we proceed with the mixing study. We conduct two simulations: one with spherical particles of uniform radius and another with particles having two different radii. Our findings reveal that as for lower stirrer speeds, particles tend to aggregate initially and remain in the center. However, with further increase in stirrer speed, particles tend to accumulate near the tank corners due to the circulation induced in the fluid due to the stirrer motion. We use an open-source software, PySPH, adapting and integrating the coupled model to conduct the current study.

Electric Field Calculations in Aspherix® and CFDEM®coupling

Philippe Seil

DCS Computing GmbH, Linz

The behavior of particle systems is often influenced by electric fields: from triboelectric charging of powders to electrostatic filters, these effects play a decisive role in many applications. However, accurate modeling of Coulomb forces in the framework of the Discrete Element Method (DEM) is challenging due to the long range of the Coulomb potential. Traditional molecular dynamics (MD) methods like Ewald sums or the Barnes-Hut method cannot be applied to real-world geometries and lack support for boundary conditions on the resulting electric field. To overcome these limitations, Kohlemainen et al. [1] proposed a split approach: the far field is calculated on a Eulerian grid, while the near field is calculated directly from particle-particle interactions. Furthermore, a correction is used to blend these two field contributions. We implemented this approach in Aspherix® and CFDEM®coupling. A validation example, also showcasing the effect of the correction term, is shown in Fig. 1. Separation of calculations produces accurate results, keeps the DEM simulation local and thus efficient, and allows imposing Neumann and Dirichlet type boundary conditions on the electric field. In addition to field calculation, we also implemented triboelectric charge transfer during collisions. We present the general feasibility of this approach, show validation studies for all components, and give an outlook on possible applications.

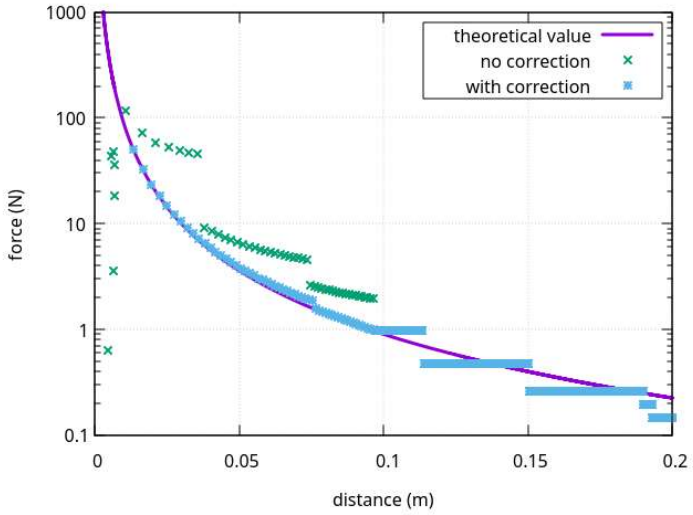


Fig. 1: Force between two particles of opposite charge. For larger distances, the field (and thus force) is a stair step because it is computed on a grid. For a distance < 0.1m (the chosen cutoff distance), the near field is calculated directly and added to the far field. Without correction term, the force shows strong deviations from the theoretical value. With correction term included, the simulated force agrees well with the theoretical value.

[1] Kolehmainen, Jari, et al. "Effect of humidity on triboelectric charging in a vertically vibrated granular bed: Experiments and modeling." *Chemical Engineering Science* 173 (2017): 363-373.

Validation of Coupled DEM-FEM Simulations

***Augusto Moura*, Marcel Kwakkel, Christoph Kloss**

DCS Computing GmbH

Coupled simulations enable the modelling of more complex and realistic applications than what is possible with a single approach. For example, fluid-structure interactions can only be properly simulated by coupling CFD and FEM simulations to study the reciprocal effects of fluid and solid on each other. Of particular interest to this work is the coupling of DEM and FEM models to simulate the interaction between solid bodies and bulk material. This is of importance to many industrial applications in multiple fields. Mining, agricultural, and pharmaceutical industries, to name a few, all deal with processes involving the transport, loading, and packing of bulk material, which will cause deformations in the tools, machinery, and packaging used in these processes. Coupled DEM-FEM simulations allow the modelling of such applications, assisting in process design and enabling prediction of behaviour and potential failures. As with any simulation workflow, coupled simulations must be validated to ensure results are accurate. This work aims at validating the coupled DEM-FEM functionality between the DEM solver Aspherix and the FEM solver Elmer built into Aspherix. Validation is performed against the experimental and numerical results in Dratt and Katterfeld [1]. The experiment consisted of a stream of material falling on top of a fixed beam. The deformation of the beam was then measured over time until the stream of particles ceased. The experimental setup is illustrated in the figure. A simulation was set up in Aspherix to replicate the experimental results, to compare the deformation of the beam with the experimental results for validation of the coupled DEM-FEM implementation in Aspherix.

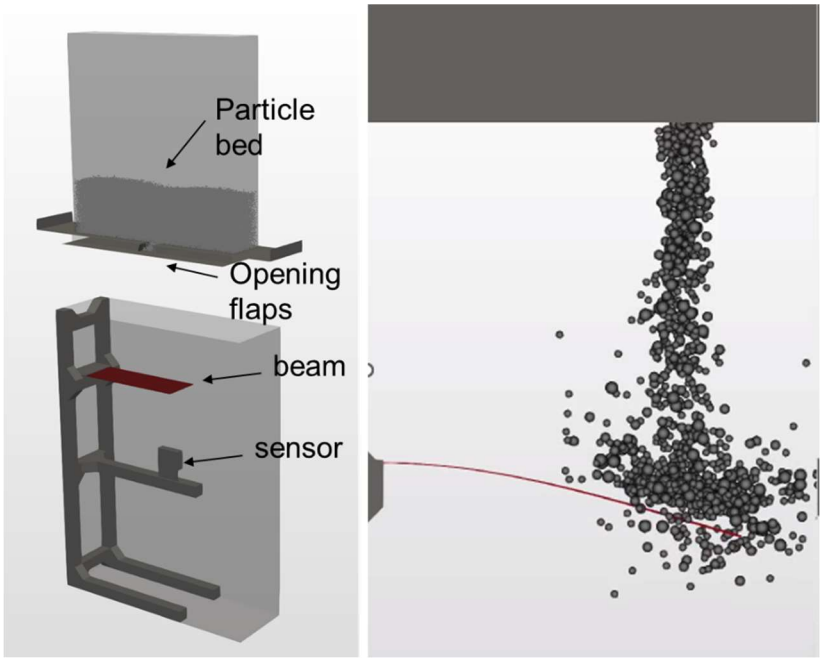


Figure 1: Experimental setup (left) and simulation results (right)

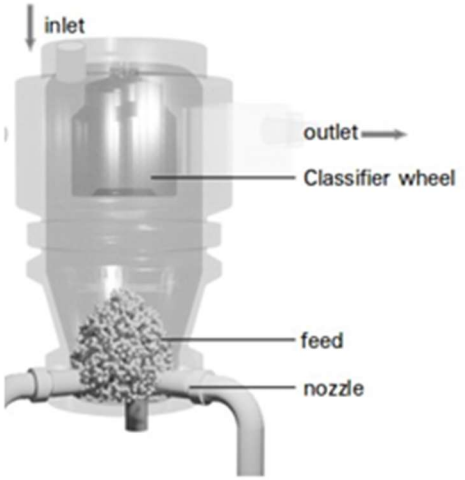
[1] Dratt, M., Katterfeld, A. Coupling of FEM and DEM simulations to consider dynamic deformations under particle load. Granular Matter 19, 49 (2017). https://doi.org/10.1007/s10035-017-0728-3

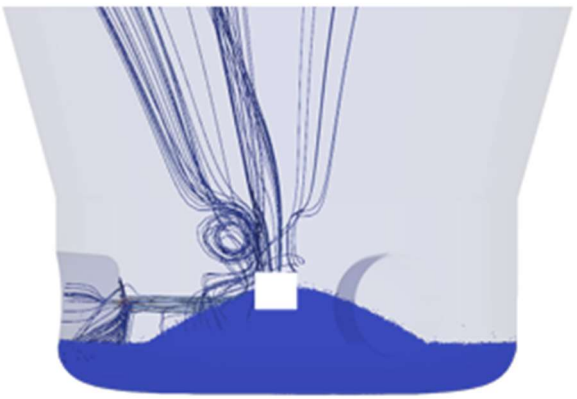
CFD-DEM Analysis on Effect of Hold-Up on Grinding Rate in an Opposed Jet Mill

Jobin Raju, Jan Henrik Finke, Christoph Goniva, Carsten Schilde

DCS Computing GmbH and TU Braunschweig

The critical role of 'hold-up' -the amount of material in a milling chamber at any given time- in jet milling processes underscores its significance in determining the grinding rate. This aspect is pivotal for achieving optimal grinding rates in continuous milling operations. Utilizing Computational Fluid Dynamics-Discrete Element Method (CFD-DEM) simulations alongside appropriate particle breakage and population balance models (PBM) facilitates the prediction of grinding rate evolution based on particle collision dynamics. In this study, we conduct a comprehensive CFD-DEM analysis on an opposed jet mill across various hold-up levels within the milling chamber. Additionally, we introduce a numerical approach to assess the evolution of grinding rates for different smaller particle size classes, using the collision distribution of the maximum sized particles employed in the CFD-DEM simulation. Contrary to conventional empirical formulations, which often lack adaptability to novel mill designs, the use of CFD-DEM simulations offers an effective alternative for gathering particle collision data and calculating grinding rates. While empirical equations are typically contingent on specific shapes, sizes, and capacity ratios, they frequently yield inaccurate predictions for innovative mill designs. Over the past few decades, empirical formulation-based PBMs have remained prevalent in granular comminution studies. Our study showcases a pioneering approach by employing a CFD-DEM-based PBM solution procedure, varying the hold-up in the investigated jet milling system. This methodological advancement holds promise for streamlining machine testing processes and expediting design iterations in industrial research, ultimately facilitating the optimization of mill designs. As this methodology continues to evolve, it stands to significantly enhance efficiency in industrial research endeavours.





DCS Invited

(abstracts with * not peer-reviewed)

A Cloud-Based Platform for Engineering and Scientific Applications*

***Augusto Moura*, Philippe Seil, Andreas Aigner,**
Christoph Döberl, Matthias Roiss, Christoph Kloss

DCS Computing GmbH

European-funded projects such as MarketPlace [1] and OpenModel [2] promote integration and dissemination of simulation and modelling workflows, bridging the gap between third-party software and promoting innovation. Engineering and scientific workflows seldom begin with complex simulations. There are myriad analytical and empirical correlations used for estimates and initial design, or for the solution of simpler problems. Despite their simplicity compared to advanced simulations, they are important stepping stones in a complete workflow. Scripting languages such as Python are of great use, allowing for the fast solution and reproduction of workflows. Python is the preeminent scripting language for such applications, simple yet powerful and versatile, with a multitude of differing solutions online (of variable quality). Simple as it may be, it still presents a learning curve to be overcome. Engicloud aims to aggregate and simplify these workflows. Offering a pre-made collection of Python calculators for a wide range of engineering and scientific applications, it allows the user to assemble complex workflows, automating the calculations in an intuitive graphical interface. Reports are automatically generated with theory and methodology of the used calculators and produced results to enable dissemination of results with colleagues and collaboration within work groups. Finally, calculators are fully editable, streamlining the code required to integrate into the platform and letting users to focus on the relevant calculations. Engicloud will streamline development of analytical and process modelling, and allow companies and research groups to coordinate, maintain and share their workflows between teams and departments.

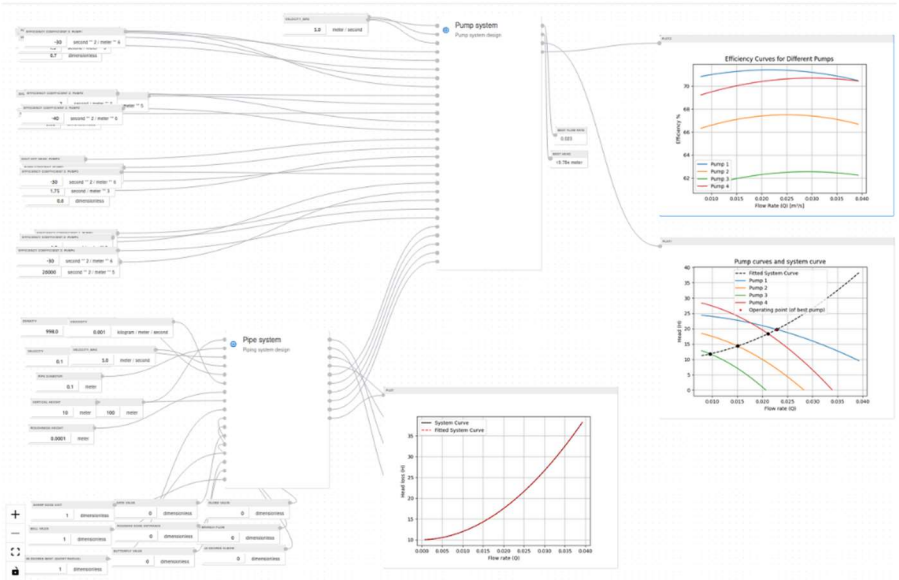


Figure 5: Schematic of a pump specification worflow in Engicloud. Given the pump curves, a user can automatically select the best pump by providing the pipe system parameters.

[1] Goldbeck, G., et al. (2023). MarketPlace - a Digital Materials Modelling Marketplace. Zenodo. https://doi.org/10.5281/zenodo.8330333
[2] Natalia Konchakova, et al. (2022). Position Paper: Open Innovation in Horizon Europe (Version 1: Jan. 2022). Zenodo. https://doi.org/10.5281/zenodo.5848552

OVITO for Custom Post Processing of Simulation Results*

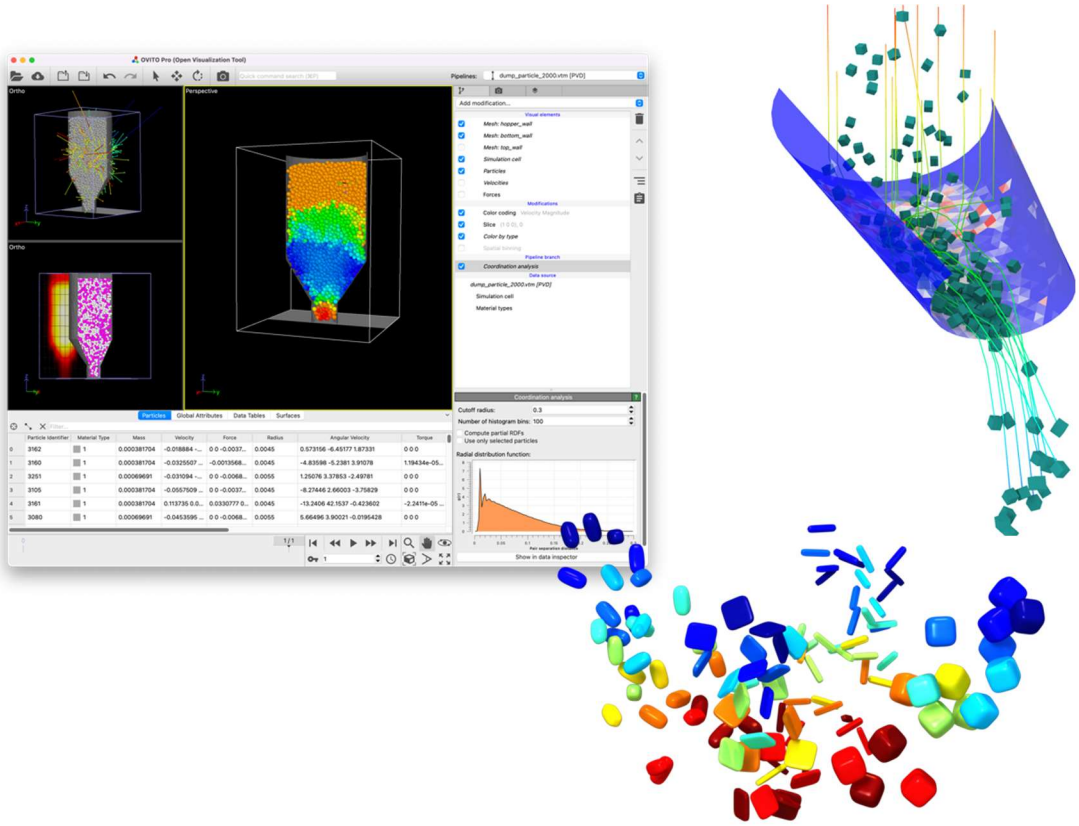
Dr. Alexander Stukowski

OVITO GmbH

OVITO (Open Visualization Tool), a leading scientific data visualization and analysis software, stands out for its adept handling of particle-based simulation models across all length scales. Developed by modeling experts in Germany, OVITO offers a high-performance platform, leveraging state-of-the-art algorithms to efficiently post-process and visualize large particle datasets of diverse kinds and shapes. These capabilities extend also to mesh-based and volumetric data, providing comprehensive analysis and visualization options for a wide range of models.

A key highlight of OVITO is its fully interactive data pipeline system paired with a user-friendly graphical interface, which collectively lower the entry barrier for new users and facilitate the creation of high-fidelity, insightful visualizations and the exploration of data.

For complex problems, however, in particular in academic research, custom solutions are commonly needed to answer novel scientific questions. In fact, the development of new data analysis methods may be the main goal of the research. This presentation showcases how OVITO greatly helps in analyzing simulation datasets and addressing such needs. A significant aspect of OVITO's utility is its powerful Python API, which enables users to leverage the fundamental capabilities provided by the software and easily build problem-specific algorithms. User extensions developed with this interface seamlessly integrate into the software and can be published and shared with others. This significantly broadens the analytical possibilities available to researchers and the scientific community.



Mixing of Passive Scalars in Turbulent Viscoelastic Wakes and Jets analysed by Direct Numerical Simulations

***Mateus C. Guimarães*[1, 2], *Fernando T. Pinho*[3], *Carlos B. da Silva*[2]**

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Direct numerical simulations (DNS) of spatially evolving turbulent planar jets and wakes of polymer solutions are performed to study the mixing of passive scalars in free turbulent shear flows of viscoelastic fluids. The FENE-P rheological model is adopted to describe the viscoelasticity of the long chain, high molecular weight, dilute polymer solutions, and the DNS is based on a highly accurate code (Guimarães *et al*., "Direct numerical simulations of turbulent viscoelastic jets", *J. Fluid Mech*., vol. 899, 2020, p. A11; Guimarães *et al*., "Turbulent planar wakes of viscoelastic fluids analysed by direct numerical simulations", *J. Fluid Mech*., vol. 946, 2022, p. A26), that employs pseudo-spectral and 6th-order compact finite difference schemes, and the shock-capturing scheme of Kurganov and Tadmor. The FENE-P model is based on the freely-joint bead-spring chain model, where spheres connected by massless springs are used to mimic the effect of the polymers on the flow.

The dumbbell model is obtained when the number of beads is equal two. The model uses the principle of coarse graining, and a single dumbbell represents a large ensemble of polymer chains, instead of a single chain. Figure 1 illustrates our DNS of turbulent planar jets. We show that viscoelasticity leads to a strong suppression of small-scale scalar mixing in the fully turbulent far-field, but large and intermediate scale stirring can be suppressed or enhanced, depending on the flow region and the rheological parameters of the viscoelastic fluid. Initially, at the high-elasticity portion of the far-field, large scale stirring is reduced by the presence of the polymers, and so is the spreading and decay rates of the passive scalar. In contrast, farther downstream, at the low-elasticity region of the far-field, the opposite effect is observed. The influence of viscoelasticity is non-monotonic. Finally, we demonstrate that the Reynolds analogy for transport of momentum and scalar is not valid for free turbulent shear flows of viscoelastic fluids.

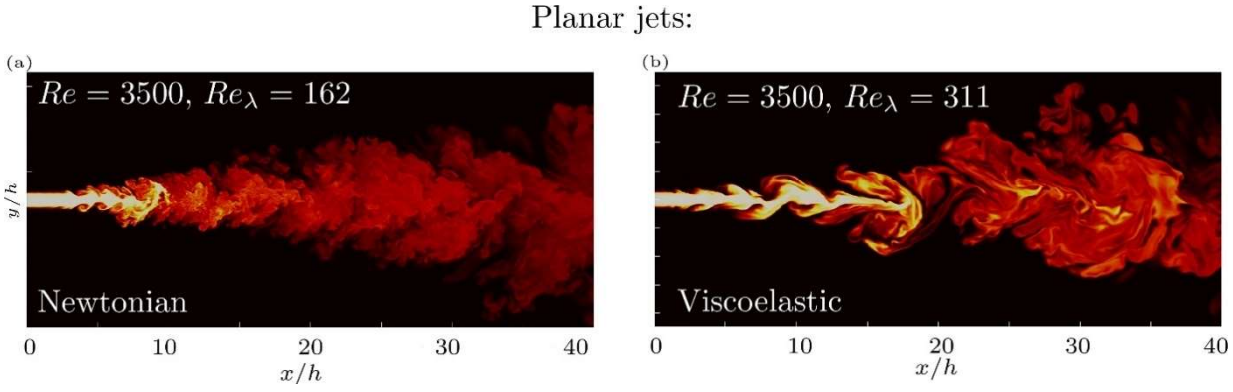

Figure 1: Two-dimensional contours of instantaneous passive scalar for turbulent planar jets of: (a) Newtonian, and (b) viscoelastic fluids.

Modeling the Coupling among Different Processes in Biological Systems*

***Alessandro Giammarini*, Alfio Grillo, Luigi Preziosi, Rugiada Scozzari, Michele Fronterrè**

Politecnico di Torino, Cantene s.r.l.

The study of complex systems, as the biological ones, requires developing advanced mathematical methods, both in Modeling and in Numerics. In particular, the evolution of biological systems is the outcome of several internal processes, and of the interaction with the environment, thereby resulting in highly nonlinear problems. In biomechanics, tissues are often described as saturated biphasic media, where the solid phase represents the contributions of cells, protein links, and extracellular matrix, whereas the fluid phase represents the interstitial fluid responsible for the transport of nutrients and drugs.

Macroscopically, the flow of the fluid through the pores of a tissue is often described by Darcy's Law, which relates the fluid velocity to spatial pressure gradients. The deformation of the solid phase plays an important role when studying inelastic phenomena [1] occurring within it (Figure 1), memory effects [2] (Figure 2), fluid flow, transport of chemicals. These cases have been studied by recurring to extensive FEM with the aid of the commercial software COMSOL® and ABAQUS®.

Within the collaboration with Cantene s.r.l. our goal is twofold: (i) we aim to gain an advanced knowledge of the technical features of Aspherix®; and (ii) we aim to simulate anelastic interactions between the solid phase of a porous medium and the particles transported by the fluid.

[1] Di Stefano, S., Giammarini, A., Giverso, C., Grillo, A., Z. Angew. Math. Phys. 73, 79 (2022).

[2] Gunda, S. Giammarini, A. Ramirez-Torres, A., Natarajan S., Barrera O., Grillo A., Math. Mech. Solids, In press.

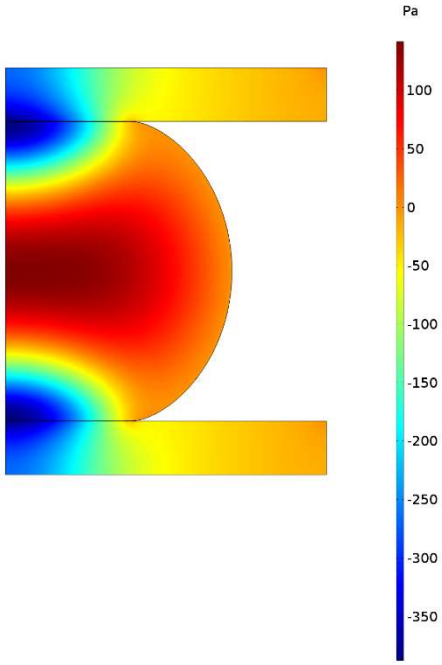

***Figure 6**: Pressure field during a simulated compression-release test for a multicellular aggregate of spherical shape placed between two plates. The simulation was performed by the software COMSOL Multiphysics® v. 5.3.*

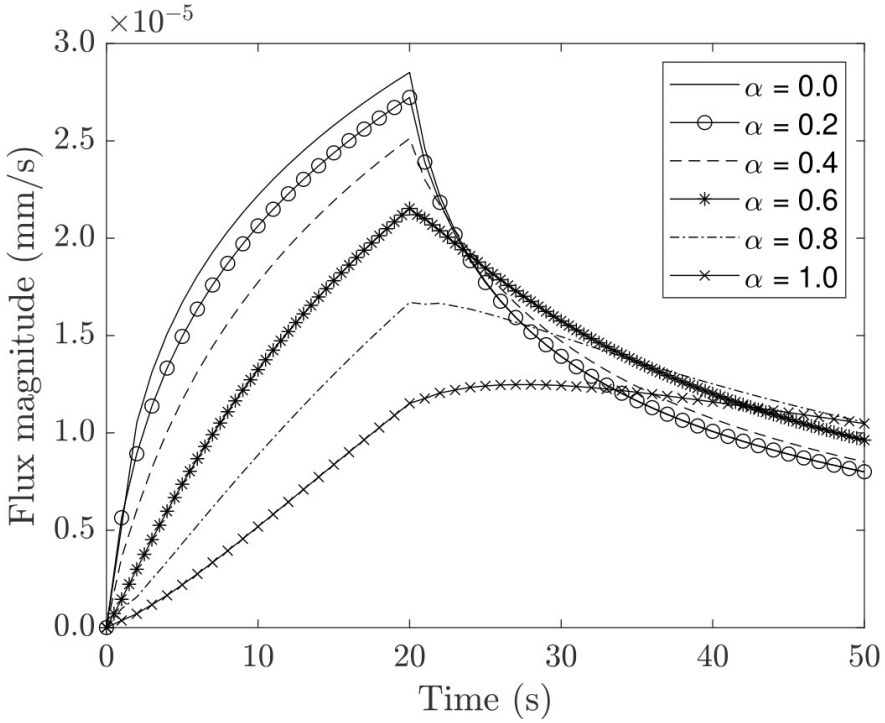

***Figure 7**: Time evolution of the magnitude of the filtration velocity for a specimen of cylindrical shape, evaluated at a boundary node placed on the lateral surface, for different values of the parameter that regulates the memory effects. The simulation was performed by the software ABAQUS®.*

Software Methodology for Characterization of Cerebral Aneurysms*

Jozsef Nagy

eulerian-solutions e.U.

The treatment of patients with cerebral aneurysms poses multiple challenges to physicians from rupture to treatment risk assessment and their consequences to the patient's health. Risk estimation support is highly required to make the optimum decisions for individual patients. The aim of this study is to develop the workflow of a simulation method for the analysis of hemodynamics and structural mechanics of cerebral aneurysms as well as its possible clinical implementation.
In this study a workflow is presented, where medical imaging data is taken and converted into CAD data (STL format) to use as geometric input for simulations. Fluid-Structure Interaction (FSI) simulations are utilized in the inflow vessel, the outflow vessels as well as aneurysm sacs. Simulations in over 450 patient data were able to statistically determine parameters, which are suitable to distinguish between stable aneurysms as well as aneurysms close to rupture.
The presented workflow and results will be used for future clinical considerations of patients with unruptured cerebral aneurysms. A software suite with a graphical use interface has been created for qualitative and quantitative interpretation of hemodynamics as well as structural mechanics. With this, it is possible for medical personnel without simulation background to run sophisticated Fluid-Structure interaction simulations with ease and in future to make optimized decisions for patient treatment.

Fig. 1: Initial segmentation step (left) and final evaluation step (right) within the implemented GUI

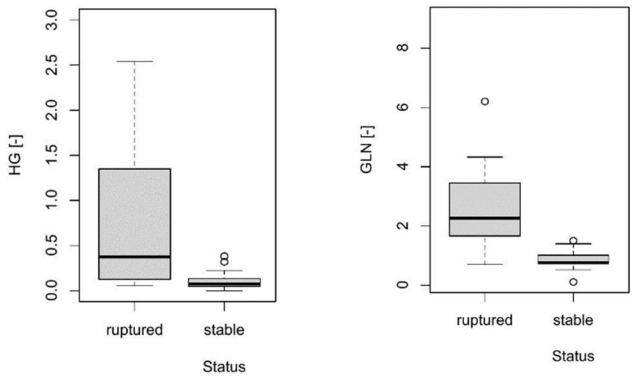

Fig. 2: Box plots of characteristic parameters obtains in FSI simulations for ruptured as well as stable aneurysms

Imprint

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