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Fachgruppe Mehrphasenhydrodynamik:

Vorträge und Poster

Utilization of Novel Magnetic Resonance Imaging and Bubble Size Distribution Measurements to Validate Multiphase LBM-Based CFD Simulations in the Ambr® 250 Bioreactor

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The Ambr® 250 system is a key tool in bioprocess development, providing a scale-down model of production conditions while allowing extensive parameter variation across up to 24 vessels in parallel operation. Cultivation results are comparable to traditional 2–5 L development scales (Xu et al., 2017) and characteristics such as shear stress align with production-scale conditions (Šrom et al., 2024). This flexibility supports media evaluation, feeding strategy optimization, and process set-point assessment. The small working volume and high throughput makes the system highly effective for rapid and parallel process screening.

Although the Ambr® 250 platform has been studied extensively (Tai et al., 2015; Xu et al., 2017; Villiger et al., 2018; Manahan et al., 2019; Šrom et al., 2022; Fang et al., 2024), recent advances enable deeper insights into its operation.

In this work, we present the first analysis of the Ambr® 250 using magnetic resonance imaging technology. This noninvasive approach provides high resolution visualization of fluid dynamics, mixing behavior, and stirrer dependent gas hold up, parameters that are difficult to capture with conventional methods. These findings can improve understanding of microscale mixing and mass transfer, support better scalability and process robustness, and have also been applied for the characterization of the Ambr® 15 system(Legrand et al., 2022).

The generated images provide valuable data for in-depth validation of multiphase CFD simulations. Parameters such as bubble size distribution offer a strong basis for validation, although they can be affected by factors like bubble overlap (Geng et al., 2013). Magnetic resonance imaging adds an additional layer of validation by enabling high-resolution visualization of gas holdup distribution across the entire three-dimensional geometry or selected planes of interest. This resolution is significantly higher than that achieved with methods such as electrical resistance tomography (ERT) (Busciglio et al., 2017) . For the CFD simulations, the lattice Boltzmann-based solver M-Star CFD (M-Star Computational Fluid Dynamics (CFD) Software, 2025) was employed, incorporating the trajectory-based bubble breakage model (Weiland et al., 2024) . The model was adapted to include the acceleration as an additional force acting on the bubble. The microbial and mammalian Ambr250 systems were tested and simulated within a parameter range of stirrer speeds from 0 to 700 rpm in 175 rpm increments and aeration rates between 0.025 and 0.1 L•min^{-1} in steps of 0.025 L•min^{-1}.

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Keywords: Bioreactor, Multiphase flow, MRI, Bubble breakage, CFD

Determination of Bubble Size Distributions in Industrial Stirred Tank Reactors using Machine Learning Image Processing

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Although significant process intensification in the field of bioprocess and pharmaceutical engineering took place during the last decades, the demand for the development and scale-up of mammalian cell culture processes with high cell densities is still increasing [1, 2]. From the multiphase engineering point of view, it is especially challenging to achieve sufficient mass transfer of oxygen while keeping shear forces by aeration and agitation under control to prevent cell damage. The volumetric mass transfer coefficient k_La is dominated by the interfacial area a between gaseous and liquid phase, which can be influenced by the bubble size distribution. Despite its importance, the determination and control of the bubble size distribution in various systems is still challenging due to the dynamical behavior of rising, coalescing and breaking bubbles and the difficult accessibility in dense bubbly flows.

In this study a workflow is presented to determine the bubble size distribution in an industrial scale aerated stirred tank reactor with a volume of 15 000 L. Despite the tank is transparent, the optical accessibility is limited due to the dense bubbly flow at higher gassing rates. To enable the measurements, a dived endoscopic camera (*Sopat GmbH*) is used that allows to take images with a spatial resolution of 2464 x 2056 pixel and a temporal resolution of $f = 5$ Hz. These images are evaluated using an own automatic image analysis software based on the Segment Anything Model by Meta® [3]. Based on a point grid the Segment Anything Model divides each image in several segments, each representing one bubble from the image. To transfer the segmentations into interpretable data a 2D-ellipse fitting algorithm is used around each segmentation. For the further data analysis, the major and minor axes of each 2D-ellipse is calculated. To obtain the volume and the surface area of the bubbles based on the 2D-data the bubbles are assumed as oblate ellipsoids.

In accordance to literature results, a significant influence of the specific power input on the bubble size distribution can be detected [2]. In a coalescence inhibited medium a Sauter diameter smaller than $d_{32} = 2$ mm was observed with over 20 000 evaluated bubbles per operating point. In addition, the automatic image analysis is validated by comparison with manually evaluated reference data, showing good agreement in the resulting bubble size distributions.

In the lecture the measurement technique as well as the evaluation algorithm will be presented and exemplary measurements for different operating points will be discussed. Furthermore, the results of the validation and a comparison between different settings for the algorithm will be shown.

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Keywords: bubble size distribution, stirred tank reactor, AI, Segment Anything Model

Dynamic Characteristics of Fluidized Bed Reactors

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Three-dimensional Eulerian–Lagrangian simulations were employed to investigate the hydrodynamic behavior of a laboratory-scale, cold-flow gas–solid bubbling fluidized bed reactor (FBR) of cylindrical geometry. This work aims to elucidate the dynamic characteristics of the FBR through the specific kinetic energy of the solid phase (k_S), defined as the total kinetic energy of all solid particles divided by the total particle mass, and to examine its correlation with key operating parameters. The simulation framework was first validated against experimental X-ray CT data, demonstrating good agreement between predicted and measured bubble size and frequency. A parametric study was then conducted to assess the effects of reactor diameter (d_R), superficial gas velocity (u_G), and bed inventory (m_S) on the hydrodynamic behaviors of the FBR. Figure 1 shows representative three-dimensional snapshots of bubbles, visualized as iso-surfaces of void fraction, interacting with particles at different reactor scales and bed inventories. In addition to k_S, other hydrodynamic parameters, including bed height h_B, pressure drop Δp, bubble surface area A_B, bubble frequency f_B, were calculated from the simulation results, and their correlations with the operating parameters were evaluated. The principal findings are summarized as follows:

- While the conventional parameters h_B and Δp show little sensitivity to changes in reactor diameter d_R, k_S increases slightly with d_R. This is attributed to the reduced influence of wall friction on particle motion. In addition, as the reactor is scaled up, the FBR's hydrodynamics transition from a regime dominated by a single bubble column to one characterized by multiple bubble columns.
- A similar trend is observed for variations in superficial gas velocity u_G: h_B and Δp remain nearly constant, whereas k_S and A_B increase markedly with u_G. This trend results from the higher momentum flux of the gas flow, which enhances momentum transfer to the solid phase via increased aerodynamic drag.
- For a fixed d_R and u_G, k_S increases moderately with bed inventory m_S; this indicates enhanced gas-to-solid momentum transfer, which is caused by the greater bed volume and the corresponding increase in interfacial contact area (e.g., bubble surface) between the phases.
- Furthermore, the bubble frequency f_B derived from the time fluctuations of local void fraction and static pressure shows consistent agreement with that evaluated from time evolution of the global parameters k_S and A_B.

These results reveal how key hydrodynamic features respond to different operating conditions, highlighting the need to include kinetic parameters (e.g., bed material kinetic energy, bubble frequency) in FBR performance evaluations, rather than relying solely on static measures. This approach is vital, as hydrodynamics directly control the mixing and heating processes essential for efficient thermochemical conversion.

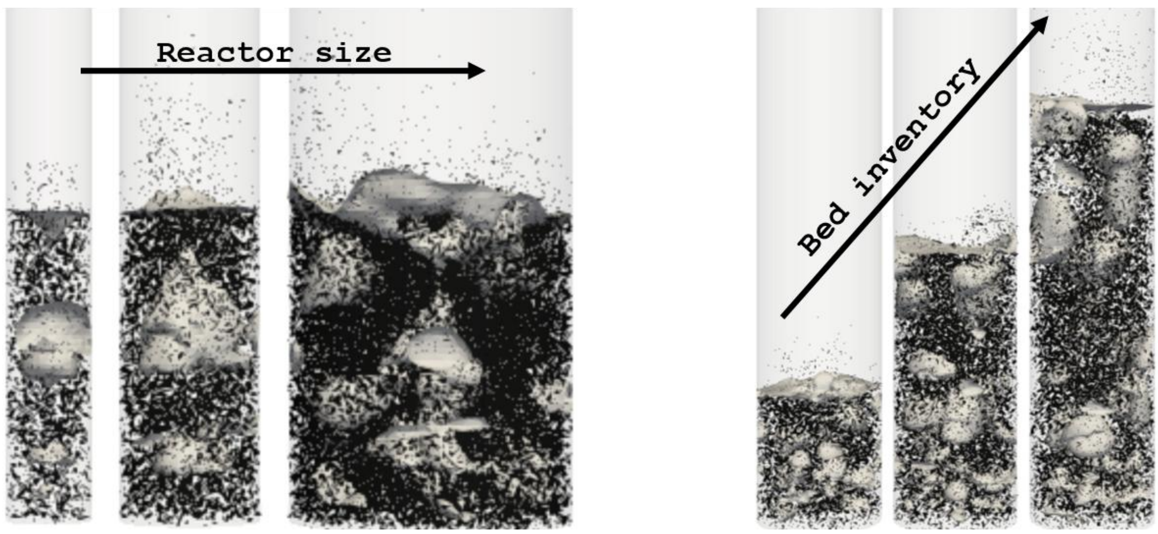

Figure 1: Snapshots of void fraction iso-surfaces illustrating bubble structures for different reactor diameters and bed inventories.

Keywords: Gas-solid flows, bubbling fluidized bed, hydrodynamics, Eulerian-Lagrangian simulation, kinetic energy

Numerical investigations on flow hydrodynamics in two-phase and three-phase flows for slag reduction experiments with hydrogen

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In this present work, a computational fluid dynamics (CFD) model is devised to study and understand the flow characteristics of two-phase and three-phase flows with chemical reactions in metallurgical gas-slag-metal systems. This study is motivated by the goal for CO2-neutral production and recovery of valuable non-ferrous metals, e.g. copper, nickel, lead, tin and zinc from slags. The metallurgical industry is facing major challenges in transforming existing processes in terms of substitution of fossil fuels, considering costs and safety of plant operation and maintaining product quality. Experimental investigations of slag reduction processes focus mainly on understanding the complex chemistry between slag and various reducing agents in the gas phase, including hydrogen. Hence, numerical models enable a detailed investigation of flow characteristics between gas and slag phase as well as thermochemical interactions at the reactive interphase, where mass transfer and chemical reactions occur.

To study the hydrodynamic interactions between the gas, slag and potential liquid metal phase, a CFD model has been developed in reference to an experimental study, in which a lance was introduced into a molten slag concentrate through which a mixture of hydrogen and argon is injected. [1] A Volume-of-Fluid approach has been used to resolve and track the interface between the phases, enabling a detailed modeling of the multiphase flow characteristics. Simulations have been carried out to investigate the influence of varying gas flow rates and lance configurations on bubble formation and rising, on splashing of the liquid phase and overall mixing within the two- and three-phase flow. Furthermore, hydrogen conversion for the reduction reactions with tin oxides and iron oxides was tracked and the reduction performance for each flow configuration evaluated. It was obtained that the reduction performance depends on the design of process parameters. An increase of gas volume flow rate leads to a higher interphase area between gas and liquid due to larger bubbles but decreases the hydrogen conversion due to a higher bubble rising velocity and therefore lower bath residence time. Although reducing the hydrogen conversion, higher gas volume flow rates can reduce the duration of reduction experiments, as the total amount of hydrogen necessary to reach the thermochemical equilibrium is faster provided to the slag bath. Additionally, larger bubbles with higher rising velocities lead to a more turbulent flow within the slag bath, improving the mixing behavior. Too high gas volume flow rates lead to slag droplet output through increasing the liquid splashing. It can be concluded that the design of slag reduction experiments can be optimized by means of CFD studies by investigating the bath hydrodynamics, which can hardly be investigated in situ due to high temperatures and corrosive atmospheres.

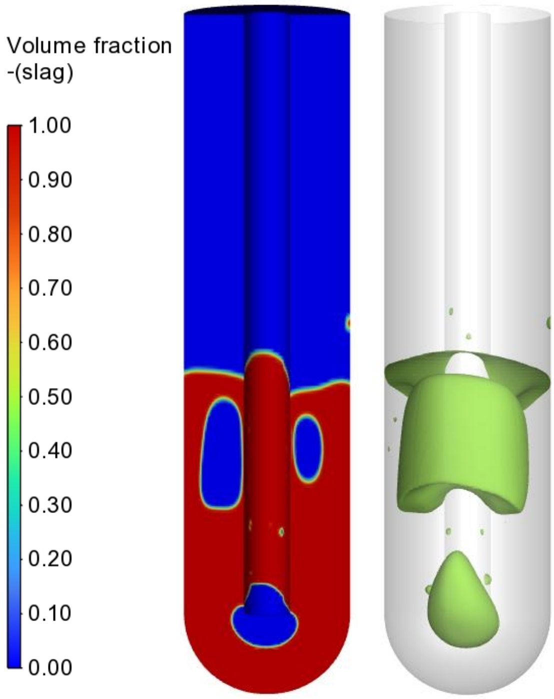

Fig. 1: Contour of phase volume fraction in flow field (left) and interface between gas and liquid (right)

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Keywords: CFD, reactive gas-liquid-systems, hydrogen, slag reduction

Optimizing CO_2 Capture: A Study of $Ca(OH)_2$ Carbonation in a Three-Phase Stirred Tank Reactor

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The permanent storage of carbon dioxide through carbonation reactions, a method known as mineral sequestration, emerges as a promising approach in CO_2 capture and storage research [1]. It finds particular application in the cement industry, which is responsible for 8 % of human-made carbon dioxide emissions. Silicate minerals are suitable materials for mineral carbonation due to their abundance of magnesium and calcium [2].

Wet carbonation represents a potential mineral carbonation process route involving three coexistent mechanisms within a three-phase reactor: carbon dioxide bubbles partially dissolve in the aqueous phase, while calcium or magnesium is leached from the mineral particles and reacts with CO_2 to form calcium or magnesium carbonate, respectively. Wollastonite ($CaSiO_3$) is selected as a primary reactant candidate for carbonation experiments due to the higher reactivity of Ca-silicates in comparison to Mg-silicates [3]. The main challenges to address in making aqueous carbonation a competitive process for CO_2 storage are the slow reaction rates due to the rate-limiting dissolution of calcium silicate and low energy efficiency. To overcome these problems, it is crucial to optimize the reactor design and operational parameters to improve the mass transfer and reaction kinetics.

This study presents experimental investigations on the carbonation of $Ca(OH)_2$ in a customized stirred-tank reactor. Although $Ca(OH)_2$ is an artificial material and not intended for industrial scale-up, it offers a simplified and fundamental system for analysing the response of the reaction to the reactor characteristics, before transitioning to more complex and less reactive materials in future studies. The effects of key operating parameters—stirring rate, gas flow rate, and solid loading—on carbonation rate were systematically evaluated. Results show that, keeping other process variables unchanged, higher stirring rates significantly reduce reaction time.

Additional experiments focused on bubble characterization within the reactor's tank were conducted using an inline endoscope at two different positions: one facing the rotor–stator system and the other at the mid-section of the tank. The bubble size distribution (BSD) was measured under varying stirring rate and gas flow rate conditions. The results showed that increasing impeller speed led to a progressive reduction in the bubble Sauter mean diameter due to the intensified shear forces acting on the bubbles. This reduction in bubble size increases the interfacial area, thereby improving gas–solid mass transfer and accelerating carbonation kinetics.

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Keywords: CO_2 capture, mineral carbonation, three-phase stirred tank reactor, bubble size distribution

Dreidimensionale Modellierung des Filtrationsprozesses in komplexen Filterstrukturen unter Verwendung eines gekoppelten Physics Informed Neural Networks mit einer Smoothed Particle Hydrodynamics Methode

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Die effiziente Entfernung fester Partikel und flüssiger Tröpfchen ist in vielen industriellen Prozessen von entscheidender Bedeutung. Das Hauptziel besteht darin, eine hohe Abscheideeffizienz zu erreichen und gleichzeitig den damit verbundenen Druckverlust zu minimieren. Dieses Spannungsfeld stellt eine zentrale Herausforderung bei der Gestaltung von Filtermedien dar, bei der es gilt, die Filtrationsleistung zu optimieren, ohne die Energieeffizienz oder die Betriebssicherheit zu beeinträchtigen. In den letzten Jahrzehnten haben sich sowohl experimentelle Techniken als auch numerische Modellierungen erheblich weiterentwickelt. Dennoch bleibt das Verständnis aufgrund der mikroskopischen Natur der Filtration begrenzt. Experimente leiden häufig unter eingeschränkter Reproduzierbarkeit und erfordern kostspielige Versuchsmedien. Konventionelle numerische Ansätze, wie die Finite-Volumen-Methode, können die relevanten Transportmechanismen zwar auflösen, jedoch erfordern die dabei auftretenden kleinen räumlichen und zeitlichen Skalen extrem feine Gitter und Zeitschritte. Diese Einschränkungen machen klassische Simulationen der Strömungsmechanik (CFD) teuer und teilweise unpraktisch.

In dieser Arbeit [1] wird ein Modellierungsansatz zur Simulation des Filtrationsprozesses vorgestellt, der ein Physics Informed Neural Network (PINN) mit der Smoothed-Particle-Hydrodynamics-Methode (SPH) koppelt. Mit Hilfe des PINN werden die dreidimensionalen Geschwindigkeits- und Druckfelder innerhalb des Faserverbunds direkt aus den Navier–Stokes-Gleichungen, ohne auf Trainingsdaten angewiesen zu sein, bestimmt. Das resultierende Strömungsfeld wird an den SPH-Solver weitergegeben, der die Tröpfchenbahnen, den Aufprall der Tropfen auf die Fasern als auch die Bewegung der Fluidfilme berechnet. Da sowohl PINN als auch SPH gitterfreie Verfahren sind, entfällt die komplexe Gittererstellung. Sobald die abgeschiedenen Tröpfchen groß genug werden, um das Strömungsfeld zu beeinflussen, wird ihre geometrische Information an das PINN übertragen, das anschließend mittels Transfer Learning das Strömungsfeld neu berechnet. Der Vergleich zwischen dem durch die PINN-Modelle vorhergesagten Strömungsfeld und den mit einem CFD-Solver berechneten Ergebnissen für vier repräsentative Filterstrukturen zeigt eine sehr gute Übereinstimmung zwischen PINN und CFD (siehe Abb. 1).

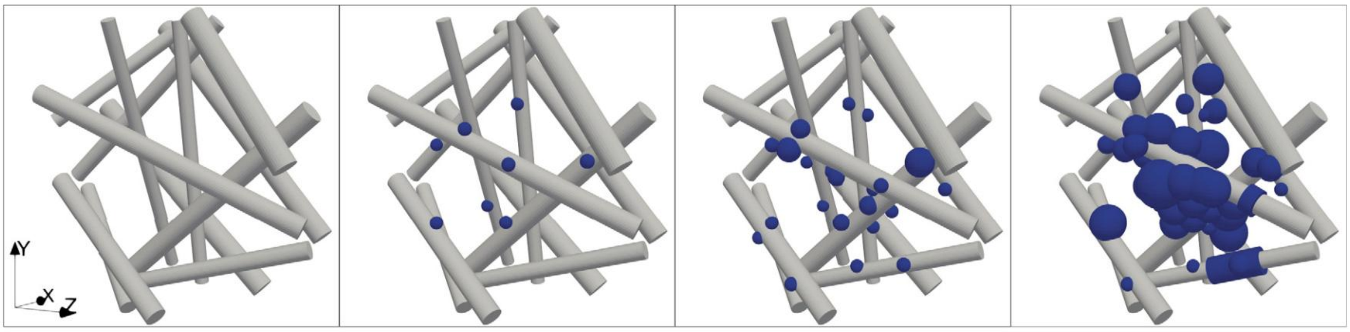

Abb. 1: Zeitliche Entwicklung der Abscheidung von Öltröpfchen und des resultierenden Fluidfilms für eine Anfangsporosität der Struktur von $\varphi = 0{,}942$.

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Keywords: Ölfiltration, Smoothed Particle Hydrodynamics (SPH), Physics Informed Neural Networks (PINN), Machine Learning (ML), Filterstruktur

Bubble Migration in Turbulent Bubbly Jets

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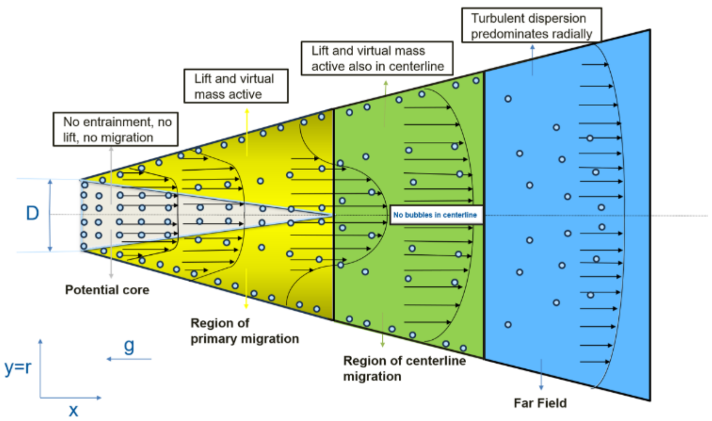
Turbulent bubbly jets occur in a wide range of industrial processes, such as chemical reactors or flotation cells, where they are used to enhance mixing and contact between the phases. Beyond their practical importance, they also represent a fundamental topic in modern fluid dynamics research. Compared with their single-phase counterparts, bubbly jets are much less studied and exhibit a variety of distinctive phenomena which are only partially explored and an understanding of which is largely lacking.

This study focusses on one of these phenomena, namely the migration of bubbles away from the centerline of the jet, an indication of which was found in a recent computational study [1] and is also confirmed experimentally [2]. However, as of yet there seem to be no investigations of the mechanism causing this migration and its dependence on the flow parameters.

The present work approaches these questions by means of a multiphase CFD simulation of turbulent bubbly jets using an Euler–Euler / RANS approach. A baseline model that was applied successfully to a variety of bubbly flows [e.g. 1,3] together with the numerical setup for the turbulent jet geometry from Ref. [1] has been used as a starting point. Initial comparison against the experimental data from Ref. [2] showed that adjustments of the models for drag and bubble-induced turbulence as well as the liquid velocity profile at the nozzle were necessary. Reasons for these adjustments leading to a reasonable agreement with the measurements are discussed.

Upon validation of the model, the mechanisms driving bubble migration within the jet are investigated, showing that the lateral drift of bubbles from the jet core towards its periphery for the conditions of the experiment [2] originates primarily from the lift force. Noting that the jet Reynolds number in [2] has a relatively low value of ~3000, the analysis is extended to higher Reynolds numbers to clarify how the relative importance of the various interfacial forces changes. The results show that with increasing Reynolds number, the influence of the lift decreases, while pressure gradient and virtual mass effects become increasingly important. The changing significance of these forces is further analyzed by dimensional considerations. Finally, a division of the jet into regions according to the dominant mechanisms is proposed as summarized in the figure below.



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Keywords: Turbulent jets, disperse multiphase flow, bubble migration, lift force, Euler-Euler two-fluid model, CFD simulation

Fibre dispersion dynamics in a Jet-in-Crossflow configuration: Experimental and numerical advances of interactions with vortical structures and rigid walls

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Abstract

The transport of non-spherical particles in confined turbulent flows drives efficiency in processes ranging from paper manufacturing to wastewater filtration and chemical reactors. In these systems, the complex interplay between fibres, flow structures, and bounding walls dictates the final particle orientation and spatial distribution. Standard RANS approaches often struggle to capture these dynamics accurately, as they typically treat particles as point-masses without the spatial coherence necessary to model fibre rotation correctly, nor do they account for the hydrodynamic alterations caused by wall proximity. This study investigates the dispersion of rigid fibres ($D_p \approx 40\mu m$ with variable aspect ratio between 2 and 10) injected via a vertical jet into a horizontal turbulent water channel, specifically aiming to bridge the gap between efficient numerical modeling and the complex physics of fibre-wall and fibre-vortex interactions.

We characterize the flow field and fibre dynamics simultaneously using high-speed shadowgraphy combined with Particle Tracking Velocimetry (PTV). To capture the full downstream evolution of dispersion, we extended the experimental database to include measurement profiles at 50, 100, and 200 mm from the injection point. On the numerical side, we utilised the Euler/Lagrange framework coupled with a RANS (k−ω SST) flow field. In order to address the limitations of previous studies, we refined the physical fidelity by integrating three specific components. First, we introduce a probabilistic injection model based on experimental aspect ratio distributions to capture real polydispersity (or shapes). Second, we implement advanced hydrodynamic force and torque correlations (e.g., Chéron et al., 2024) that explicitly account for wall-proximity effects in shear flows. Third we apply a fibre dispersion model based on a filtering technique (Cholesky decomposition) to generate coherent velocity fluctuations along the fibre dimension. These new implementations are coupled with a rigorous hard-sphere wall collision model (Quintero et al., 2021) that accounts for the actual impact point and rotational momentum exchange.

The comparison of numerical results with the extended experimental profiles demonstrates that the synergistic implementation of variable aspect ratios, wall-corrected hydrodynamic forces, and spatially correlated dispersion significantly enhances prediction accuracy compared to standard models. Specifically, this comprehensive modelling framework correctly captures the vertical fibre spread and effectively prevents the unrealistic rapid settling often observed in simplified simulations. Furthermore, the model reproduces the subtle changes in rotational dynamics, capturing the characteristic orientation angles observed experimentally in both the channel core and near-wall regions at different downstream positions. These results highlight that accurate prediction of fibre transport in complex confined flows requires not just a robust wall collision model, but a holistic inclusion of real shapes, wall-bounded hydrodynamics, and spatially coherent turbulence.

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Keywords: Non-spherical particles, Jet-in-crossflow, Fibre dispersion, Shadowgraphy, Euler/Lagrange approach, Wall collision modeling.

Measurement of liquid foam flow through a diverging nozzle

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The pneumatic foam theory describes the transport of liquid through continuously rising foam in a vertical column [1]. For a constant cross-sectional area, it is assumed that the foam moves similarly to a plug flow with an even distribution of the liquid phase. To verify the pneumatic foam theory in the case where the foam flows through a cross-sectional expansion, we measured the liquid fraction distribution and local velocity of a stationary foam flow in a vertically aligned, divergent nozzle using optical and radiographic methods [2].

In this contribution [3], the experimental results are presented and discussed in comparison with the theoretical predictions assuming different models of foam permeability. Radiography revealed that the liquid fraction decreases with increasing cross-sectional area in the nominal flow direction, which is consistent with the pneumatic foam theory [4]. But, the measured liquid fraction was higher overall than predicted. In the radial direction, it was found that the liquid fraction increases slightly towards the nozzle wall. The corresponding velocity profiles were measured using X-ray-based particle tracking (Figure 1). These also deviate from the expected plug flow.

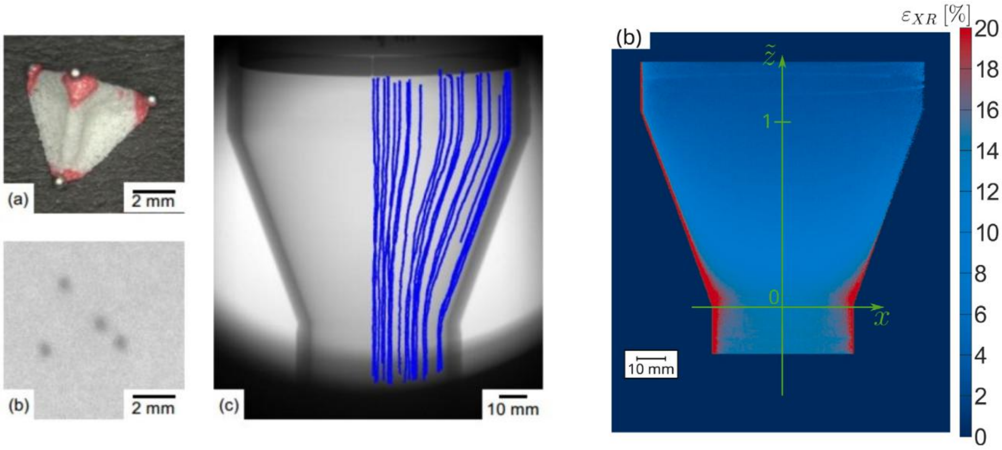

Figure 1: X-ray particle tracking velocimetry, (a) Close-up image and (b) X-ray image of a tracer particle for foam flow. (c) Overlay of 23 tracks of tracer in a nozzle. (d) liquid fraction distribution from radiography [3].

Due to the radial inhomogeneity of the liquid content and velocity, the convective liquid transport through the nozzle is lower overall than predicted by pneumatic foam theory. This makes a divergent nozzle particularly well suited for limiting liquid transport in foam columns.

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Keywords: Foam column, Pneumatic foam theory, Nozzle flow, Radiography, X-ray particle tracking.

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TU Dresden | Hörsaalzentrum

Strömungsprofile in einem düsenbasierten Mischsystem für Biogasfermenter

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Motivation:

Industrielles Mischen findet als Grundoperation der mechanischen Verfahrenstechnik in vielen pharmazeutischen, chemischen und biochemischen Prozessen Anwendung.
Eine in den letzten Jahren sehr stark gewachsene Anwendung sind Biogasfermenter, in welchen das gasproduzierende Gärsubstrat durch Rühren in Bewegung gehalten wird. Wartungsarbeiten, Austausch von Ersatzteilen oder andere Arbeiten in der harschen, explosionsgefährdeten Umgebung des Gärbehälters sind mit großen Aufwand verbunden. Durch einen Mischeraufbau ohne innenliegende Teile wird die Wartung und Reparatur deutlich einfacher und billiger.

Material & Methodik:

Ein alternativer Ansatz zum klassischen Rühren von Suspensionen ist die Erzeugung einer Strömung im gesamten Behälter durch Absaugen und Eindüsen des Mediums. Die Konvektion im Mischbehälter erfolgt also durch dezidierte Entnahme und Zuführung von Flüssigkeitsvolumina. Versuche wurden in einem experimentellen Aufbau im Labormaßstab mit 1,4 L umgesetzt, dargestellt in Abbildung 1a. Magnetventile öffnen die Druckluftzufuhr und schieben Volumina aus externen Behältern zeitperiodisch gesteuert über Düsengeometrien in den Behälter. Ebenso entnehmen sie über Druckabsenkung in den Vorlagebehälter gezielt Volumen aus dem Mischbehälter. Die Betriebskenngrößen Druck und Füllstand sowie Videosequenzen der Partikelbewegung wurden aufgenommen. Nach Aufbereitung der Videorohdaten (siehe Abbildung 1c.) wurde durch softwarebasierte Auswertung der Partikelbahnen (siehe Abbildung 1d) eine Geschwindigkeitsverteilung ermittelt. Aus den Betriebskenngrößen und der Geschwindigkeitsverteilung wird der Mischprozesse hinsichtlich Effizient bewertet. Es ergibt sich ein Mischverfahren, das auf Einbauten im Behälter vollständig verzichtet.

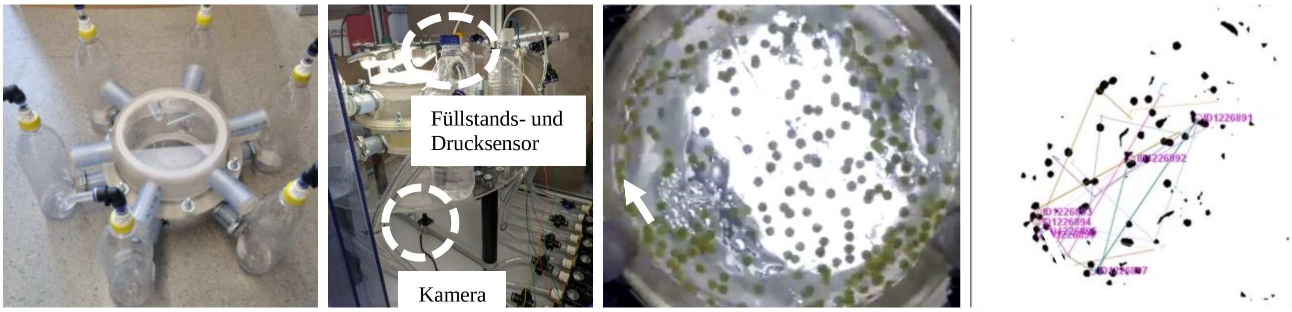

Abbildung 1a: Mischkammer und Vorlagebehälter; b:Prozessüberwachung; c/d: Rohvideo und softwarebasierte Auswertung der Partikeltrajektorien

Keywords: Mischtechnik, Suspendieren, Fermenter, Biogas

Experiments and Numerical Studies on Dual Gas-Assisted Sheet Nozzles

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Liquid sprays are widely spread among chemical industry e.g. for burner nozzles or gas cleaning, as well as for food production, medical purpose or even agricultural application. Although there are countless experimental and numerical studies on the subject of sprays, the design of nozzles for distinct operating conditions is still highly empirical and often subject to trial and error. In particular, the issue of scaling from laboratory scale to technical application, remains a major challenge. Against this background, atomization research at KIT – ITC/EBI aims to develop the fundamentals for scaling gas-assisted nozzles. Parallel to the experimental work, numerical simulations of the primary breakup are carried out and validated using the experimental data. This approach enables further insight which is elsewhise difficult or impossible to obtain experimentally. Our aim is to develop a Virtual Spray Test Rig, that allows for targeted nozzle design, with only a small number of expensive experiments remaining in the future.

In conventional jet-type nozzles, the liquid is released via a centrally located pipe (the liquid jet), while the gas stream for atomization is issued via a concentric annular gap at the nozzle outlet. However, experimental studies have shown that the scalability of such jet nozzles to higher mass flow rates is limited [1]. For this reason, dual gas-assisted sheet-type nozzles were used for the experiments presented here. In this nozzle design, the liquid flows through a ring-shaped gap at the nozzle orifice and is atomized by an inner gas jet accompanied by an outer annular gas flow, surrounding the liquid sheet. This type of nozzle showed better atomization performance in initial tests compared to jet nozzles and has great potential for scale-up [2]. Here, first results concerning the influence of liquid sheet thickness on the resulting droplet size measured with a Phase Doppler Anemometer will be presented. The experiments revealed a distinct influence of the liquid sheet thickness at the nozzle orifice on the downstream droplet size distribution. This impact increases with increasing liquid viscosity. Furthermore, a pulsating effect during primary breakup at the nozzle orifice was observed via high-speed camera images, s. Fig. 1 (left side of each picture). The origin of this pulsation was detected based on data from the accompanying CFD simulations, s. Fig 1 (right side of each picture).

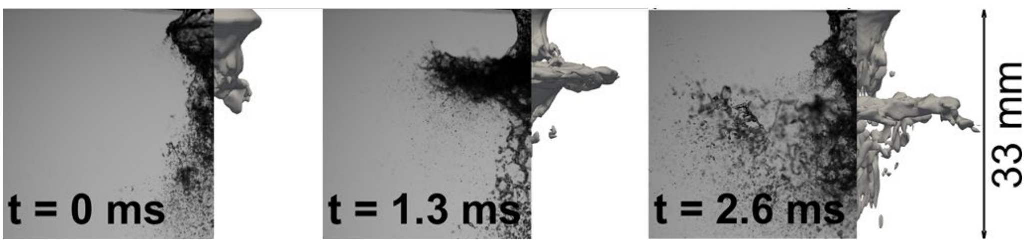

Figure 1: Pulsation during primary breakup - temporal evolution (left side experiment / right side of the picture CFD) [3]

With our ultimate aim of developing a Virtual Spray Test Rig that allows for prediction of primary breakup phenomena and finally even the resulting drop size distribution of gas assisted nozzles, the presented experimental and numerical results mark an important, but intermediate step towards this goal.

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Keywords: nozzle scaling, sheet nozzle, atomization, numerical simulation

A CFD–DEM Framework for Evaporating Droplets in Spray Drying

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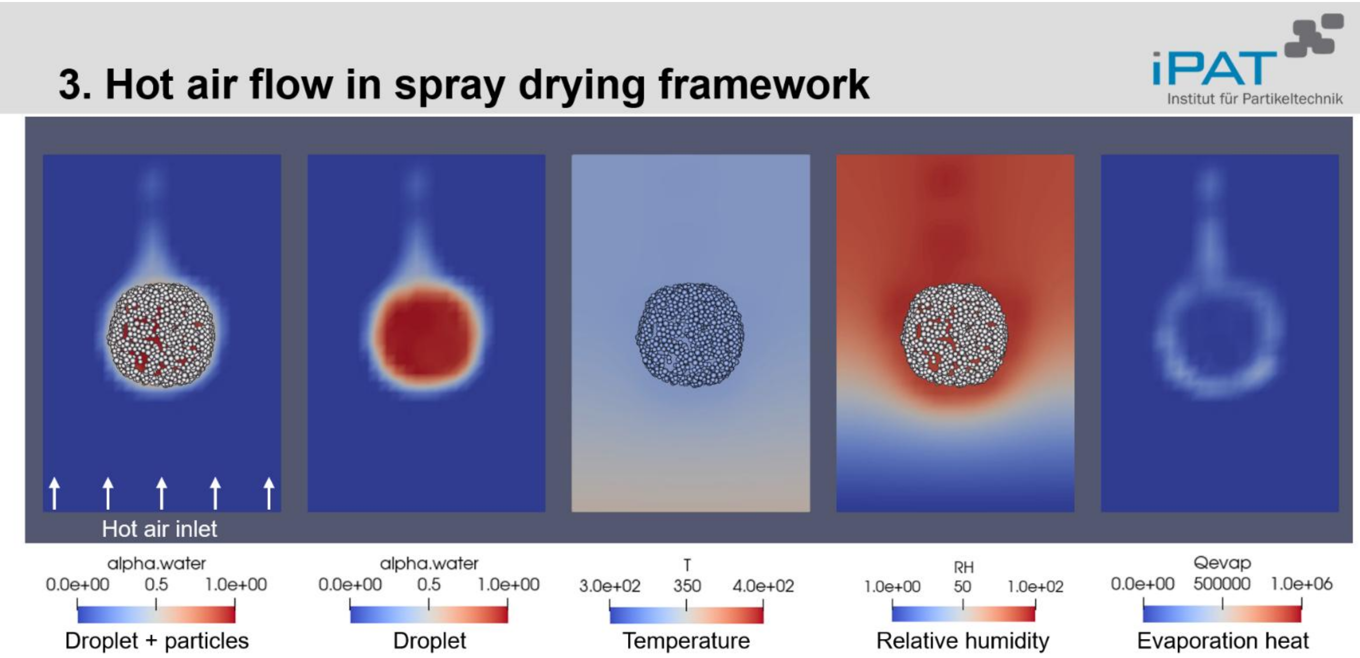
Spray drying requires predictive tools that resolve droplet–gas interactions while capturing heat, mass, and momentum exchange in a humid, particle-laden environment. We present a CFD–DEM framework that integrates volume-of-fluid (VOF) interface tracking with coupled temperature and humidity fields and two-way coupling to dispersed solids. The liquid–gas interface is advanced consistently with evaporation so that droplet shrinkage, latent cooling, and vapor addition to the gas phase remain synchronized. A segregated pressure–velocity procedure drives the carrier flow, while micro-iterations between temperature, humidity, and the interfacial source maintain thermo-mass consistency without relying on case-specific tuning. The DEM side exchanges momentum and (optionally) heat with the fluid and accounts for local porosity effects typical of dense spray regions. Algorithmic safeguards—interface compression, volume-conserving corrections in the VOF band, bounded sources, and property regularization—provide robustness across meshes and operating conditions relevant to spray dryers. Demonstration cases in hot crossflow reproduce physically consistent droplet shrinkage, stable humidity fields, and the expected latent-cooling behavior as droplets approach wet-bulb conditions. The framework is intended as a building block for process-level questions in spray drying, including sensitivity to inlet conditions, nozzle placement, residence time control, and droplet–particle interactions.



Keywords: spray drying; evaporating droplets; humidity and temperature coupling; VOF; CFD–DEM; two-way coupling; OpenFOAM.

Numerical Modeling and Experimental Validation of the Single Electrospray Process: A Foundation for Hetero-Aggregate Synthesis

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Introduction

Precise morphological control of hetero-aggregates is critical for energy applications. Bipolar electrospray synthesis achieves this through the controlled collision of oppositely charged droplets [1]. To predict the resulting particle composition, we are developing a comprehensive Euler/Lagrange model of this process. This study presents the foundational step: the numerical modeling and experimental validation of a single electrospray system, which is a prerequisite for simulating the complex bipolar aggregation.

Numerical Method

Numerical simulations utilize a fully coupled Euler/Lagrange framework implemented in OpenFOAM. The Eulerian phase solves the Navier-Stokes, energy, and species equations, coupled with Poisson's equation for the electrostatic field and ionic charge transport. In the Lagrangian phase tracking discrete droplets are followed through the flow field, incorporating Schiller-Naumann drag, the Abramzon-Sirignano [2] evaporation model and Coulomb explosions.

Results and Discussion

Initial validation (Figure 1, left) confirms the expected increase in spray radius with flow rate. However, while simulations match the trend at low flow rates, they underpredict the radius increase at higher flow rates, with the largest deviation observed at the lowest flow rates. These discrepancies are attributed to the uncertainty in the initial droplet size distribution, which is based on scaling laws and estimation rather than direct measurement. Moreover, it should be mentioned that the measurement of the spray radius was quite simple and gives only a qualitative dependence. Figure 1 (right) presents a separate analysis investigating the dependency of the simulated spray radius on Coulomb Explosions (CE). The results demonstrate the significant effect of CE on spray shape, particularly at low flow rates where CE are most frequent, underscoring the critical need to accurately model this phenomenon.

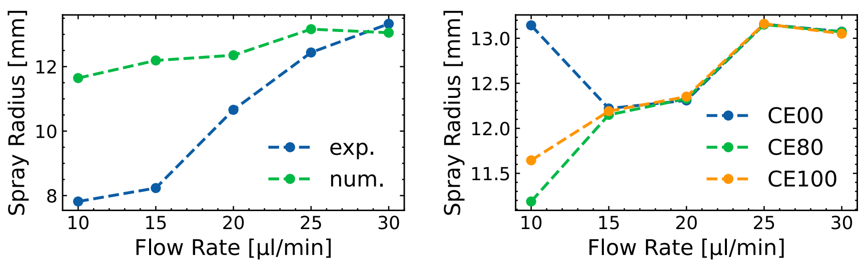

Figure 1: Measured and simulated spray radii across five flow rates (left); simulation results without CE, with CE triggered at 80% and at 100% (right).

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Keywords: Electrospray, Euler-Lagrange, Hetero-aggregates, Coulomb Explosions, Droplet Dynamics.

Sprühkühlung mit Öl-Aerosolen in Fertigungsprozessen

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Kühlschmierstoffe (KSS) werden in Fertigungsprozessen wie z.B. bei der Zerspanung eingesetzt. Sie vermindern die Reibung und die erzeugte Reibungswärme und tragen zur Wärmeabfuhr bei (Kühlen-Schmieren-Transportieren). Bei der Minimalmengenschmierung (MMS) wird der KSS (beispielsweise Öl) in einer Gasphase vernebelt und als Aerosol in die Bearbeitungszone transportiert. Die Schmierwirkung von KSS in Abhängigkeit ihrer räumlichen Verteilung wurde bereits vielfach untersucht, während die Kühleffekte im Prozess bisher kaum systematisch erfasst und bewertet wurden. Die bei einer Sprühkühlung resultierende Kühlwirkung hängt maßgeblich von der Sprayzusammensetzung (Beladung) sowie von der. Tropfengröße, Auftreffgeschwindigkeit, Benetzung sowie der thermischen Belastung ab. Da bislang unklar ist, ob auch bei der Minimalmengenschmierung sprühkühlungsähnliche Effekte auftreten, soll gezielt untersucht werden, wie und in welchem Umfang die Mechanismen bei der Sprühkühlung mit Öl-Aerosolen in Fertigungsprozessen wirken.

In einem Analgieversuch wird die Kühlwirkung bei einem durch ein Bohrwerkzeug versprühten Aerosol in Abhängigkeit von den Volumenströmen der Luft und des KSS bei der MMS untersucht. Der hierfür genutzte Modellversuchsstand (Abb. 1) umfasst eine vorderseitig angesprühte, erhitzte Metallplatte (Ti6Al4V und 42CrMo4, 20x20x2 cm), die rückseitig mit einer Thermografiekamera (ImageIR 8300 von InfraTec, Deutschland) aufgenommen wird. Die rotatorische Bewegung des Bohrers im Bohrgrund wird in eine translatorische Bewegung übersetzt und über den ansteuerbaren Verfahrtisch (OSM26-(x) OptoSigma, Frankreich) mit 4 cm/s bewegt. Die Kühlungseigenschaften durch MMS werden über die Temperaturentwicklung und den Wärmeübergangskoeffzienten analysiert, für dessen Berechnung die analytische Lumped Capacitance Methode sowie ein Algorithmus zur Lösung des inversen Wärmeübertragungsproblems [1] verwendet und verglichen werden. Die Ergebnisse erlauben eine Bewertung des Kühlpotenzials der MMS in Abhängigkeit der Luft- und Ölvolumenströme und geben Aufschluss darüber, in welchem Umfang durch MMS tatsächlich signifikante Kühleffekte z.B. in der Bearbeitungszone eines Zerspanprozesses entstehen.

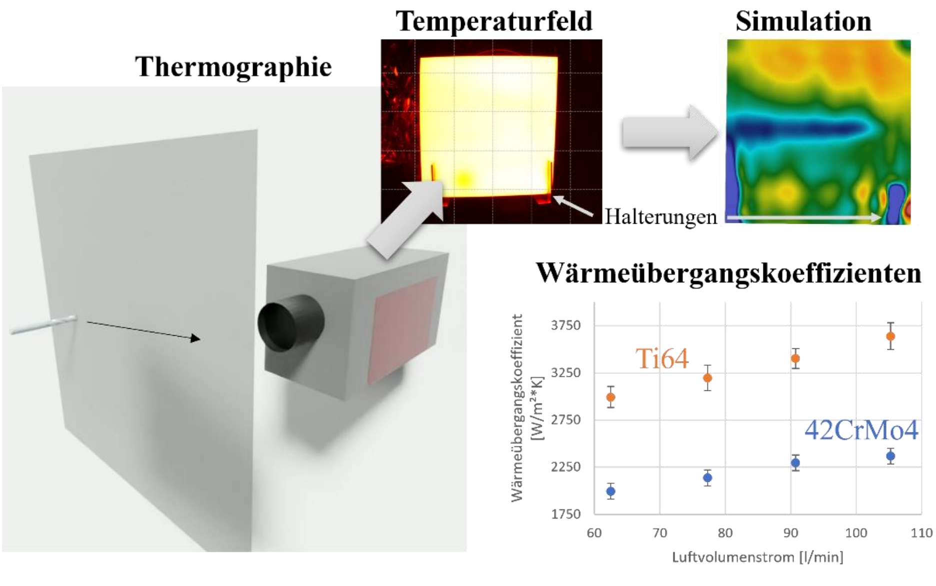

Abbildung 1 Modellversuchsaufbau, Temperaturfeld, Simulationsdarstellung und Wärmeübergangskoeffizienten von Luft.

Acknowledgement: DFG, Deutsche Forschungsgemeinschaft, Projektnummer 439950037

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Keywords: Minimalmengenschmierung, Spray cooling, Thermographie, Wärmeübergangskoeffizient.

Particle and Erythrocyte Distribution in Channel Flow at High Volume Fractions

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At this moment, at least 5000 people (U.S. [1] and parts of Europe[3] [2]) are on the waiting list for a heart transplantation, even though the number of heart transplants globally has increased from about 5000 in 2004 to 10000 in 2024 [3]. For patients requiring support of the cardiac pump function, ventricular assist devices (VADs) can be used. These devices are commonly either a centrifugal or axial turbomachine, comprising a rotor and stator. To design these VADs and minimize hemolysis (destruction of red blood cells), it is important to consider the viscosity and shear stresses involved. For that, the distribution of the red blood cells in the liquid must be considered, as the local volume fraction affects the effective viscosity. It is known that the presence of particles or cells in a fluid results in smaller system losses in blood pumps than in analog liquids of similar viscosity [4]. This effect is likely linked to lateral forces that move the cells away from the wall. The resulting depletion of particles near the wall (*cell-free layer*, CFL) reduces the effective viscosity and can reduce the shear stress acting on the cells, depending on the local velocity profile. In the narrow gaps between moving and stationary components, the local shear stresses may therefore contribute less to hemolysis than the high strains suggest, as noted by Thamsen et al. [5].
The existence and height of the CFL has been reported for many flow conditions [6, 7], but besides numerical approaches, e.g. [8,9] there are few systematic, experimental studies on how the particle distribution evolves along the streamwise direction. A major challenge in such measurements is the limited optical access across the channel height, especially at higher volume fractions. Thus, in this work, red blood cells with reduced optical density (*ghost cells*, GCs) are used to improve visibility. Their distribution evolution is compared with that of PMMA particles as they flow through a microchannel of comparable height to VAD rotor–stator gaps. The distributions are tracked in situ using astigmatism particle tracking velocimetry (APTV).
The experiments were carried out at the Institute for Fluid Mechanics and Aerodynamics at the Technical University of Darmstadt. The setup is described in detail in [10]; only a brief summary is provided here, as only minor modifications were made. As a first approximation of the axial flow state in a VAD gap, a channel flow with a height of 150 µm is generated by pumping the suspension through the channel with a syringe pump. Fluorescent particles are illuminated by a double-pulse, dual-cavity Nd:YAG laser, and astigmatism is introduced by a cylindrical lens placed in front of the CCD camera, which records double-frame images. The 3D particle positions are then reconstructed by cross-correlating the recorded images with a stack of calibration images. To isolate the effect of particle properties, measurements were performed with PMMA particles and with GCs of comparable sizes at otherwise identical flow conditions. The GCs were produced using repeated osmotic lysis based on modified methods from the literature [11,12]. A fraction of about 0.2% of the GCs was fluorescently labelled with Rhodamine 6G. An example of the obtained GCs is shown in Figure 1.

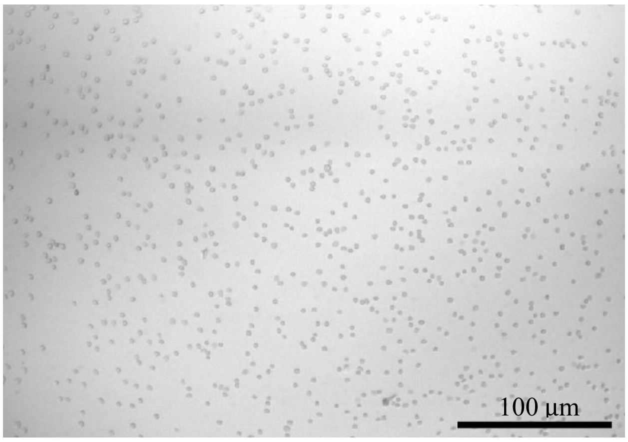

Figure 1: Bright-field microscopy image of the utilized ghost cells suspended in phosphate buffered saline (volume fraction $\Phi \approx 0.2\%$) using an adapted procedure from refs. [11] and [12].

The combined approach of both PMMA particles and GCs allows to evaluate how well blood analogue suspensions can represent the migration phenomena in real blood. Tracking the particle distribution evolution across the channel height in streamwise direction also enables uncovering the influence of the particle properties on the apparent viscosity and shear stresses, thus accelerating the development of better hemolysis prediction and improved VAD designs.

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Keywords: red blood cell, suspension flow, astigmatism particle tracking velocimetry

Lagrangian relative motion of particle-bubble pairs in gas–liquid–solid three-phase flows

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Bubble–particle relative motion governs mixing, transport, and collision processes in many natural and industrial gas–liquid–solid flows. In flotation, for instance, the relative velocity between a rising bubble and a particle controls approach and attachment efficiency. While most existing knowledge is based on Eulerian point measurements, recent advances now enable true Lagrangian tracking of individual bubbles and particles even in moderately dense bubbly flows [1,2]. We perform controlled three-phase experiments in an octagonal bubble column (11.5 cm diameter, 90 cm water height) with monodisperse bubbles of 3–5 mm generated by needle spargers under homogeneous bubbly-flow conditions. This study investigates the Lagrangian relative velocity and acceleration of bubble–particle pairs, explicitly conditioning on their spatial configuration—whether particles reside inside or outside bubble wakes. New high-resolution three-phase tracking data are currently being acquired, enabling analysis over a broader range of temporal and spatial scales; full results will be presented at the conference.

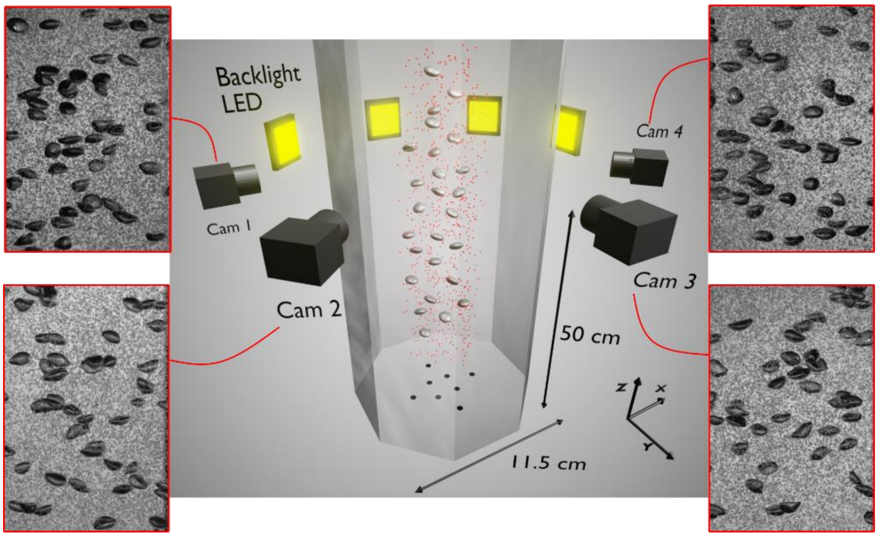

Fig. 1. Sketch of the octagonal bubble column used in the experiments (note that in the actual experiment, the number of bubbles in the column is $O(10^3)$ and approximately 50 to 100 bubbles are tracked in the field of view). The red points in the center panel represent glass beads.

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Keywords: Three-Phase Flows, turbulence moderation, particle acceleration.

Contact resolution between ellipsoids using distance parametrizations for PR-DNS

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The transport of particles in fluid flow is central to many industrial and environmental processes. Spatially resolved simulations of particle-laden flows can provide a deeper understanding of the underlying physics by accounting for interactions between particles and the fluid, as well as between particles themselves. The collision models used in these simulations rely on accurate contact points, which are only available in closed form for spheres. However, there is increasing evidence of strong shape effects on particle dynamics, and large-scale simulations with many non-spherical particles are required. Within the context of hydraulic engineering, the Institute of Fluid Mechanics [1] has conducted particle-resolved direct numerical simulations (PR-DNS) of sediment transport using a collision model [2] that required precise contact point calculation. Ellipsoids were used to model the shapes of sand grains, and contact was defined to occur at the closest points of colliding particles. Figure 1 illustrates the scenario.

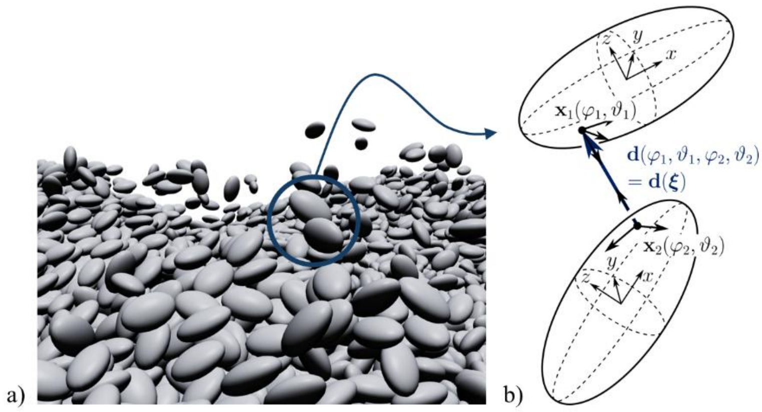

Figure 1: Contact detection in PR-DNS. a) Mobile bed with ellipsoidal particles, b) distance minimization for closest points.

This contribution addresses the computation of closest-point pairs for ellipsoids used in collision models. The underlying objective is a parametric minimum-distance problem, $\min d(\boldsymbol{\xi})$, that must be solved iteratively to determine contact points [3]. Existing approaches typically cast this problem as either an optimization or a root-finding formulation. Unfortunately, many available methods lack a unique solution or sacrifice accuracy for computational efficiency. With increasing particle volume fraction, however, collision events become more frequent and eventually dominate the dynamics in dense regimes. This creates a demand for reliable, fast distance algorithms. Several candidate methods are, therefore, adapted and evaluated for ellipsoids. Based on these findings, a combined method for distance computation is presented. The parametric problem is split into subtasks that are successively solved with tailored algorithms to ensure uniqueness and practical runtimes in the present setting. The resulting method outperforms the base methods and a well-established distance algorithm in terms of computational cost.

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Keywords: PR-DNS, non-spherical particles, ellipsoids, multiphase flow, contact detection, optimization

Radial reaction fronts with particle precipitation

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Radial reaction fronts can be employed to produce particulate materials, with broad applications ranging from soil remediation and stone conservation to the formation of functional barrier layers and particle synthesis [1,2]. Here, we investigate the spatiotemporal dynamics of radial reaction fronts in precipitation of mineral particles from salt solutions.

The radial injection of reactive salt solutions (Na_2CO_3 and $CaCl_2$) produces precipitation fronts of $CaCO_3$, where the evolving density, viscosity, and permeability distribution gives rise to distinct hydrodynamic regimes: particle advection, flow clogging, and gelation. By combining experiments in radial and capillary cells with variable gravity conditions during parabolic flight, we identify how reactant buoyancy and particle sedimentation modulate front dynamics and structure formation.

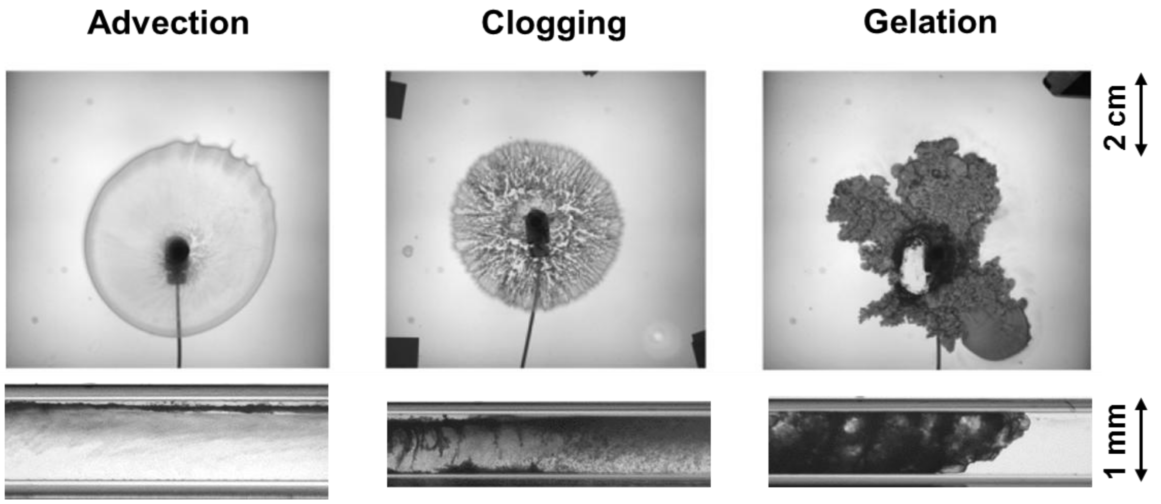

Figure 1: The three typical hydrodynamic regimes as they appear in experiments with calcium carbonate formation, i.e., Na2CO3 injected into CaCl2: particle advection, flow clogging and gelation regimes. The upper row shows the pattern formation in radial reactor cells in top view, while the lower row shows the precipitate reaction front in square capillaries in side view. In the snapshots of the upper row, the vector of gravity points into the viewing plane; in the snapshot of the lower row, the vector of gravity points downwards.

Our studies provide a unified framework for understanding pattern formation in the mixing zone of the two reactant solutions, paving the way for controlled, sustainable design of soft and mineral-based functional materials in natural and engineered environments.

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Keywords: particle-laden flow, reaction-diffusion-advection, hydrodynamic instabilities, micro gravity, precipitation

A numerical study of the influence of rotating flow on secondary droplet breakup in entrained-flow processes

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The utilization of alternative feedstocks such as bio-based pyrolysis oils is a key factor towards CO_2-free production in chemical industry. Overall gasification efficiency is highly dependent on droplet-scale aero-hydrodynamic interactions in liquid fuel sprays. In swirl gasification burners, secondary atomization of fuel droplets dominates the momentum exchange, evaporation, and mixing of the liquid feedstock. In this work, droplet breakup in an entrained-flow gasifier is numerically studied by varying the swirl intensity of the rotating gas flow and the upstream pressure of the inlet feedstock (from the nozzle) based on a simple pressure swirl atomizer. We found a pronounced impact on the droplet-size distribution of the spray, which is further examined by plotting volumetric distributions, calculating the Sauter Mean Diameter, and evaluating the probability distribution. Macroscopic variation in spray dispersion dynamics and the gas-liquid momentum ratio are also evident. The numerical shear breakup is modeled using the Kelvin-Helmholtz Rayleigh-Taylor (KHRT) breakup model, and the liquid feedstock is fed into the reactor under non-reacting inert conditions. Lagrangian droplet tracking is implemented to trace the breakup of primary droplets into secondary droplets.

Keywords: Secondary droplet breakup, Swirl flow, Entrained-flow gasification, Multiphase CFD simulation.

CFD Modeling of Two-Phase Flow in a Porous Ceramic under Plasma-Assisted Wastewater Treatment Conditions

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In this study, we present an integrated experimental and CFD-based investigation of two-phase air–water flow in a porous alumina ceramic used for plasma-assisted water treatment. A three-dimensional CFD model based on the Volume of Fluid (VOF) approach was constructed using a geometry obtained from X-ray computed tomography of the ceramic (Fig. 1a). This CT-derived representation preserves the actual pore arrangement. Transient simulations were conducted over a wide range of inlet water flow rates from 3.0 to 100 L h^{-1}, covering the operating window of the plasma reactor. From the simulations, the evolution of water volume fraction, wetted surface area, liquid film thickness, liquid hold-up, and residence time was derived.

The numerical results show that liquid distribution inside the ceramic changes markedly with increasing flow rate. At low inlet flow rates, water enters the pore space as thin films that spread along the ceramic surface under the influence of capillary forces. These conditions lead to moderate pore saturation and long residence times exceeding 8.2 s, while average film thicknesses remain around 0.36 mm. As the inlet flow rate is increased, inertial effects begin to outweigh capillary retention, causing the liquid to accumulate in pore cavities and form thicker films. This transition is clearly visible in the water volume fraction distributions shown in Fig. 1a, where the cases of 7.0 L h^{-1} and 20.2 L h^{-1} demonstrate the enlargement of saturated regions and the thickening of the flowing liquid layer. The hydrodynamic consequences of increasing flow rate are reflected in liquid hold-up and residence time, summarized in Fig. 1c. Liquid hold-up increases steadily with flow rate, rising from approximately 4 % at 3.0 L h^{-1} to nearly 28 % at 100 L h^{-1}, indicating extensive pore filling at high hydraulic load. In contrast, residence time decreases continuously from more than 8 s at the lowest flow rate to less than 2 s at the highest flow rate, consistent with the increasing velocity of the liquid through the pore network. These findings indicate a shift from capillary-dominated flow at low flow rates to inertia-dominated flow at higher flow rates, with important implications for plasma–liquid contact. The experimental degradation of indigo carmine mirrors these hydrodynamic trends. Under low-flow conditions, where thin films and long residence times prevail, degradation efficiencies reached up to 33.4 ± 1.8 mg L^{-1}. These observations highlight the crucial balance between liquid throughput and hydrodynamic conditions that support effective plasma-liquid interaction [1-2].

Overall, the combined CFD and experimental analysis demonstrates that the operating flow rate imposes fundamental trade-offs in plasma-assisted wastewater treatment. Higher flow rates promote improved surface wetting but simultaneously limit residence time and increase liquid shielding effects, which reduce contact between the liquid phase and plasma-generated reactive species.

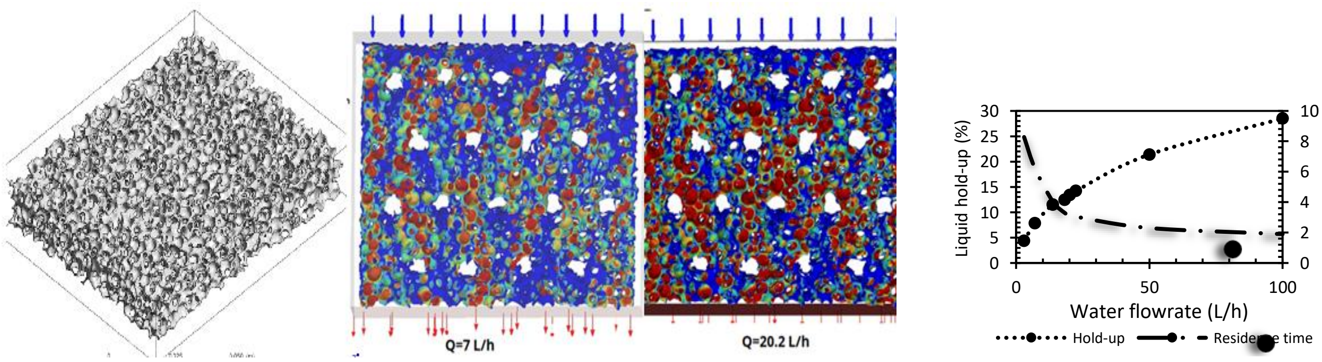

Fig. 1. (a) Computational domain reconstructed from X-ray CT data; (b) water volume fraction distribution within the porous ceramic at inlet flow rates of 7.0 and 20.2 L h^{-1}; (c) liquid hold-up (%) and residence time (s) as a function of water flow rate.

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Keywords: Multiphase modeling, Low-temperature plasma (LTP), CFD simulations, Wettability, Porous ceramic

Stofftransport und relativer Gasgehalt in einer Blasensäule im Pilotmaßstab – Experimente unter industriellen Prozessbedingungen

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Am Engler-Bunte-Institut des Karlsruher Instituts für Technologie (KIT) wird die Dreiphasen-Methanisierung als eine Schlüsselkomponente zum dynamischen Betrieb von Power-to-Gas-Prozessketten (PtG-Prozessketten) untersucht. Bei der Methanisierung werden herkömmlicherweise Festbettreaktoren eingesetzt, in denen die gasförmigen Reaktanden (bei PtG-Prozessen H_2 und CO_2) direkt mit dem festen Katalysator in Kontakt kommen (= Zweiphasensystem) und dort zu den Produkten H_2O und CH_4 reagieren. Im Fall der Dreiphasen-Methanisierung ist der Reaktor dagegen eine Slurry-Blasensäule, bei der feine Katalysatorpartikel in einer Flüssigkeit suspendiert und durch Edukt- und Produktgase fluidisiert sind. Die Suspension wird in der Blasensäule von den Reaktionsgasen durchströmt, welche sich in der Flüssigkeit lösen und anschließend am Katalysator reagieren. Dabei sorgt die Flüssigkeit als dritte, inerte Phase für eine starke Durchmischung, einen guten Wärmeübergang und bringt zusätzliche thermische Masse in das System ein, die dynamische Lastwechsel glättet und damit eine bessere Lastflexibilität im Vergleich zu Festbettreaktoren garantiert.

In einer abgeschlossenen Promotionsarbeit [1] wurde ein reaktionskinetischer Ansatz zur Beschreibung der Dreiphasen-Methanisierung aufgestellt und ein Blasensäulenreaktor mit einem dynamischen axialen Dispersionsmodell modelliert. Eine experimentelle Validierung des Modells war jedoch nicht Teil der Arbeit.

Zur Validierung des Modells unter realen Prozessbedingungen mit Reaktion wurde daher eine Pilotanlage am KIT Energy Lab 2.0 errichtet, welche mit einem Blasensäulenreaktor von 260 mm Innendurchmesser ausgestattet ist. Der eingereichte Beitrag soll diese Pilotanlage und die mit ihrer Hilfe erzielten Erkenntnisse vorstellen. Besonders hervorzuheben sind: (a) Das Reaktorkonzept ermöglicht den lastflexiblen Betrieb. (b) Im stationären Betrieb liegt eine starke Temperatur- und Druckabhängigkeit des Umsatzes vor. (c) Die Limitierung durch (äußeren) Stofftransport und/oder Reaktionskinetik kann mit bisher vorliegenden Daten und Modellen nicht ausreichend genau beschrieben werden. [2]

Zur Klärung des letztgenannten Punktes sind daher weiterführende Experimente zu Stofftransport und Hydrodynamik erforderlich. Hierzu wurde an der Pilotanlage eine Rückführung des Gases im geschlossenen Kreislauf nachgerüstet, angetrieben durch einen Turbinenverdichter. Die Anlage kann nun in zwei verschiedenen Modi betrieben werden: (a) Methanisierungsbetrieb und (b) geschlossener Gaskreislauf (ohne Reaktion). Im geschlossenen Kreislauf können über eine dynamische Messung des Druckabfalls während der Gasabsorption volumetrische Stoffübergangskoeffizienten ($k_L a$) ermittelt werden [3]. Zudem wurde mit der Nachrüstung der mögliche Betriebsbereich für Hydrodynamikversuche (z. B. Messung des relativen Gasgehalts) deutlich erweitert.

Im nächsten Schritt wurden umfangreiche Messungen zum Stofftransport und zum relativen Gasgehalt ("Gasgehalt") mit CH_4, CO_2 und N_2 in Dibenzyltoluol (Abkürzung DBT, Flüssigphase bei der Dreiphasen-Methanisierung) durchgeführt – der Einfluss von festem Katalysator soll in zukünftigen Experimenten ermittelt werden.

Da die Diffusionskoeffizienten der Gase in DBT mit steigender Temperatur stark zunehmen, wurde im betrachteten Temperaturbereich (100 °C bis 260 °C) auch ein starker Anstieg der $k_L a$-Werte festgestellt. Während bei 100 °C in einem weiten Bereich von Gas-Leerrohrgeschwindigkeiten (0,01 bis 0,2 m/s) gemessen wurde, liegt bei 260 °C die maximal mögliche Gasgeschwindigkeit bei 0,03 m/s. Die gemessenen $k_L a$-Werte sind jedoch bezüglich der Diffusionskoeffizienten so konsistent, dass die Daten gut auf den Temperaturbereich der Dreiphasen-Methanisierung (260 °C – 330 °C) extrapolierbar sein dürften.

Messungen zum Gasgehalt wurden bei Temperaturen bis 320 °C, Drücken bis 20 bar und Gas-Leerrohrgeschwindigkeiten bis 0,2 m/s durchgeführt. Hierbei konnte für das betrachtete Stoffsystem der starke Einfluss der Gasdichte auf den Gasgehalt nachgewiesen werden, was sich auch mit der gängigen Literaturvorstellung deckt [4].

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Keywords: pilot scale bubble column, gas holdup, mass transfer, elevated pressure and temperature

Analysis of CO_2 Mass Transfer in Ionic Liquid–Water Mixtures by Thermophysical and Taylor Bubble Studies

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Understanding the multiscale mechanisms governing CO_2 absorption in ionic liquid (IL) based solvent systems is essential for the development of next-generation separation technologies. The behavior of these solvents emerges from different and interconnected phenomena: molecular interactions define thermophysical properties, such as viscosity and diffusivity, which in turn shape fluid dynamics and ultimately control gas–liquid mass transfer in contactors. In this work, we investigate this chain of dependencies for aqueous mixtures of 1-ethyl-3-methylimidazolium acetate (EMIM OAc) and 1-butyl-3-methylimidazolium tetrafluoroborate (BMIM BF_4), two hydrophilic ionic liquids that have gained significant attention for CO_2 capture [1].

A comprehensive dataset of viscosity, density, surface tension and electrical conductivity was collected for different IL–water compositions, both before and after CO_2 absorption. This allows us to quantify not only how CO_2 uptake alters the liquid microstructure, but also to understand the intricate correlations between composition, intermolecular interactions and macroscopic transport behavior. These measurements aim to help connect the molecular scale to the mass-transfer performance.

To assess the impact of these property changes on gas–liquid mass transfer, CO_2 absorption of Taylor bubbles in vertical capillaries of circular shape with varying but defined hydraulic diameters is studied. In this configuration, single Taylor bubbles are held stationary while high-speed imaging captures the evolution of the bubble volume, allowing the measurement of the CO2 uptake by the liquid phase. From the transient development of the bubble volume, liquid-side mass transfer coefficients k_L are extracted following established methodologies as described [2, 3, 4].

The combined thermophysical and Taylor bubble analysis highlights a strong coupling between solvent composition, CO_2-induced structuring and mass transport performance. Increasing IL content leads to higher viscosity and lower diffusivity, and the viscosity further increases upon CO_2 absorption. These effects translate into measurable shifts in the mass transfer coefficient k_L, demonstrating how subtle molecular reorganizations propagate across scales to influence macroscopic mass transfer.

Overall, the results provide new insight into the dynamic behavior of ionic liquid–water mixtures under CO_2 absorption conditions and support the rational design for larger scale ILs based gas–liquid contactors, including bubble column processes. This multiscale framework represents a step toward predictive and optimized formulations for energy efficient carbon-capture technologies.

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Keywords: Taylor Bubble, CO_2 mass transfer, Ionic liquids, Thermodynamic properties, Carbon capture

Modulierte Blasenbildung zur Verbesserung des Stofftransportes bei kleinen Volumenströmen

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Die Gaseinspeisung in einer Blasensäule erfolgt häufig über eine Lochplatte, die über einer Gasverteilerkammer angebracht ist, um beim Ausströmen eine gleichmäßige Gasverteilung zu ermöglichen. Bei kleinen Volumenströmen zeigt die Lochplatte jedoch eine ungleichmäßige Gasblasenbildung: Nur ein Teil der Löcher ist aktiv und trägt zur Bildung von Gasblasen bei. Der Volumenstrom verteilt sich ungleichmäßig über dem Querschnitt und führt zu lokal größeren Gasblasen. Das führt zu Inhomogenitäten der Strömung und des Stoffaustauschs innerhalb der Blasensäule. Eine kontrollierte Modulation des Gasdrucks an den Einspeiser-Öffnungen bietet die Möglichkeit, diesem Effekt entgegenzuwirken.

In diesem Beitrag werden die Ergebnisse einer Untersuchung vorgestellt, bei dem der für die Blasenbildung notwendige Druck an allen Öffnungen gleichzeitig erzeugt wird. Das ermöglicht den Betrieb des Einspeisers bei gleichem Gesamtvolumenstrom mit allen Löchern. Im Vergleich zu einem konstanten Volumenstrom entstehen dadurch kleinere Gasblasen und führen damit zu einem verbesserten Sauerstoff-Transport in die Flüssigphase.

Die Experimente werden in einer vollautomatisierten Blasensäule durchgeführt. Zunächst wird durch Spülung mit Stickstoff im Fluid gelöster Sauerstoff aus der Flüssigphase verdrängt und anschließend alternierend Messungen mit kontinuierlichem bzw. druckmoduliertem Sauerstoffvolumenstrom durchführt. Die Messung des gelösten Sauerstoffs erfolgt mittels einer optischen Gelöstsauerstoffsonde. Abhängig vom Volumenstrom zeigen sich in den Untersuchungen Verbesserungen von bis zu 15% des Stoffübergangskoeffizient (K_la) für den Sauerstofftransport bei der druckmodulierten Einspeisung.

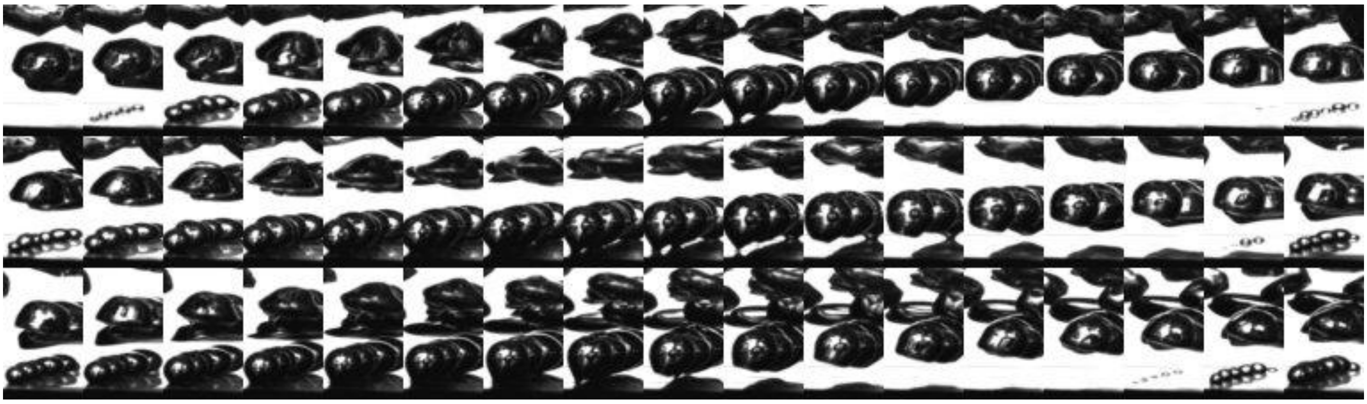

Abbildung 1: Bildserie der synchronen Blasenentstehung an einer Lochreihe der Lochplatte mit einer Modulationsfrequenz von 30 Hz. (Zeitreihe startet links oben und endet rechts unten)

Keywords: Blasensäule, Stofftransport, Blasenbildung, kontrollierte Gasblasenbildung

Radiographic measurements of liquid foam flow around a cylindrical obstacle

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When a fluid such as air or water flows around an obstacle at a certain velocity, vortices are formed and detach periodically at the back of the obstacle, depending on its shape and size. In flowing liquid foam as a gas-liquid two-phase system, such vortex shedding has not yet been reported. Several experimental studies have used optical measurements in order to investigate a two-dimensional flow of liquid foam around a circular obstacle [1-3]. In a similar three-dimensional flow configuration around a cylindrical obstacle, we have combined neutron and X-ray radiographic measurements to experimentally determine both the volumetric liquid fraction of the foam and its flow velocity [4]. This conference contribution presents experimental results at different cylinder diameters, foam bubble sizes, and superficial gas velocities. Neutron radiography has revealed the local distribution of the liquid fraction in the foam and, in particular, resolved the bubble layering near the cylinder wall [5]. X-ray radiography was used to monitor the liquid fraction distribution in repeated measurement runs and, more importantly, to measure the foam velocity around the cylinder by Lagrangian particle tracking [6]. Notably, the tracer particles used here also enable measuring the local vorticity of the flowing foam. All experimental data will be made available for comparison with numerical simulations. With regard to potential vortex shedding, future studies will need to address liquid foam flowing around a three-dimensional obstacle at higher superficial gas velocity than applied here. In this case, spatially resolved measurements of the liquid fraction might be particularly suitable for flow characterisation.

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Keywords: Gas-liquid flows, Liquid fraction, Particle tracking velocimetry, Neutron radiography, Vorticity, X-ray radiography

CFD investigations of mixing of micron-sized aggregates in an Opposed Jets Fluidized Bed

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Fine aggregates are considered as essential elements in the production of a wide range of food, pharmaceutical as well as other chemical products. In process industry, mixing of such particles is a crucial operation which controls the quality, texture and attributes of the final product. For instance, formation of hetero-aggregates mainly depends on effective mixing and blending of different homo-aggregates [1]. However, mixing becomes quite challenging while dealing with cohesive particles because of strong inter particulate forces, mostly van der Waals or capillary forces. A strong external force is required to overcome the cohesive forces and eventually, to agitate and mix such aggregates. With several advantages, mixing of such aggregates can be carried out in gas phase regime using fluidized bed systems. However, gas-solid environment yields to turbulent multiphase flows in such cases. Hence, it is important to understand the internal hydrodynamics of the apparatus for the optimum performance [2]. In the current study, a two-way coupled Euler-Lagrange CFD model has been developed for the investigation of hydrodynamics and mixing of micron sized aggregates in an opposed jet fluidized bed. In total two phases were selected including air as a gas phase whereas TiO_2 was considered as the solid phase. Micron-sized particles were placed in the apparatus at known quantity and different streams of air jet were injected with the help of three nozzles mounted in the bottom and the side walls. As a result, fluid dynamically different zones were formed such as stressing zone and mixing zone (Fig. 1). Increasing jet injection, the suspension and mixing of particles is improved. However, very high air injection results in formation of wall bounded layer of particles which negatively effects the mixing. Further investigations are being carried out for the parametric optimization with respect to different particle types, size distribution and mass loading.

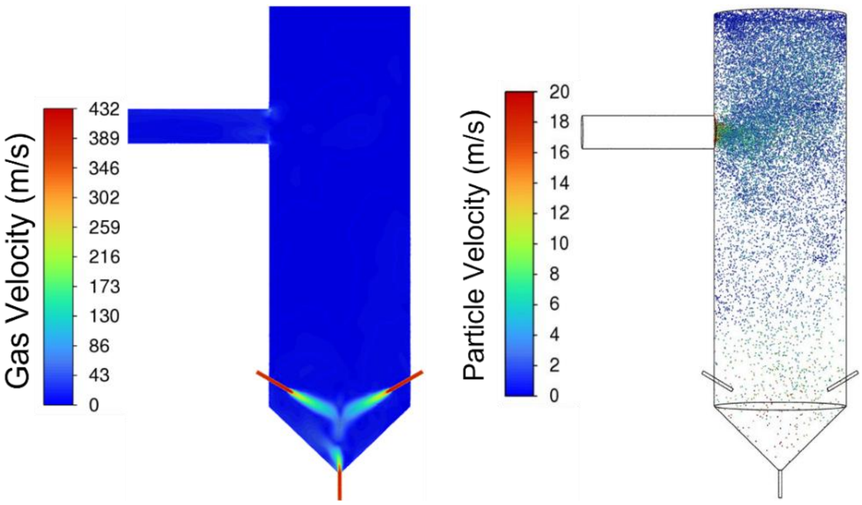

Figure 1: Velocity profile of gas and solid phase

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Keywords: Multiphase flow, CFD, particle mixing, fluidized bed.

Modification of the flow structure of liquid jets by dispersed bubbles and particles

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Turbulent jets are used in process engineering to efficiently mix different phases such as particles or bubbles in liquids or to intensify the rate of particle-bubble collisions [1]. Compared to the single-phase case, two-phase jets (particles or bubbles in liquid) are not extensively investigated and for the three-phase jet (liquid, particles and bubbles) virtually no scientific studies exist. The present investigation focuses on the vertically upwards pointing axisymmetric jet. The single-, two-, and three-phase case of liquid jet, particulate jet, bubbly jet and particle-bubble-laden jet are considered. The quantities of interest in the system are the velocities and locally resolved volume fractions of all phases. Experiments are performed for the bubbly jet in a cylindrical water tank with a $D = 5\,mm$ nozzle. The local bubble size, speed and volume fraction are measured with an optical-fiber Doppler probe by A2 Photonic Sensors [2]. Simulations of bubbly, particulate and three-phase jets are performed in a Eulerian multi-fluid framework, calculating their local velocity and volume fraction field. Full sets of unsteady Reynolds-averaged Navier–Stokes (URANS) conservation equations (mass and momentum) are applied to each phase [1][3].

A prominent feature found in the near-field of the two-phase bubbly jet is shown in Figure 1: the bubbles are expelled from the jet center soon after leaving the nozzle, only to again spread over the whole cross-section of the jet at a farther distance. This effect is observed in both, the simulations and experiments. Differences in the position of the dip along the jet centerline and its distinctness can be attributed to the non-uniform inflow velocity profile in the experiment vs. the idealized constant profile of the simulations. The bubbly and particulate two-phase cases quickly reach a stationary state in the simulations. In contrast, the three-phase jet, with both bubbles and particles becomes highly transient and the gas/solid fractions greatly vary in time. Here, the interaction of bubbles and particles, and their effect on the liquid flow field have to be studied more closely.

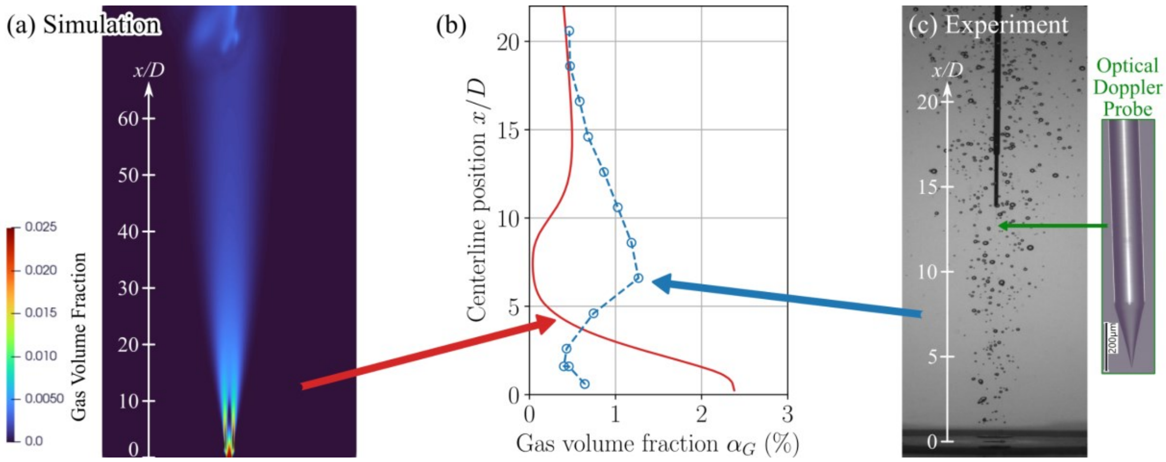

Figure 1: Near-nozzle dip of the gas volume fraction (GVF) in the jet center $\dot{V}_L = 1.96$ L/min, $\dot{V}_G = 0.05$ L/min). (a) Euler-Euler simulation GVF snapshot. (b) Centerline profile of the GVF from simulation (solid red) and experiment (dashed blue). (c) Shadowgraph image of the experimental bubbly jet and the optical Doppler probe.

Acknowledgements

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Keywords: Turbulent jet, disperse multiphase flow, optical Doppler sensor, Euler-Euler two-fluid model

Large Contact Angle Hysteresis Enhances Post-Impact Droplet Oscillations

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Droplet impact on solid surfaces plays a critical role in a wide range of applications, including inkjet printing, spray cooling, surface coatings, and microdroplet chemistry. Precise control of droplet-surface interactions is essential, but the fundamental mechanisms governing this process are still not fully understood. In this study, we demonstrate that large contact angle hysteresis (CAH) on hydrophobic nanoporous surfaces significantly amplifies post-impact droplet oscillations. This reveals the critical influence of CAH on the redistribution of impact energy and the modulation of droplet-surface interactions. Using shape mode decomposition via Legendre polynomials and Fast Fourier Transform (FFT) spectral analysis, we show that surfaces with larger CAH excite and sustain higher-order droplet shape mode oscillations, leading to persistent capillary waves even after contact line pinning. The observed amplitude modulation and multiple frequency components within individual shape modes reveal nonlinear energy transfer between different modes. These amplified and coupled oscillations are shown to promote daughter droplet coalescence. This study presents a framework for understanding the role of CAH in storing and redistributing impact energy through nonlinear mode excitation and establishes CAH as a critical design parameter for controlling fluid dynamics on solid surfaces.

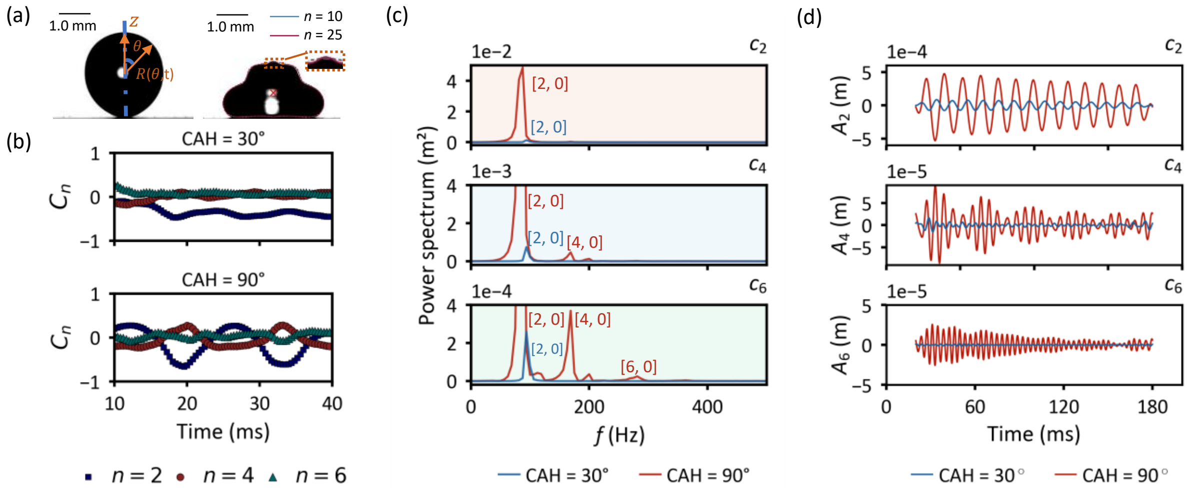

FIGURE 1. Shape mode decomposition of droplet shape oscillations. (a, left) Droplet contour extracted from image analysis, used to obtain the radial amplitude $R(\theta, t)$. (a, right) Shape mode decomposition of the droplet interface, showing mode $n = 10$ (blue dashed line) and mode $n = 25$ (red solid line). Scale bar: 1.0 mm. (b) Evolution of the shape mode amplitude of three modes, n = 2,4,6 and 8, on two different CAH surfaces. (c) Fast Fourier Transform (FFT) analysis of the shape modes c_2, c_4 and c_6. (d) Band pass filter for the shape modes c_2, c_4 and c_6.

Keywords: droplet oscillation, contact angle hysteresis, shape mode decomposition, daughter droplet, mode excitation

Optische Charakterisierung der Zusammensetzung von Lacktröpfchen im Flug

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Die Qualität von Beschichtungen in der Spritzlackierung hängt maßgeblich von der Zusammensetzung der Lackteilchen ab, die während des Zerstäubungsprozesses entstehen. Diese sogenannten dynamischen Lackteilchen bestimmen entscheidend die Homogenität, den Farbton und die Oberflächenstruktur des Endprodukts. Trotz des hohen Automatisierungsgrades moderner Lackierprozesse existiert bislang keine geeignete Methode, um die Zusammensetzung einzelner Lackteilchen im Flug zum Substrat zu überwachen. Die vorliegende Arbeit beschreibt ein neuartiges optisches Verfahren und eine dazugehörige Vorrichtung, mit denen die Zusammensetzung dynamischer Lackteilchen anhand ihrer zeitlich aufgelösten Lichtstreusignale charakterisiert wird.

Das Verfahren basiert auf der Analyse der zeitlichen Abfolge von Lichtstreuintensitäten [1], die entstehen, wenn ein Lackteilchen einen geformten Lichtstrahl passiert. Die zeitabhängige Lichtstreuung wird von zwei oder mehr Detektoren erfasst. Aus der Reihenfolge der Signalmaxima lässt sich bestimmen, ob das Lackteilchen als semi-transparent oder nicht-transparent einzustufen ist. Durch statistische Auswertung vieler solcher Ereignisse kann die relative Anzahl semi-transparenter Teilchen N_{rel} bestimmt werden, die Rückschlüsse auf die Zusammensetzung der Lackteilchen erlaubt.

Die experimentelle Validierung erfolgte durch die Analyse von Lacktröpfchen in einem Spray, die aus Materialien mit unterschiedlichen Gewichtsverhältnissen zwischen Basislack und Farbkonzentrat hergestellt wurden $C_m = \{3\%, 5\%, 11\%, 13\%, 17\%, 23\%\}$. Die Tröpfchen wurden hinsichtlich ihres Transparenzgrades klassifiziert und gezählt. Aus den resultierenden Häufigkeiten wurde N_{rel} berechnet und mit dem jeweiligen Mischverhältnis C_m verglichen. Die Ergebnisse zeigen eine deutliche Korrelation zwischen N_{rel} und C_m (siehe Abb. 1): Mit zunehmendem Anteil des Farbkonzentrats sinkt der Anteil semi-transparenter Lackteilchen. Dieses Verhalten bestätigt die Eignung des vorgestellten Verfahrens zur quantitativen Charakterisierung der Zusammensetzung dynamischer Lackteilchen im Beschichtungsprozess.

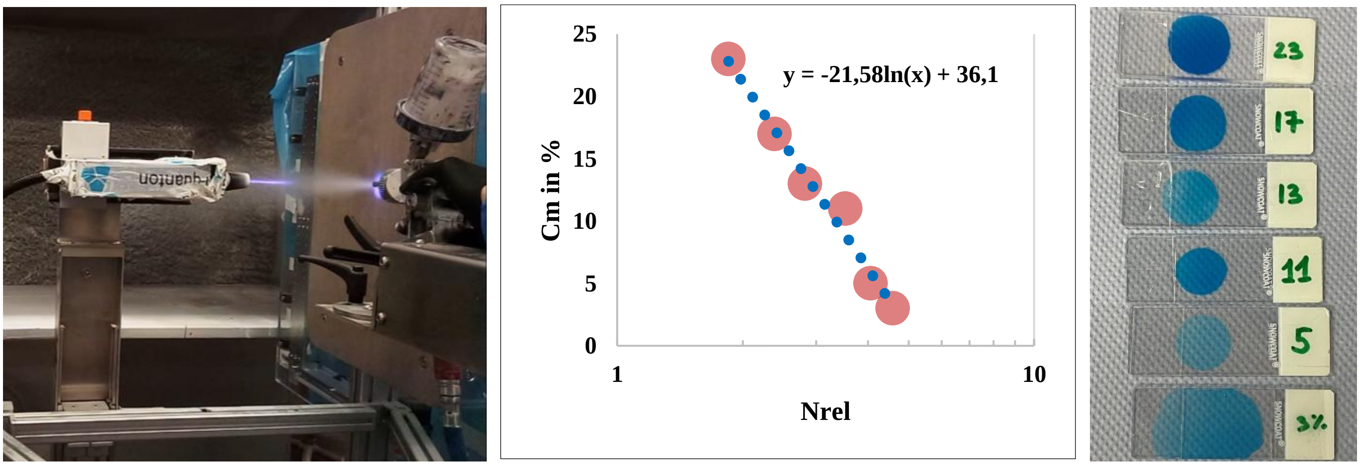

Abbildung 1: *(links)* Experimenteller Aufbau mit der Messsonde und einem pneumatischen Zerstäuber. *(mitte)* Korrelation zwischen dem Gewichtsmischverhältnis C_m und der relativen Anzahl semi-transparenter Lackteilchen N_{rel}. Mit abnehmendem Anteil des Farbkonzentrats steigt die Anzahl semi-transparenter Lackteilchen. *(rechts)* Lackproben der untersuchten Materialien. Die unerwarteten visuellen Unterschiede in der Transparenz resultieren aus geringfügigen Abweichungen im Abstand zwischen den Objektträgern.

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Keywords: Spritzlackierung, Transparenzanalyse, Prozessüberwachung, semi-transparente Lackteilchen

Charakterisierung eines LNH3-Sprays und der Lichtstreuung an einzelnen LNH3-Tröpfchen

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Die optische Messtechnik zur Tröpfchencharakterisierung in dichten Sprays stellt eine besondere Herausforderung für alle auf Vorwärtsstreuung basierenden Verfahren dar – darunter Laserbeugungs-, Phasen-Doppler- und bildgebende Techniken. Ursache hierfür sind die starke Abschwächung der Lichtintensität durch Absorption im Sprühstrahl sowie Mehrfachstreuung, die die für die Auswertung relevante Lichtstreuung überlagert und verfälscht. Hinzu kommt, dass der optische Zugang häufig durch den experimentellen Aufbau begrenzt ist, wodurch der Einsatz vorwärtsstreuungsbasierter Messverfahren weiter eingeschränkt oder sogar unmöglich wird. Solche dichten Sprays mit limitiertem optischem Zugang treten insbesondere bei Flash-Boiling getriebener Zerstäubung auf, wie beispielsweise beim Einsatz von flüssigem Ammoniak (LNH3) als Brennstoff. Zusätzlich zum primären Strahlzerfall führt die thermodynamische Instabilität unter Flash-Boiling-Bedingungen dazu, dass Tröpfchen durch interne Blasenbildung expandieren und zerplatzen. Um die Einschränkungen vorwärtsstreuungsbasierter Methoden zu umgehen und Tröpfchen mit Dampfblasen zu detektieren, wird in dieser Arbeit ein auf Rückstreuung basierendes Messverfahren, TSTOF (Time-Shift Time-of-Flight) [1], eingesetzt. Das TSTOF-Messinstrument erfasst die Lichtstreuung zweiten Grades, sodass das detektierte Signal das Tröpfchen zweimal durchläuft (siehe Abb. 1 (*links*)) und damit auch Informationen über dessen inneren Aufbau enthält. Bei TSTOF werden vier Lichtstreusignale pro Tröpfchen aufgezeichnet, aus denen Tröpfchengeschwindigkeit und -größe redundant bestimmt werden können.

Ein solches TSTOF-basiertes Messinstrument wird in dieser Arbeit zur Charakterisierung eines LNH3-Sprays unter verschiedenen Betriebsbedingungen verwendet. Der Versuchsaufbau ist in Abb. 2 (*mittig*) dargestellt; ergänzend kommen Hochgeschwindigkeitskameras zum Einsatz. Weiterhin wird die Leistungsgrenze des TSTOF-Verfahrens unter den vorliegenden Bedingungen bewertet, indem Messungen nahe am Düsenaustritt durchgeführt wurden. Darüber hinaus wird die Lichtstreuung einer Tröpfchenkette (siehe Abb. 3 (*rechts*)) qualitativ analysiert, um das Streuverhalten von Tröpfchen mit Dampfblasen zu untersuchen.

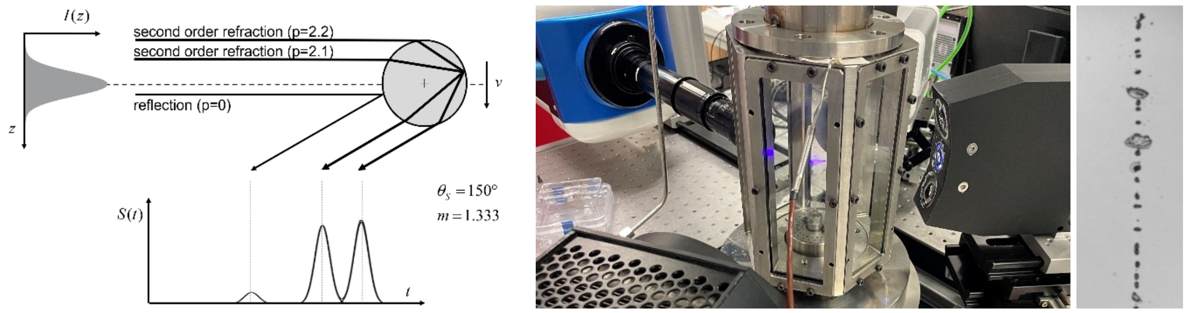

Abbildung 1: (links) 2D-Darstellung der Lichtstreuung eines transparenten Tröpfchens an einem Gauß-Strahl. Ein sich durch den gaußförmigen Lichtstrahl bewegendes Tröpfchen transformiert dessen Intensitätsverteilung in ein zeitliches Signal, das als Time-Shift-Signal bezeichnet wird. (mittig) Experimenteller Aufbau mit der Brennkammer und einer Ultra-Hochgeschwindigkeitskamera kombiniert mit einer Messsonde eines TSTOF-Messinstruments (ParticleTensorAI®) (rechts) Aufnahme einer LNH_3-Tröpfchenkette mit wachsenden Dampfblasen. Im Bild sind mehrere geplatzte Tröpfchen deutlich erkennbar.

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Keywords: LNH3-Spray, Gasinklusionen, Tröpfchen
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Deep Learning–Based Flow Reconstruction from Lagrangian Particle Tracking in Bubbly Flows

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Lagrangian Particle Tracking (LPT) has become one of the most frequently used 3D flow measurement methods in the recent years. The measured Lagrangian data is then often used for high-resolution flow field reconstructions, e.g. for pressure determination or flow structure identification. Although powerful data assimilation and deep learning-based methods that use physical constraints and regularizations to interpolate flow fields from LPT data exist for single-phase flows [1], such tools have rarely been used for dispersed multi-phase flows, like bubbly flows. On one hand, additional physical constraints due to gas-liquid interfaces are present that require dedicated treatment. On the other hand, the experimentally measured data is highly non-uniform and sparser than that of single-phase flows due to the hindered optical access by bubbles. To address these additional challenges, we are developing a deep learning-based methodology incorporating modern Transformer network architecture and suitable physical constraints. To develop this methodology, we sample artificial tracers from high-fidelity bubbly flow DNS data [2] that aims to mimic realistic experimental LPT measurements in bubbly flows. We also use the DNS data to validate the achieved flow reconstruction. Preliminary results demonstrate the potential of our method for dispersed multi-phase flows, showing promising reconstruction quality.

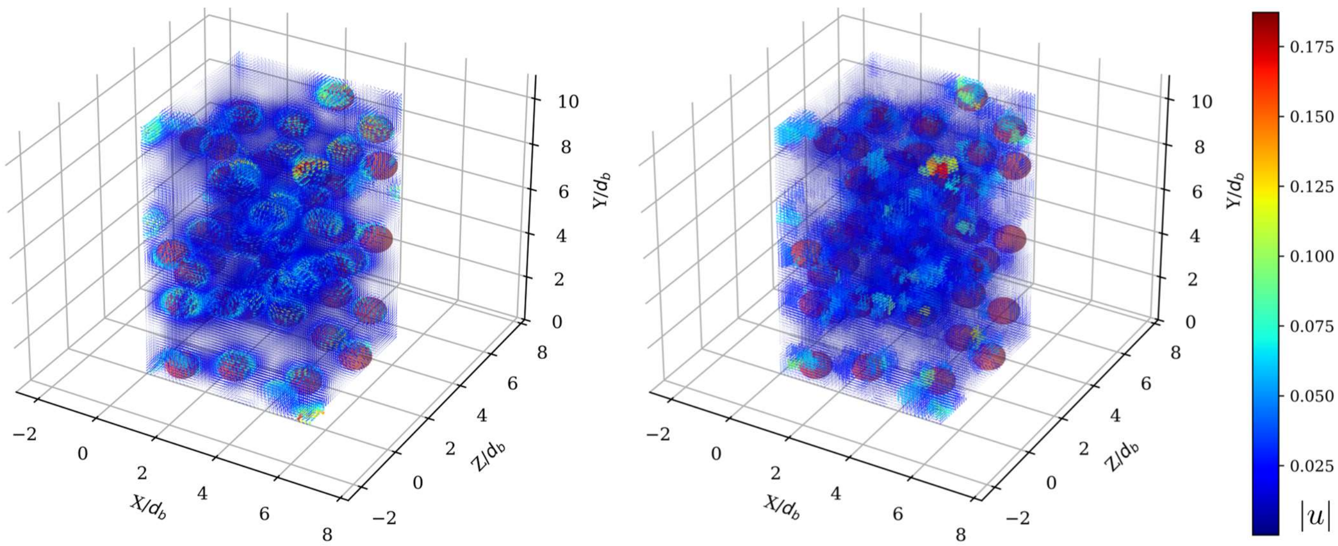

Figure 1: Preliminary flow reconstruction results from sparse measurements. Left: DNS flow field around bubbles (red spheres); Right: Prediction of the developed method with $O(10^3)$ sampled data points mimicking an experimental measurement.

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Keywords: Lagrangian Particle Tracking, Bubbly Flows, Flow Reconstruction

Investigation of Biomass Particle Dynamics and Bubble Behavior in a Pseudo-2D Multi-Solid Fluidized Bed

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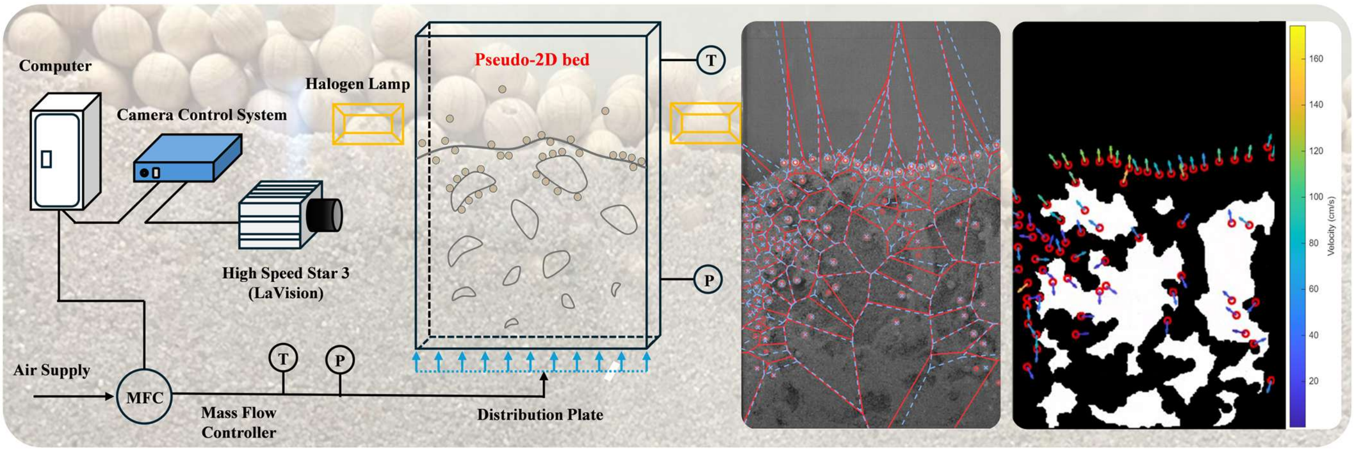
The pyrolysis of biomass represents a promising thermochemical pathway for the sustainable conversion of waste resources into valuable fuels and platform chemicals. The hydrodynamics of such systems in pyrolysis fluidized beds critically influence gas–solid contact efficiency, heat transfer, and reaction uniformity, yet remain insufficiently understood. In this study, a pseudo-two-dimensional (2D) multi-solid fluidized bed [1] was employed to investigate bubble behavior and biomass particle dynamics in a system consisting of sand as inert material and monodisperse spherical biomass particles as the reacting fuel. A high-speed imaging system coupled with Particle Tracking Velocimetry (PTV) was utilized to capture bubble evolution [2] under different superficial gas velocities, while the Voronoi algorithm and a Relaxation Probability Tracking approach [3] were applied to segment the flow domain into local regions and to support the prediction of individual biomass particle trajectories.

The results reveal a pronounced dependence of flow structure and particle distribution on gas velocity. At low velocities, the bed exhibits distinct stratification as lighter biomass particles accumulate in the upper region owing to density contrast and limited bubble activity. As the gas velocity increases, bubble size, rise velocity, and coalescence frequency grow substantially, leading to intensified particle agitation and a transition from stratified to well-mixed states. The degree of mixing continues to improve at higher velocities as bubble-induced turbulence promotes vertical circulation and interphase exchange. Correlation analysis indicates that the spatial distribution and motion of biomass particles are strongly coupled with bubble dynamics, particularly in bubble wakes and near boundary regions. These findings provide new insights into the fundamental fluidization behavior of multi-solid biomass systems and provide a scientific basis for the design and optimization of biomass pyrolysis fluidized bed reactors.



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Keywords: Fluidized bed; Pyrolysis; Bubble dynamics; Particle Tracking Velocimetry; Voronoi algorithm; Multi-solid System

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Analyse der Tiegelausströmung beim Aluminothermischen Schweißen: Von analogen Laborversuchen zu digitalen Prognosen

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Das aluminothermische (AT) Schweißverfahren wird aufgrund seiner Einfachheit, Robustheit und Portabilität als ein wichtiges Verfahren zum Reparaturschweißen von Schienen eingesetzt. Das Verfahren basiert auf einer stark exothermen Reaktion einer Thermit®-Portion aus Eisenoxid, Aluminium und Legierungsbestandteilen. Dabei bilden sich flüssiger Thermit®-Stahl und Schlacke mit einer Temperatur von über 2000 °C, die sich aufgrund ihrer Dichte im Einweg-Reaktionstiegel trennen und nacheinander in die darunterliegende Gießform ausströmen. Für eine fehlerfreie Schweißnaht ist der Zeitpunkt des Durchbruchs der Schlacke (leichte Phase) entscheidend: Läuft die Schlacke mit dem Stahl ein, können Fehlstellen aufgrund der Schlacke in der Schweißnaht entstehen, wodurch deren mechanische Qualität beeinträchtigt wird. Daher ist ein detailliertes Verständnis der Zweiphasenströmung und der Bedingungen, die zum Schlackedurchbruch führen, von großer Bedeutung.

Zur Analyse des Ausströmverhaltens wurde ein Laborprüfstand konstruiert, für den ein Einweg-Reaktionstiegel aus Plexiglas gefertigt wurde, um eine direkte Beobachtung der Strömungsvorgänge zu ermöglichen. Wasser und Öl wurden als Analogfluide für Stahl und Schlacke eingesetzt. Der Auslauf wurde durch einen schlagartig öffnenden Verschluss initiiert und mittels Hochgeschwindigkeitsaufnahmen dokumentiert. Ergänzend wurden isotherme CFD-Simulationen mit dem multiphaseInterFoam-Solver mittels OpenFOAM® durchgeführt, um das Strömungsverhalten sowohl des Wasser-Öl-Systems als auch des Stahl-Schlacke-Systems zu prognostizieren.

Im Fall des Wasser-Öl-Systems wurde eine gute Übereinstimmung zwischen den Simulationsergebnissen und den Laborexperimenten festgestellt. Der Zeitpunkt des Durchbruchs des Öls (leichte Phase) wurde in der Simulation im Vergleich zu den experimentellen Werten um etwa 8 % unterschätzt. Die Simulationen des realen Stahl-Schlacke-Systems zeigten bezüglich des Durchbruchs ein ähnliches Strömungsverhalten, wobei der Durchbruch der Schlacke im Vergleich zum Zeitpunkt des Öl-Durchbruchs im Wasser-Öl-System deutlich später erfolgte. Ursache hierfür ist die höhere Oberflächenspannung zwischen Stahl und Schlacke, welche den Eintritt der Schlacke verzögert und dafür sorgt, dass die Schweißlücke zunächst vollständig mit Stahl gefüllt wird.

Insgesamt wurde der Durchbruch der leichteren Phase (Öl bzw. Schlacke) sowohl in den Laborversuchen als auch im Realsystem als unvermeidbar identifiziert. Während er im Wasser-Öl-System früh erfolgt, tritt er im Stahl-Schlacke-System deutlich später auf, was ein vorteilhafter Effekt für die Qualität aluminothermischer Schienenverbindungen darstellt.

Keywords: Aluminothermisches Schweißen, CFD, Mehrphasenströmungen, OpenFOAM®, Stahl-Schlacke, Tiegelausströmung, Wasser-Öl.

Danksagung:
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Heat Transfer and Grid Turbulence at Equivalent Artificial Roughness Density over Flat Plates

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Abstract

Fluid mechanics and local Nusselt numbers at turbulent flow over rough flat plates and for the near wall area are detailed presented in Schlichting [1].

The local Nusselt number as a function of the local Reynolds number is based on the Dipprey and Sabersky experiments, with the equation derived initially by Th. von Karman and developed to integrate further available approximated measurements [1], including improved macroscopic parameters for the viscous Reynolds number [2]. The surface equivalent artificial roughness density with cylindrical elements was adjusted to be equivalent to the spherical elements at full "sand roughness", resulting to a good agreement for the near wall local Nusselt numbers at near wall viscous flow [3].

Average Nusselt numbers are presented at fully turbulent flow over rough flat plates with cylindrical vertical elements at equivalent artificial roughness density.

The design of the rough flat plates, including now more detailed knowledge of the grid turbulence with increasing number of cylinder rows, can be improved similar to the application of staggered tubes in bundles at very low Reynolds numbers [4]. The necessary roughness elements including height, diameter and pitch can be optimized for final construction of the selected rough plates for low or high temperature heat exchangers, but also electrochemical, naval or space applications.

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Keywords: Rough Flat Plates, Full Turbulent Flow, Vertical Cylindrical Roughness Elements, Viscous Reynolds Numbers, Near Wall Nusselt Numbers, Heat Exchangers.

Energy Pathways in Venturi-based Swirling-Flow Hydrodynamic Cavitation Devices: Correlating Shockwaves and Radical Formation with Cloud Collapse

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Hydrodynamic cavitation (HC) refers to the formation, growth, and violent collapse of vapor bubbles in a flowing liquid when local pressure drops below vapor pressure. Upon collapse, cavitation bubbles create extreme localized conditions (high temperature and pressure) that produce intense shear forces and chemically reactive species like hydroxyl radicals (·OH) (Nöpel and Ayela [1]). However, currently, there are no established correlations between operating conditions, HC device design, and performance parameters that are essential for engineering and operating technical systems (Šarc et al. [2]). This work explores 3D-printed HC devices shown in Fig. 1, featuring internal flow-guiding structures that induce controlled swirling flows. As discussed by Simpson and Ranade [3], these flows stabilize cavitation cloud formation and collapse, which leads to enhanced radical formation rates while reducing energy losses and material wear.

The device performance is evaluated by correlating mechanical energy release (quantified via propagating pressure shockwaves from cavitation cloud collapses) as proven by Gawandalkar and Poelma [4] and chemical energy generation (monitored through salicylic acid dosimetry as done by Arrojo et al. [5]). Integrated pressure transducers record collapse-induced pressure waves, while ·OH radicals oxidize salicylic acid into 2,5-dihydroxybenzoic acid, which is measurable via HPLC, providing radical formation data. The combination of pressure and dosimetry data enables the first direct correlation between mechanical and chemical cavitation effects in complex swirling reactor geometries. Additionally, the first results from tomographic high-speed imaging will be presented showing transient vapor cloud structures and dynamics.

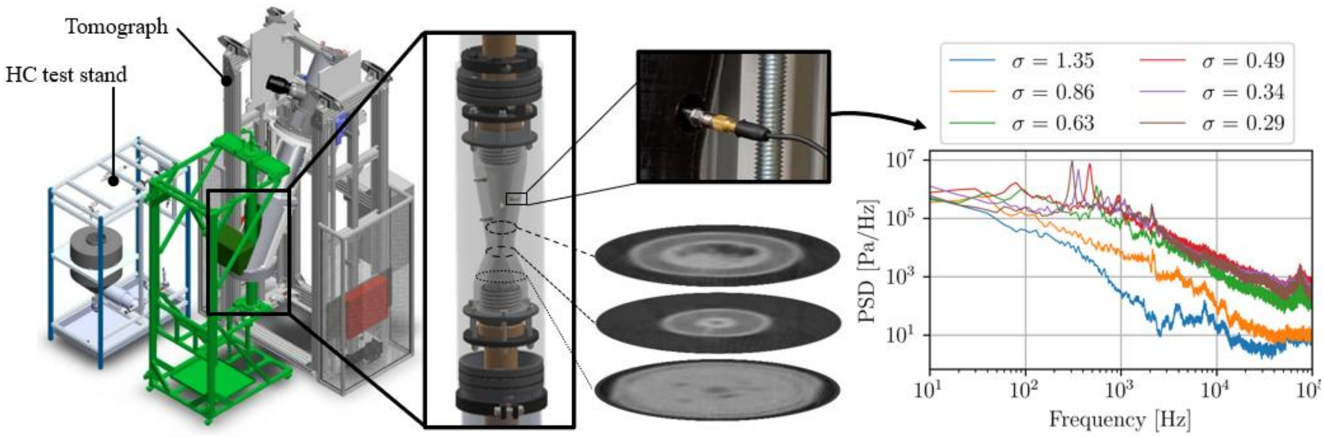

Figure 1. Fast X-ray tomography scanner with integrated HC test-rig and installed Venturi with integrated swirling element. Tomography images cavitation clouds, while the dynamic pressure sensors detect shockwaves resulting from cloud collapses.

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Keywords: Hydrodynamic cavitation, swirling flow, radical formation, pressure shockwaves, high-speed tomography.

Experimental study of parameters influencing spray cooling processes

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Abstract

Minimum quantity lubrication (MQL) is a machining technique characterized by the application of liquid sprays at very low flow rates. The primary purpose of the spray is to provide localized cooling and lubrication at the cutting zone, which contributes to extending tool life and improving the surface quality of the machined workpiece while significantly reducing liquid consumption compared to conventional flood cooling. As a result, MQL has gained increasing attention as a more sustainable and environmentally friendly machining approach. The performance of an MQL spray is governed by a variety of parameters. These include the thermophysical properties of the cooling lubricant as well as operational parameters like liquid flow rate, air pressure, and the resulting droplet size and velocity distributions. The complex interaction between these factors determines the ability of the spray to penetrate the cutting zone and efficiently remove heat from the tool-workpiece interface. In this study, three different liquids are analyzed experimentally: water, a water-based emulsion (Samnos Standard), and a pure oil (Econi FAE 49). The latter two fluids are commercially available and specifically formulated for MQL applications. The sprays are generated using a Leo spray nozzle manufactured by HPM Technologie GmbH. This nozzle features a coaxial design with two concentric orifices, where pressurized air is supplied through the inner orifice, inducing a pressure drop that draws the liquid through the outer orifice according to the Venturi principle. The influence of varying liquid flow rates and air pressures on the cooling performance of the spray is systematically investigated. To quantitatively assess the cooling capacity of each spray configuration, an inverse heat transfer problem (IHTP) is solved. This approach allows the transient heat flux at the cooled surface to be determined from experimental temperature measurements, providing a robust means of comparing the thermal performance of the different fluids and operating conditions [1]. An Inconel 718 plate with a diameter of 140 mm and a thickness of 5 mm was heated using an induction heater to temperatures above 500 °C. The plate was then allowed to cool naturally while the spray nozzle was positioned using a traverse system. When the plate temperature reached approximately 450 °C, the spray was initiated. All temperatures were measured on the rear surface of the plate (opposite to the cooled surface) using a PI640i infrared camera manufactured by Optris GmbH. Transient temperature measurements from 100 locations were used as input to solve the inverse heat transfer problem (IHTP). The results indicate that, for certain configurations, the cooling performance is comparable to that obtained using compressed air alone, suggesting that the liquid provides a negligible contribution to heat removal. This behavior is attributed to the inability of the liquid droplets to overcome the Leidenfrost effect, which limits effective liquid-surface contact at high surface temperatures. Furthermore, the specific cooling performance is evaluated using the ratio of the maximum heat flux to the liquid flow rate, offering a quantitative measure of the cooling efficiency of each configuration.

Acknowledgement

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Keywords: Spray cooling, minimum quantity lubrication (MQL), cooling efficiency, experimental study.

Experimentelle Parametrierung des Wandkollisionsverhaltens von Holzspänen für CFD-DEM-Simulationen

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Die Spanerfassung durch leistungsfähige Absaugvorrichtungen ist wesentlich für den Arbeits- und Brandschutz bei der spanenden Holzbearbeitung, ist aber auch Voraussetzung für eine hohe Oberflächengüte der gefertigten Werkstücke. Für die Entwicklung energieeffizienter und gleichzeitig leistungsfähiger Absaugungen in der Industrie werden Simulationswerkzeuge, wie z.B. die Software Simcenter STAR-CCM+, zunehmend interessant. Der Weg der Späne nach ihrer Freisetzung an der Werkzeugschneide wird entscheidend durch Kollisionen mit dem Werkzeugkörper und den Wänden der umgebenden Absaughaube bestimmt. Um das Kollisionsverhalten von Holzspänen in einer CFD-DEM-Simulation realistisch abbilden zu können, müssen geeignete Parameter für die Kollisionsmodellierung gefunden werden. Die bei der spanenden Holzbearbeitung entstehenden Späne besitzen einen breites Größen- und Formspektrum [1], was eine besondere Herausforderung für die Parametrierung darstellt.
In Simcenter STAR-CCM+ kann das Hertz-Mindlin-Modell zur Abbildung des Kollisionsverhaltens verwendet werden. Dieses enthält drei Parameter: den statischen Reibungskoeffizient sowie den normalen und tangentialen Restitutionskoeffizient. Die Restitutionskoeffizienten quantifizieren den Impulsverlust während der Kollision aufgrund teilelastischen Materialverhaltens. Sie beeinflussen die Dämpfungskraft im Kollisionsmodell. Der tangentiale Impulsverlust bei schrägen Wandkollisionen wird bei flacheren Auftreffwinkeln wesentlich stärker vom statischen Reibungskoeffizient als vom tangentialen Restitutionskoeffizient beeinflusst, das Rutschen des Partikels entlang der Wand dominiert das Verhalten („gross-slip“). Der tangentiale Impulsverlust steigt mit steilerem Auftreffwinkel an, da sich das Rutschen verringert und ein wachsender Anteil der translatorischen kinetischen Energie in Rotationsenergie umgewandelt wird [2].
Zur Bestimmung der Kollisionsparameter wurden Prallversuche mit realen Spänen, welche durch Zerspanung von Spanplatten gewonnen wurden, durchgeführt. Das Größenspektrum der Späne wurde auf die Siebklasse 500 µm – 630 µm reduziert. Die massereichen Späne dieser Fraktion sind für die Spanerfassung von Spanplattenspänen besonders relevant. Für die Versuche wird mittels einer Schwingrinne ein annähernd konstanter Massestrom an Spänen erzeugt, anschließend werden diese durch einen Ejektor beschleunigt. Eine Spaltblende reduziert die Höhe des Partikelstrahls und schirmt die dahinter liegende Prallplatte weitgehend von der Strömung ab. Ihr Anstellwinkel gegenüber dem Partikelstrahl kann in einer Ebene beliebig verändert werden. Die Kollisionen der Späne mit der Prallplatte werden mit einer Hochgeschwindigkeitskamera gefilmt.
Mithilfe eines Particle-Tracking-Verfahrens werden die Spantrajektorien aus den Hochgeschwindigkeitsaufnahmen ermittelt. Aus den Geschwindigkeiten vor und nach der Kollision wird der effektive Restitutionskoeffizient normal und tangential zur Wand ermittelt. Der Restitutionskoeffizient beschreibt das Verhältnis der Werte der jeweiligen Geschwindigkeitskomponente nach der Kollision im Vergleich zur Geschwindigkeit vor der Kollision. Die ermittelten Werte weisen eine erhebliche Streuung auf, die aus der Formvielfalt der Späne resultiert. Im statistischen Mittel zeigt der wandnormale Restitutionskoeffizient nur eine sehr geringe Abhängigkeit vom Auftreffwinkel, während der tangentiale Restitutionskoeffizient im Wesentlichen dem oben beschriebenen Zusammenhang für vollständiges Rutschen folgt. Aus den Daten der effektiven Restitutionskoeffizienten werden Modellwerte für den normalen Restitutionskoeffizienten und den statischen Reibungskoeffizienten abgeleitet. Eine zusätzliche tangentiale Dämpfung ist von untergeordneter Bedeutung.
Zur Überprüfung der Modellparameter wurde ein CFD-DEM-Modell des Versuchsstands in Simcenter STAR-CCM+ erstellt. Es wurden Simulationen mit den ermittelten Kollisionsparametern bei verschiedenen Anstellwinkeln der Prallplatte zunächst für eine glatte metallische Prallfläche durchgeführt und mit den experimentellen Daten verglichen.
Analoge Versuche wurden mit anderen Materialien der Prallfläche, die sich durch eine erhöhte Oberflächenrauheit oder Elastizität auszeichnen, durchgeführt.

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Keywords: Parametrierung, Kollisionsmodellierung, Prallversuch, Holzspäne

Striation-Based Mixing Time in Two-Dimensional Power-Law Non-Newtonian Vortices

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In vortex-dominated flows, mixing is often characterized by progressive striations produced by the shearing action between rotating layers. Fundamental questions pertinent to vortex structures as mixing mechanisms include how effective the mixing is and how long it takes to achieve it. This study investigates the striation thickness and associated mixing time in two-dimensional, non-Newtonian, power-law vortices with a focus on deviations from Newtonian Lamb–Oseen vortices. Striation thickness, as a kinematic mixing metric defined by the tracking of the temporal evolution of striation thickness along material trajectories, is used to define a mixing time associated with advective stretching. Molecular diffusion is excluded in order to isolate the intrinsic mixing potential of the vortex that arises from advective stretching alone. Mixing times are computed for a range of power-law indices and viscosity coefficients, and compared systematically with their Newtonian counterparts. The results demonstrate how non-Newtonian rheology modifies the temporal decay of angular velocity and stretching rates. This leads to significant changes in striation thickness evolution and mixing time. Shear-thinning behavior, in particular, alters the rate at which striation evolves relative to the Newtonian case. This results in mixing times that cannot be inferred from effective viscosity alone. Though limited to two-dimensional kinematics and single-vortex dynamics, this study offers essential insights into the influence of power-law rheology on mixing performance in vortex-dominated flows. This has direct relevance to engineering applications, such as activated sludge basins in wastewater treatment facilities, where coherent vortical structures play a dominant role.

Keywords: Mixing time, Striation thickness, Power law non-Newtonian fluid, Two-dimensional vortex, Similarity solution, Lamb–Oseen vortex

Enabling Control of Dynamic Aeration via Neural MPC

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Dynamic aeration applies pulsed oscillations to the gas flow, thereby controlling both the frequency and the amplitude of the gas flow rate. This method shows promising potential for increasing oxygen mass transfer and increasing the energy efficiency with special focus on the biological wastewater treatment process. Industrial adoption, however, encounters barriers such as the lack of a validated causal (first-principles) model of the process, which is necessary when deploying traditional Model Predictive Controllers (MPC). On the other hand, model-free approaches, e.g. PID or Advanced Regulatory Control (ARC), do not handle strong nonlinearities well and are not a good solution for using two or more manipulated variables (MV) to control one common controlled variable (CV).

Therefore, we propose a Neural Model Predictive Controller that relies on a data-driven approach. We first designed and deployed an empirical digital twin of the aeration process; to include the effects of the pulsation frequency on the volumetric mass transfer coefficient (K_{La}), an empirical term was proposed and fit to CFD data from [1] using a least squares method. For model identification, we ran 16 experiments with differing excitation signals on the air flow rate. These signals were designed to excite the system over the full actuation space for Pulse Width Modulation (PWM) frequency and gas flow amplitude, including boundary cases (frequency = 0, Amplitude = 0) and the full range of measurable values. The resulting datasets were used to train, validate, and test a Long Short-Term Memory (LSTM) Recurrent Neural Network (RNN), which serves as the internal model for the Neural MPC.

This framework allows the controller to coordinate multiple MVs to control a unique CV using only standard plant signals, namelys dissolved oxygen (DO) and gas flow rate. We discuss practical requirements and report design-phase results, outlining limitations and next steps toward pilot testing. To assess the capacity of the controller in handling both MVs to optimally regulate the DO setpoint, we ran closed loop simulations in the digital twin environment. The results show that the dynamic aeration control strategy improves oxygen transfer efficiency; this is achieved by the controller finding a solution that allows lower ga flow rates and reduced energy consumption, while keeping the same DO reference compared to standard operation.

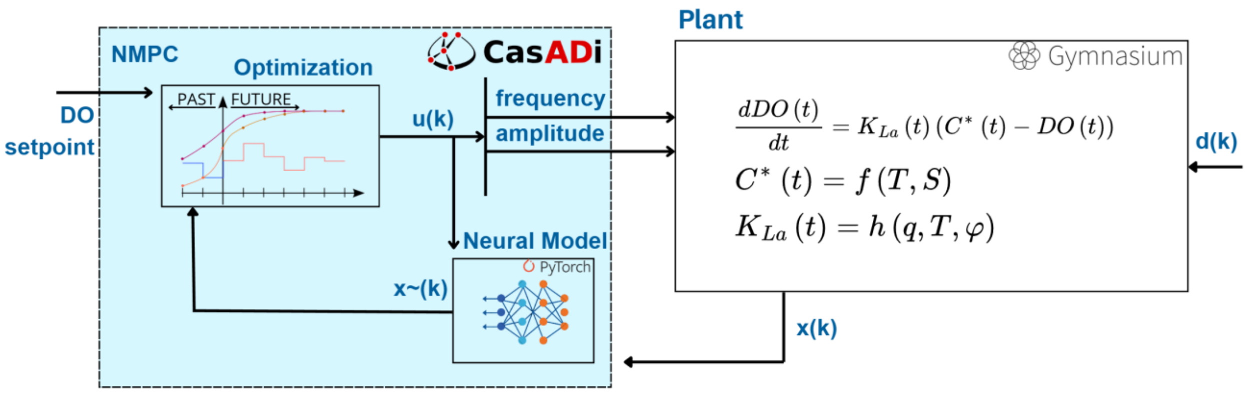

Figure 1- Neural MPC Controller Design Structure

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Keywords: Neural Model Predictive Controllers (NMPC), Recursive Neural Networks (RNN), Data-driven modeling.

Investigation of an Aerated Stirred Tank Reactor with Lagrangian Sensor Particles

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The investigation of the spatio-temporal flow inside industrial-sized vessels, e.g., biogas fermenters or wastewater treatment plants, is inherently difficult with commercially available sensor systems. Therefore, so-called Lagrangian Sensor Particles (LSPs) are developed at HZDR [1]. LSPs are autonomous data loggers deployed inside the vessel where they follow the flow while collecting motion (acceleration, angular velocity, pressure) and process data (temperature). The measured pressure is converted into the axial position of the LSP by applying Pascal's law, and the axial velocity is given by the time derivative of the axial position.

LSPs have already been used to characterize a single-phase stirred tank [2]; however, many processes consist of at least two phases. The 3 LSPs were deployed for 1 h in an aerated CSTR with a working volume of 1400 l, equipped with a 3-bladed pitched blade turbine and 2 disc diffusers. The results for down-pumping, aeration and the combination of both are shown in Fig. 1. From the probability of presence, it is concluded that better mixing is reached by combining the opposing stirring and aeration. Especially in the vicinity of the surface and bottom of the reactor. The downwards velocity is slowed down by the upwards-directed aeration, indicating the buildup of compartments in the vessel.

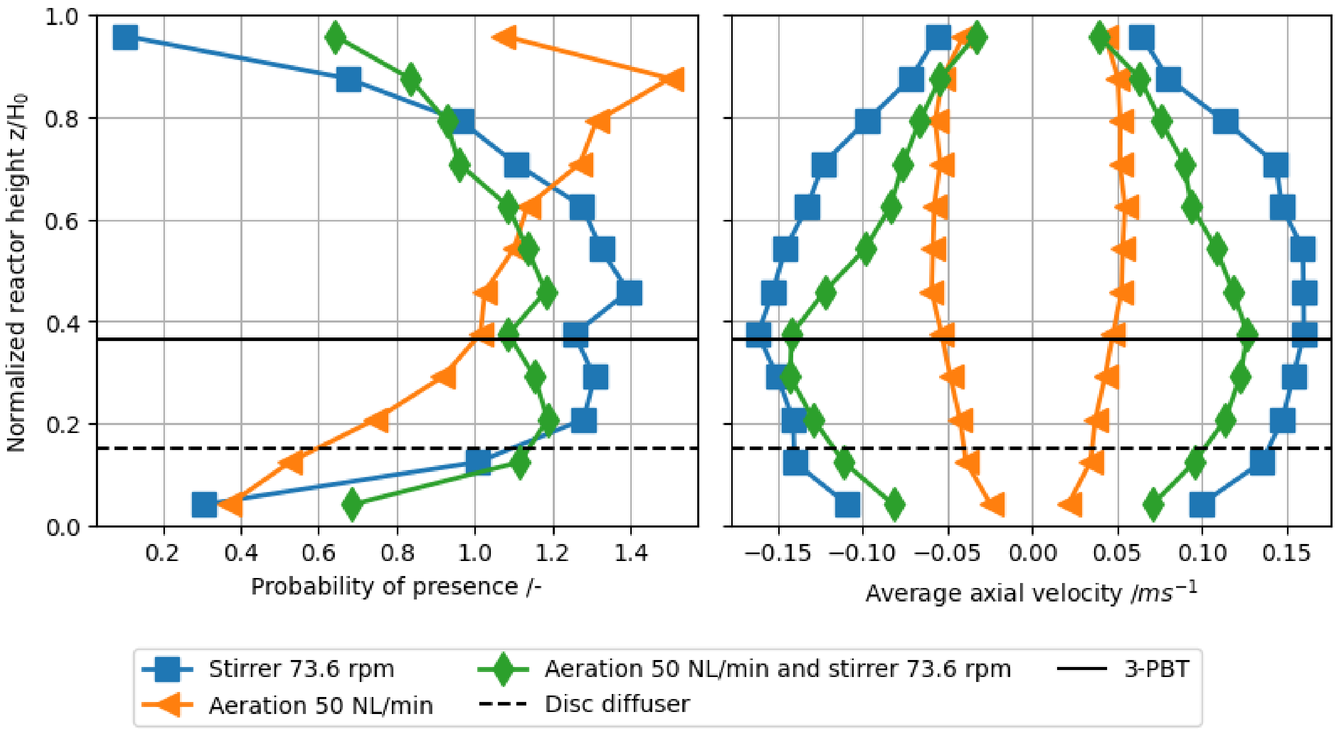

Figure 1: Axial probability of presence (left) and axial velocity (right) for different flow regimes. The height has a resolution of 6.3 cm.

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Keywords: Lagrangian Sensor Particles, Flow Followers, Aerated Stirred Tank Reactor

Direct numerical simulations of bubbles growing on electrodes

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The growth of gas bubbles nucleated at solid surfaces plays a crucial role in various processes. Particularly in water electrolysis, bubbles adhering at the electrodes reduce the reaction area and impede mass transfer, thereby causing additional energy losses. We perform direct numerical simulations to investigate the behavior of surface bubbles in electrochemical environments by using a geometric volume-of-fluid (VOF) method implemented in Basilisk [1] combined with a two-field phase change model of Gennari et al. [2]. We first studied diffusion-driven growth of gas bubbles at micro-cavities in uniformly supersaturated solutions. We focus in detail on how surface wettability influences the early stages of the bubble evolution, thereby comparing with results from optical measurements and theoretical analyses. Hydrophobicity is found to support faster growth [3,4]. In the next step, we simulated bubbles growing on micrometre-sized electrodes (resembling catalytic islands) in differently saturated electrolytes, where dissolved gas is continuously produced at the wetted part of the electrode. Our results show that bubbles may approach dynamic equilibrium states at which they neither grow nor shrink, as shown in Fig. 1. The equilibrium arises from the balance of local influx near the bubble foot and global outflux, and may occur during both, pinning and expanding wetting regimes of the bubbles. To identify the parameter regions of bubble growth, equilibrium and dissolution, our simulation results are found to agree with an analytical solution extending the work of Zhang & Lohse [5] by considering the modified gas fluxes along the bubble interface. As bubble dynamics and electric field mutually influence each other, we discuss the influence of the electrode size and surface structuring and draw conclusions on how to possibly enhance the efficiency of electrolysis [6].

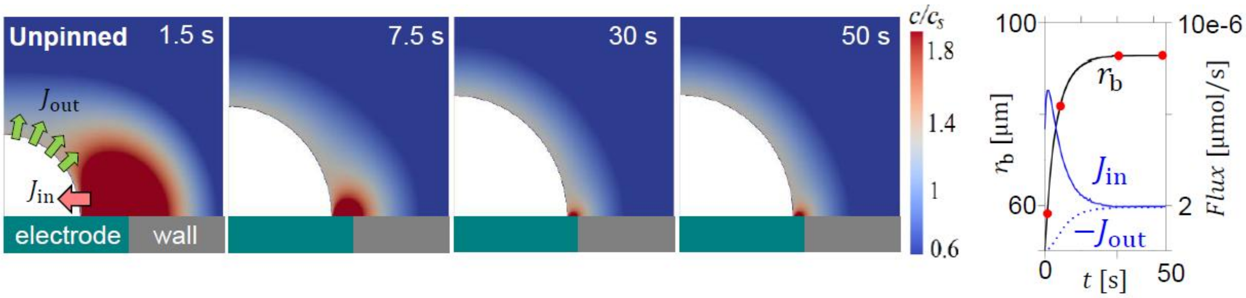

Fig. 1. Growth and equilibrium of an unpinned hydrogen bubble on a micro-electrode.

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Keywords: bubble dynamics, electrolysis, wetting, structured surface, volume-of-fluid

Fachgruppe Agglomerations- und Schüttguttechnik:

Vorträge und Poster

Development of recycling strategies by agglomeration for shifting residue streams connected to the green transformation in steel industry

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The European steel industry is focusing increasingly on climate-friendly production routes. Consequently, on one hand, the number of blast furnaces (BF) in operation is expected to decline in the upcoming decades, while the importance of direct reduction (DR) processes is set to increase. On the other hand, electric arc furnaces (EAFs) and smelters will become more prevalent, while the number of converters (BOFs) will decline. All metallurgical process routes produce residues in the form of dust, sludge or slag. [1, 2] But the transformation in steel industry will alter the proportions and composition of these specific residues. Existing internal processing equipment, such as sintering plants, will be phased out. This will create new challenges for residue processing and recycling strategies, most of which will require agglomeration.

This contribution focuses specifically on dust generated by the BOF and EAF processes. New EAFs will be operated using directly reduced iron (DRI) instead of steel scrap, which has been the state of the art until now. Since scrap contains zinc, the zinc content of the resulting EAF dust in integrated steelworks will be reduced, while the total amount of EAF dust increases. The currently dominant zinc recovery processes, will then no longer be economical. At the same time, the mass flows of BOF dust will decrease. The processing of mixtures with shifting compositions of BOF and EAF dust will be of great importance in the coming years due to transformation in steel production. The favorable recycling process itself depends on the specific grain size of the dust fraction, the chemical composition, the share of the dust fraction and the recycling purpose.

The contribution gives different possible options for the internal and external recycling of EAF and BOF dusts supported by test results for the granulation and briquetting of these materials at different thermal conditions. For example, EAF dust and BOF fine dust can be agglomerated well in a granulation drum. The resulting agglomerates can be used, e.g, in the cement industry or, depending on the zinc content, for zinc recovery. Mixtures of EAF dust and BOF coarse and fine dust were briquetted which allows for an internally recycling to BOF.

Acknowledgements

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Keywords: iron and steel production, BOF, EAF, residues, dust, agglomeration

Recycling künstlicher Mineralien (EnAM) mittels FluidFM®-Technologie und selektiver Umbenetzungsagglomeration – Der steinige Weg von Modell-Schlacke zur Real-Schlacke

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Das von der Deutschen Forschungsgemeinschaft (DFG) geförderte Schwerpunktprogramm SPP2315 mit dem Titel „Engineered Artificial Minerals (EnAM)“ befasst sich mit der Schlackephase pyrometallurgischer Prozesse. Nach dem Abkühlen liegt die Schlacke entweder als homogene amorphe Struktur vor oder bildet Kristalle, deren Entstehung thermodynamisch determiniert ist. Diese Kristalle, die als „Engineered Artificial Minerals (EnAM)“ bezeichnet werden, fungieren als Speichermedium, in dem sonst stark verdünnte Elemente (Wertstoffe wie Lithium (Li)) angereichert werden können [1]. Die Freisetzung der EnAMs erfolgt mittels eines speziell angepassten Zerkleinerungsverfahrens. Im Rahmen der Schlackenaufbereitung ist es essenziell, die freigesetzten wertstoffhaltigen EnAMs von den übrigen Bestandteilen der Schlackephase (Gangart) zu separieren. In der Praxis hat sich im Rahmen der Kohle- und Erzaufbereitung die selektive Umbenetzungsagglomeration als eine gängige Methode zur Abtrennung wertvoller Mineralien erwiesen, welche auf einem Dreiphasensystem beruht [2]. Das untersuchte System setzt sich aus zwei flüssigen Phasen und einer heterogenen festen Phase zusammen, welche typischerweise in einem Rührbehälter in Wasser suspendiert ist. Die zweite flüssige Phase, die auch als Bindemittel bezeichnet wird, wird entweder in die kontinuierliche Phase dispergiert oder als Emulsion zugegeben. Die hydrophoben Tröpfchen des Bindemittels (meist auf Ölbasis) haften bevorzugt an Partikeln mit besseren Benetzungseigenschaften, was zur Bildung von Agglomeraten führt [3]. Die Separation dieser Agglomerate kann durch Fest-Flüssig-Trennung vom Rest der Suspension erfolgen.
Bei der selektiven Umbenetzungsagglomeration ist die Verwendung von hydrophoben Bindemitteln üblich. Um die Agglomeration der EnAMs zu ermöglichen, ist eine selektive Hydrophobierung dieser erforderlich. Kontaktwinkelmessungen stellen eine etablierte Methode zur Analyse der Benetzungseigenschaften und der gezielten Hydrophobierung von Partikeln dar. Bei zerkleinerten Schlackepartikeln, die aus verschiedenen Mineralphasen und auch aus Mehrphasenpartikeln bestehen, erweist sich diese Technik als unzulänglich. Zur Analyse der Benetzung einzelner Mineralphasen durch geeignete Bindemittel, wurde eine Methode unter Verwendung der Fluid-Rasterkraftmikroskopie (FluidFM®) entwickelt [4]. Mittels dieser Technik ist es möglich, Kontaktkräfte zwischen Mikro-Bindemitteltropfen und einzelnen Partikeln beziehungsweise Mineralphasen zu quantifizieren (vgl. Abbildung 1). Im Rahmen dessen werden grobe Schlackepartikel eingebettet und poliert, um die EnAMs und Gangartphasen freizulegen. Diese werden anschließend mittels BSE/EDX-Bildgebung untersucht und lokalisiert, um die gezielte Kontaktkraftmessung am FluidFM® zu ermöglichen. Diese Ergebnisse tragen zur Verfeinerung (Optimierung) der Hydrophobierung der verschiedenen Mineralphasen bei, sodass eine Trennung mithilfe selektiver Umbenetzungsagglomeration möglich ist. Das FluidFM®-System gestattet zudem Experimente in einem Suspensionsmedium, sodass die Zugabe von oberflächenaktiven Substanzen und/oder die Modifikation des pH-Werts realisiert werden können, um den Einfluss dieser Faktoren auf die Hydrophobie und damit auf die Kontaktkräfte zu bestimmen.

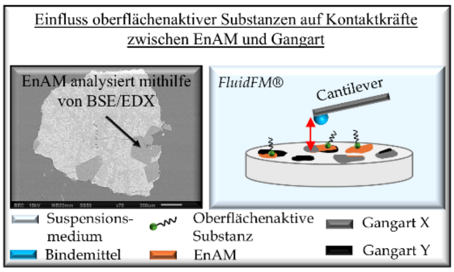

Abbildung 1: Schematische Darstellung der FluidFM®-Messungen.

Ziel der vorliegenden Studie ist es, die Veränderung der Kontaktkräfte zwischen den Mineralphasen und dem Bindemittel durch den Einsatz oberflächenaktiver Substanzen (Tenside und/oder Depressoren) zu demonstrieren. Die Ergebnisse der FluidFM®-Messungen sollen hinsichtlich der Ausbeute der EnAMs mit Agglomerationsversuchen unter Nutzung derselben oberflächenaktiven Substanzen korreliert werden. Der Fokus der Untersuchung liegt dabei auf der Übertragung der Versuche von einem Modell-Schlackesystem auf die Real-Schlacke und die damit verbundenen Herausforderungen durch das Vorhandensein eines komplexen Mehrphasensystems.

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Keywords: Selektive Umbenetzungsagglomeration, Benetzung, EnAM, Schlacke, Fluid-Rasterkraftmikroskopie

Continuous spray fluidized bed agglomeration: Influence of process conditions on growth behavior and internal structure

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Spray fluidized bed agglomeration (SFBA) is an important particle enlargement technique widely applied in the pharmaceutical, food, detergent and chemical industries to improve the flowability, dispersibility and handling properties of fine powders. In this process, a binder solution is sprayed onto fluidized particles, generating liquid bridges that promote coalescence and subsequent agglomerate growth as the binder dries. Although SFBA has been extensively studied, most investigations focus on batch configurations or overall process stability, leaving limited insight into how specific operating parameters influence agglomeration behavior and internal agglomerate structure in continuous systems. A clearer understanding of the relationship between process conditions and agglomerate morphology is still needed.

To contribute to this understanding, this study examines the effects of gas inlet temperature and binder concentration on agglomerate growth behavior and structural development in a continuous SFBA process [1]. Experiments were performed using porous glass beads and hydroxypropyl methylcellulose as a binder. The two operating parameters were systematically varied, and the resulting agglomerates were analyzed using X-ray micro-computed tomography to characterize their internal morphology.

The results demonstrated that gas inlet temperature and binder concentration strongly influenced agglomerate size, growth rate, and structural characteristics. Higher gas inlet temperatures promoted rapid drying and reduced liquid-bridge formation, resulting in smaller and less cohesive agglomerates, whereas increasing binder concentration enhanced liquid cohesion and produced larger, denser agglomerates with greater internal connectivity. These findings clarify the structure–process relationships governing continuous SFBA and provide valuable insight for optimizing product properties and improving predictive modelling of agglomeration processes.

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Keywords: spray fluidized bed agglomeration, particle enlargement, binder content, morphology, process stability

Evaluation of the high-shear wet granulation process using dry water

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The homogeneous distribution of the binder liquid is a particularly critical parameter in wet granulation, as it influences the quality of both the resulting granules and the tablets produced from them in the further downstream process. In conventional mixer granulation, the binder liquid is dripped or sprayed onto the powder surface. This forms wet granule nuclei, which in part must be broken up again by intensive mixing and brought into contact with the remaining primary powder. Uniform liquid distribution is highly dependent on the type of liquid addition, the selected process parameters and the powder formulation [1,2]. Inhomogeneous liquid distribution can lead to the formation of oversized granules or to insufficient wetting for agglomeration of primary particles, resulting in a lower yield in the required granule size range. This often also arises in innovative continuous wet granulation processes due to strongly limited mixing time [3-5].
An innovative approach to potentially improve the liquid distribution is the use of dry water in the wet granulation process (route "A" in Fig. 1). Dry water consists of micrometer-sized water droplets surrounded by a network of hydrophobic fumed silica particles. This structure means that, despite its high mass fraction of water (up to 98%), dry water appears macroscopically as a dry, free-flowing powder. When the powder is subjected to sufficiently high shear stress, the water droplets are broken up again [6]. These properties can be used in wet granulation to distribute the liquid – now in the form of an apparently dry powder – homogeneously by mixing under low stress without moistening the primary material. In the subsequent granulation step, the dry water is broken up and released under intensive shearing to agglomerate the powder. To determine the suitability of dry water for wet granulation of pharmaceutical powders, a blend of microcrystalline cellulose (Vivapur®102) and lactose (Granulac®80) is granulated in a batch high shear granulator (TMG, Glatt GmbH) using dry water (made with Aerosil®R812S) and polyvinylpyrrolidon (Kollidon®90F) as the binder (shown exemplarily in Figure 1). Prior to the granulation process, all components are gently mixed in a cube mixer (KB 20, ERWEKA GmbH) to generate a homogeneous blend. Afterwards, the blend is granulated in the high shear granulator in two phases: At first, a dedicated step to break down the dry water particles and make the liquid available for granulation and secondly, a mixing step to form the final granules. The influence of different formulation parameters, e. g. the water mass fraction in the dry water or the binder content, as well as of varying process parameters, e. g. the impeller speed, is investigated. The distribution of the liquid is determined by adding a colour tracer to the liquid prior to producing the dry water. The tracer can be analysed via UV-vis spectroscopy after extraction from the final granules. The results of the runs using dry water are compared to granules obtained from conventional high shear wet granulation (route "B" in Fig. 1).

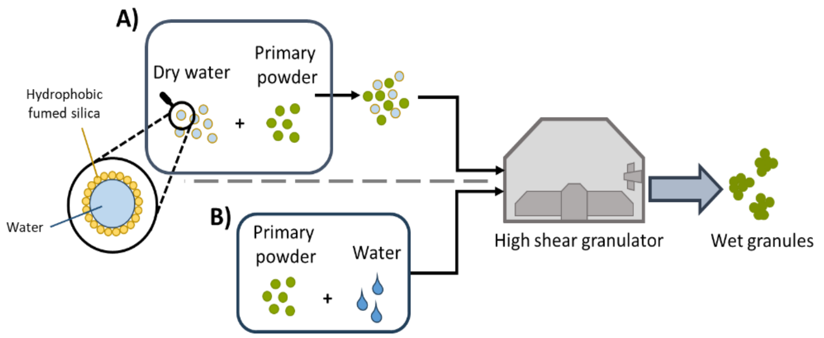

Figure 1: Exemplarily processing route for the wet granulation with dry water (A) and for the conventional reference process (B).

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Keywords: Wet Agglomeration, High Shear Granulation, Dry Water

Prozess- und Granulierleistung in der zweistufigen Planetwalzengranulation

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Einleitung

Für die kontinuierliche Schmelzgranulation stellt die Planetwalzengranulation eine vielversprechende Technologie dar. Beim herkömmlichen einstufigen Prozessaufbau finden das Schmelzen des Binders und die Granulatbildung jedoch gleichzeitig in derselben Prozesszone statt. Dadurch lassen sich Prozess- und Granulationsleistung zwar jeweils unabhängig kontrollieren, jedoch nicht miteinander verknüpfen [1]. Ziel der vorliegenden Studie ist daher die Evaluierung eines zweistufigen Prozesses, wodurch beide Schritte zeitlich und räumlich innerhalb einer Prozesseinheit voneinander getrennt ablaufen. Erste Untersuchungen befassen sich mit der Prozessstabilität hinsichtlich Wiederholbarkeit und Reproduzierbarkeit der Prozess- und Granulationsleistung anhand von Verweilzeit- und Partikelgrößenverteilungen.

Methoden

Die Versuche wurden auf einem zweimoduligem Planetwalzengranulator (PWE 30, ENTEX Rust& Mitschke GmbH, Bochum, DE) durchgeführt. Die beiden Einzelkomponenten der Formulierung Laktose-Monohydrat (90 Gew.% Foremost Farms USA, Baraboo, USA) und Hydroxypropylcellulose (10 Gew.%, Klucel EXF Pharm, Ashland Inc., Covington, USA) wurden jeweils gravimetrisch (DDW-M-DS(R) 28, Brabender GmbH & Co. KG, Duisburg, DE) zudosiert. Die Prozessleistung wurde über die Verweilzeitverteilung (ExtruVis, MeltPrep GmbH, Graz, AT) und die Granulationsleistung wurde über Partikelgrößenverteilung (QICPIC, Sympatec GmbH, Clausthal-Zellerfeld, DE) bestimmt. Der Planetwalzengranulator lief mit einer Drehzahl von 80 min^{-1} und einem Gesamtmassenstrom von 1,0 kg h^{-1}. Das Schmelzmodul war auf 110 °C temperiert und mit fünf Standardspindeln bestückt, das Granulationsmodul mit vier. Dessen Temperatur sowie die der zentralen Spindel waren auf 150 °C eingestellt.

Ergebnisse und Diskussion

In ersten Untersuchungen des zweistufigen Aufbaus wurde die Wiederholbarkeit und Reproduzierbarkeit hinsichtlich der Prozess- und Granulationsleistung erfolgreich nachgewiesen (Abb.1). Die gemessenen Verweilzeitverteilungen stimmen weitgehend überein mit einem Median der Verweilzeit von etwa 90 s bei einer Standardabweichung von 1,6 %. Auch die gemessenen kumulativen Partikelgrößenverteilungen weisen untereinander eine hohe Übereinstimmung auf. Der durchschnittliche Median liegt bei 1,5 mm, die relative Standardabweichung bei 1,3 %. Weitere Studien befassen sich mit der Langzeit-Prozessstabilität, sowie dem Vergleich zwischen dem einstufigen und dem zweistufigen Aufbau. Zudem wurde der Einfluss verschiedener Prozessparameter auf die Prozess- und Granulationsleistung untersucht.

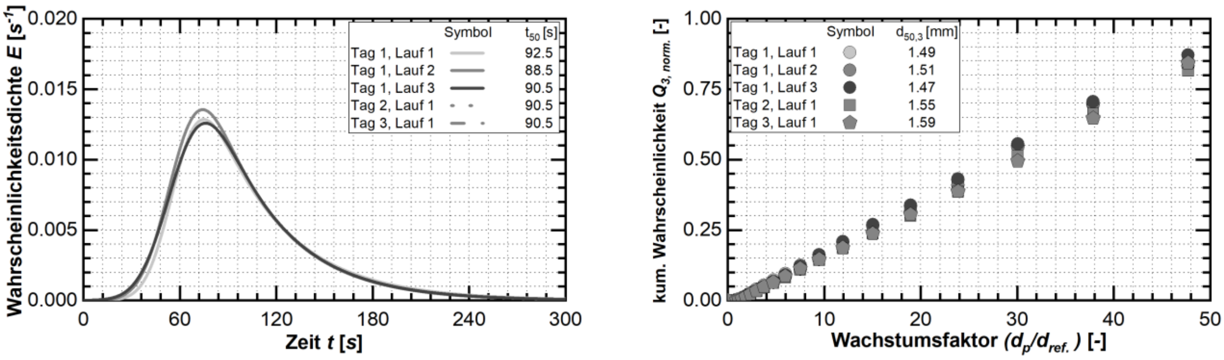

Abbildung 1. Verweilzeitverteilung (links) und kumulative Partikelgrößenverteilung in Abhängigkeit vom Wachstumsfaktor (rechts).

Danksagung

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Schlüsselwörter: Kontinuierliche Fertigung, Schmelzgranulation, Planetwalzengranulation

Detection and Machine Learning Modelling of Spray Nozzle Blockage Anomalies in Fluidized Bed Spray Granulation

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Fluidized bed spray granulation is a cornerstone technology in the pharmaceutical, food, and chemical industries [1]. However, the process is susceptible to operational disruptions, with spray nozzle blockage being a frequent and critical anomaly. This issue disrupts the homogeneous liquid distribution, leading to non-uniform product quality, process instability, component defects, and costly production downtimes. Addressing this challenge requires robust, real-time detection methods to ensure process reliability and efficiency [2, 3].

This project introduces a systematic, data-driven framework for the early detection of nozzle blockage anomalies during granulation. To monitor the process, a multi-sensor array was implemented, featuring standard process sensors monitoring temperature, superficial gas velocity, and spray pressure, complemented by pressure sensors for both the atomizing air and the spray liquid, alongside a liquid flow rate sensor. A custom-designed optical light sensor, intended to provide further insights by analysing spray patterns, is currently under development. This novel sensor utilizes an infrared (IR) light emitter and detector to analyse the spray pattern and detect particle build up by measuring changes in light intensity.

The core of the detection system is an advanced knowledge module that leverages unsupervised machine learning to identify anomalies from the collected sensor data. Following comprehensive data pre-processing, including feature engineering and Principal Component Analysis (PCA), a first comparative analysis of two distinct modelling techniques was performed. An Isolation Forest was employed to detect statistical outliers in the data, while a recurrent neural network, specifically an LSTM-Autoencoder, was used to identify temporal pattern anomalies.

Preliminary results demonstrate the efficacy of the sensor system. A significant increase in spray pressure proved to be a reliable, direct indicator of nozzle clogging. First comparative modelling studies concluded that a hybrid approach combining the Isolation Forest and the LSTM-Autoencoder provides a more robust and comprehensive detection of anomalies than either model can achieve alone. Furthermore, spray pattern analysis revealed that the nature of the blockage influences droplet characteristics: partial clogging leads to the formation of larger droplets, whereas strong clogging results in smaller droplets due to the restricted nozzle opening. This finding underscores the complexity of the failure mode and the value of multi-faceted anomaly detection.

Building on these findings, future work will expand the scope of algorithmic evaluation by testing further model architectures, with a particular focus on state-of-the-art approaches. In parallel, the unique signatures of single-model detections will be leveraged to characterize and classify different types of process failures. Ultimately, by advancing from simple detection to predictive characterization, this framework promises to significantly enhance process stability, reduce material waste, and ensure consistent product quality in fluidized bed systems.

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Gravity-driven granular flow characterization and discrete element model calibration using the FlowBoard

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The numerical simulation of granular materials is used in many areas - from food technology and pharmaceuticals to additive component manufacturing. A recurring problem hereby is the calibration of material parameters for a given granular material. The Fraunhofer IWM has developed a novel test rig called FlowBoard that enables the flow behavior of granular materials to be investigated efficiently. The analyzed property is the materials gravity-driven flow through a transparent chamber interspersed with a variable obstacle pattern. An image or video of the flow serves as a fingerprint of the flow behavior. The test rig makes it possible to carry out the measurement required for calibration within a few minutes. The corresponding material parameters are then obtained using a combination of a material database and inverse discrete element simulations of the experiment. Figure 1 compares the flow pattern of sesame seeds in the FlowBoard with the respective simulation results. This comparison confirms that the flow behavior of the granular material observed in the numerical simulation corresponds largely to its behavior in reality. The sensitivity of the observed flow pattern with respect to powder properties and the obstacle setup will be discussed. Furthermore, the FlowBoard will be compared to existing equipment used for discrete element model calibration.

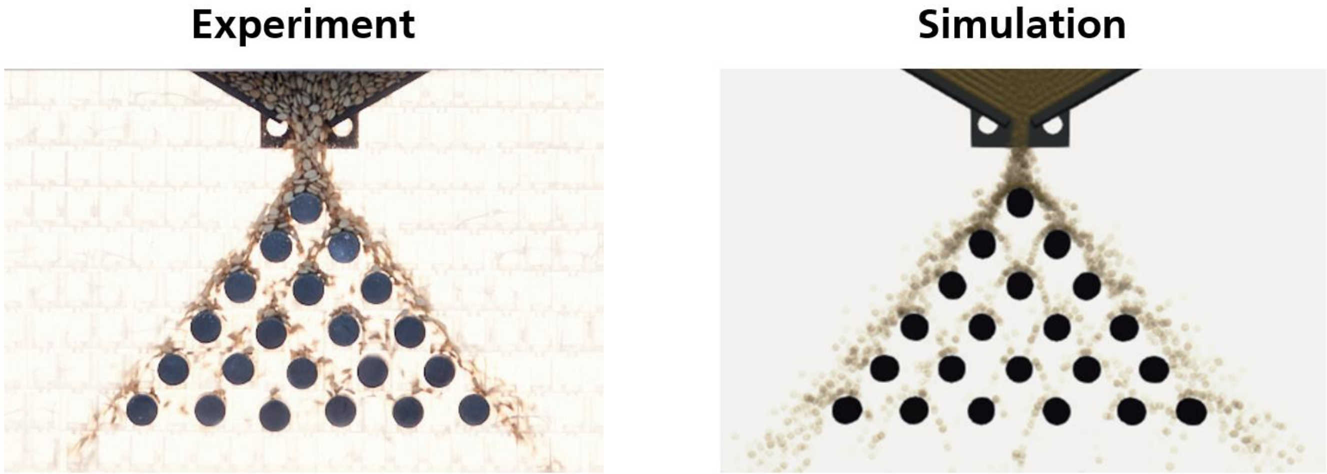

Figure 1: Comparison of the flow pattern of sesame seeds in experiment (left) and simulation (right).

Keywords: Granular flow, test rig, discrete element method, parameter calibration.

Kleiner Maßstab, große Spannungen: Exzentrisches Ausflussverhalten in einem Modellsilo einer Silozentrifuge

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Obwohl die Entwicklung der Silomechanik bereits im 19. Jahrhundert mit den Arbeiten von Janssen begann und im letzten Jahrhundert umfangreiche Forschungsarbeiten durchgeführt wurden, sind viele Fragen zum Fließverhalten in Silos und deren Auswirkung auf die mechanischen Spannungen noch unbeantwortet. Das Verständnis von Totzonen ist dabei einer der Schlüsselfaktoren, um eine Überdimensionierung oder, bei falscher Auslegung, eine Beschädigung des Silos zu vermeiden. Da sich Totzonen aufgrund von Veränderungen des gelagerten Schüttguts oder exzentrischen Entleerungen in einem bestehenden Silo verfahrenstechnisch oft nicht vollständig vermeiden lassen, ist es umso wichtiger, ihre Entstehung, ihre Auswirkungen auf das Schüttgut (z.B. Abweichung von den Anfangsspannungen im Silo) und die daraus resultierenden Lasten auf die Silowand zu verstehen. Neben der zentrischen Ausrichtung der Auslauföffnung können exzentrische Auslauföffnungen nicht immer vermieden werden. Darüber hinaus kann bei einer unzureichenden Auslegung von Austragshilfen ein exzentrischer Ausfluss ungewollt auftreten. Exzentrische Öffnungen führen in der Regel zu Totzonen und asymmetrischen Lasteinwirkungen und erfordern daher besondere Aufmerksamkeit. Im aktuellen Lastansatz für die Bemessung des exzentrischen Austrags (DIN EN 1991-4 [1]) sind mehrere Annahmen notwendig und ein stabiles und nachhaltiges Silodesign kann nicht garantiert werden. Weitergehende Forschung ist essentiell um Auswirkungen des exzentrischen Austrags zu verstehen.

In dieser Studie wird der Einfluss der Auslauföffnung im Hinblick auf das Fließprofil, die Spannungen an der Silowand und die ausgeflossene Masse unter Verwendung einer Silozentrifuge untersucht (siehe Abb. 1). Bei der verwendeten Silozentrifuge handelt es sich um einen Eigenbau der TU Braunschweig und ermöglicht die Simulation von Verdichtungsspannungen im Großmaßstab unter Verwendung eines Silos im Kleinmaßstab und der wirkenden Zentrifugalbeschleunigung a_z. Die Zentrifugalbeschleunigung berechnet sich aus dem Verhältnis der relativen Zentrifugalkraft RCF (engl. relative centrifugal force) und der Erdbeschleunigung g. Die RCF kann in der verwendeten Zentrifuge bis zu dem 115-fachen der Erdbeschleunigung erreichen. Das Silo ist horizontal in die Silozentrifuge eingespannt und durch die verbaute Kraftmessung können die Zeitpunkte und aktuellen Drehzahlen beim Ausfluss von Schüttgut aufgezeichnet werden. Ergänzend werden Spannungsmessungen an ausgewählten Stellen der Silowand durchgeführt, um die Spannungen an der Wand aufzuzeichnen.

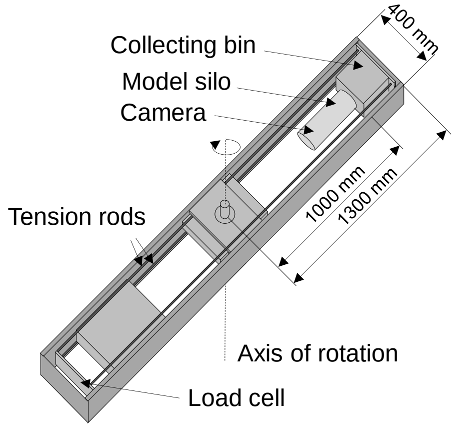

Abb. 1: Aufbau der Silozentrifuge

Im Rahmen der Präsentation werden Ergebnisse zur Anwendung der Braunschweiger Silozentrifuge zur Untersuchung des Fließverhaltens bei Verwendung exzentrischer Auslassöffnungen an einem Flachbodensilo vorgestellt. Bevor das exzentrische Ausflussverhalten in Bezug auf verschiedene Exzentrizitäten und Durchmesser diskutiert wird, wird die Position des Auslasses relativ zur Drehrichtung anhand von Spannungsmessungen betrachtet. Neben der Validierung der Silozentrifuge für die Modellierung exzentrischer Ausflussversuche in einem kleinen Modellsilo werden erste Ergebnisse zum Einfluss der Fließprofilbildung bei unterschiedlichen Exzentrizitäten und Auslassdurchmessern mit der Silozentrifuge vorgestellt. Die paramteterabhängige Ausbildung der toten Zonen kann deutlich abgebildet werden. Insbesondere die Bildung von Totzonen und die daraus resultierende Spannungen an der Silowand liefern wertvolle Erkenntnisse über das exzentrische Entleerungsverhalten in einem Silo unter hohen Belastungen. Diese Ergebnisse bestätigen die Eignung der Silozentrifuge für derartige Untersuchungen und ermöglichen es, den Lastansatz DIN EN 1991-4 [1] durch weitere Untersuchungen an das exzentrische Ausflussverhalten anzupassen, um ein stabiles und nachhaltiges Silodesign ohne Überdimensionierung zu erreichen.

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Keywords: Silozentrifuge, Exzentrische Auslauföffnung, Prozesscharakterisierung

The influence of nanoparticle and liquid surface modification on packing density, powder flow and self-aeration

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In the presented research, the authors investigated and compared the influence of two kinds of surface modification on powder flow and packing density. A nanoparticle flow aid (nanosilica), as well as two liquid organic additives (DEG and TEA), which are commonly used as grinding aids in dry grinding, were used at different concentrations. Using dry mixing, both were applied onto the particle surfaces of a sand/cement mixture, commonly used in particle bed 3D printing by Selective Cement Activation (SCA). The mixtures were first characterised by tap-density measurements, ring shear tests, and dynamic angle of repose. All surface modifications increased the packing density, determined both as bulk and tapped density. An increased bulk density was found to be advantageous for the SCA printing process in a previous work [1]. Nanosilica and TEA both result in the highest achieved packing densities, indicating a similar effectiveness in reducing attractive forces between particles. DEG and TEA slightly increased flowability ffc, albeit at higher bulk densities, while nanosilica leads to a more substantial increase. Similarly, DEG and TEA reduced the angle of repose at 40 1/min by 7 %, compared to a 65 % reduction with nanosilica. Thus, nanosilica has a much higher impact on dynamic flow behaviour than the liquid organic additives, while both nanosilica and TEA improve the packing behaviour in a similar way. Furthermore, it was found, that for all mixtures, the dynamic angle of repose is lower at 40 1/min than 10 1/min. This indicates an aeration of the powder in the experiment, leading to a fluidised behaviour and good apparent flow behaviour as described in [2]. Again, nanosilica had the strongest effect in reducing the dynamic angle of repose at higher rotational speed.

Hence, an increased self-aeration due to nanosilica seemed to be the most plausible reason for the low dynamic angle of repose. To prove it, the apparent volume of the material during the dynamic angle of repose was evaluated and showed the highest increase in volume from 10 1/min to 40 1/min for the mixture with the strongest decrease in dynamic angle of repose. Using a novel characterisation method, we were able to further investigate this phenomenon and thereby correlate the significant reduction in dynamic angle of repose with nanosilica is caused by an increased self-aeration. Accordingly, we accomplished self-aeration by rotating the mixtures in a measurement cylinder and subsequently recorded deaeration with a camera after halting rotation. The results show three main findings: 1. The highest volume directly after rotation and thus, the most incorporated air, was achieved with the nanosilica coated mixture, which also led to the lowest dynamic angle of repose. This further supports a stronger self-aeration as the reason for the lower angle of repose. 2. Higher packing densities were reached with TEA and nanosilica compared to the reference material after deaeration, as also found in bulk and tap density measurements. 3. The nanosilica coated mixture had a significantly higher deaeration half-life compared to the reference and TEA modified mixture. This indicates, that a slower dearation assumingly due to lower permeability is the reason for an increased self-aeration with nanosilica coating. As a result, an increased self-aeration due to lower permeability might be another working principle of nanoparticle flow aids for dynamic flow regimes. The organic liquid additives, which do not show increased self-aeration, are a suitable alternative to nanoparticle flow aids, if only the packing density needs to be increased as in SCA or, an increased self-aeration is unwanted, as e.g. it could promote flooding.

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Keywords: Surface modification, powder flow, self-aeration.

CFD-DEM-Simulationen vibrierter Wirbelschichten und Vergleich mit Echtzeit-MRT-Messungen

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Mechanische Vibrationen können die Qualität der Fluidisierung einer Wirbelschicht verbessern, indem sie die minimale Fluidisierungsgeschwindigkeit (U_{mf}) verringern und Kanalbildung und Partikelagglomeration minimieren [1, 2]. Die Hydrodynamik solcher Systeme ist jedoch noch unzureichend verstanden. Der Hauptgrund dafür ist, dass die räumliche Verteilung der Phasen experimentell schwer zu untersuchen ist, da die Systeme optisch undurchsichtig sind. Konventionelle Messmethoden liefern entweder nur lokale Messwerte aus intrusiven Sonden, die die Strömung beeinflussen, oder untersuchen mit optischen Verfahren pseudo-2D-Systeme, bei denen Wandeffekte eine verstärkte Rolle spielen. Daher gewinnen zur Untersuchung solcher Systeme zunehmend nicht-invasive tomographische Methoden, wie die Magnetresonanztomographie (MRT), an Bedeutung [3]. Ergänzend ermöglichen CFD-DEM-Simulationen detaillierte Einblicke in die Partikel- und Fluiddynamik während der Fluidisierung.

Die Experimente wurden an einem vertikalen 3-Tesla-MRT-System mit einer zylindrischen PMMA-Wirbelschicht (Durchmesser: 10 cm) durchgeführt. Es wurden MRT-detektierbare Geldart-B- und D-Partikel bei Leerrohrgasgeschwindigkeiten zwischen U_{mf} und $4\,U_{mf}$ unter vibrierter und nicht vibrierter Betriebsweise untersucht. Für die numerischen Untersuchungen wurde ein gekoppelter CFD-DEM-Ansatz verwendet. Die mechanischen Vibrationen wurden über eine oszillierende Gravitationsbeschleunigung modelliert. Aus den MRT- und CFD-DEM-Daten wurden Blasenpositionen, -größen und -geschwindigkeiten sowie die Bettexpansion bestimmt.

Für nicht vibrierte Wirbelschichten mit Geldart-D-Partikeln zeigen MRT-Messungen das erwartete Blasenverhalten, das in den CFD-DEM-Simulationen gut reproduziert wird (Abbildung 1a). Die aus Experimenten und Simulationen gewonnenen mittleren Blasendurchmesser stimmen zudem mit etablierten Literaturkorrelationen überein (Abbildung 1b). Darüber hinaus konnte experimentell (Abbildung 1c) sowie in Simulationen (Abbildung 1d) strukturierte Blasenbildung in der 3D-Wirbelschicht beobachtet werden. Dieses Phänomen ist durch ein periodisches, räumlich geordnetes Blasenmuster charakterisiert. Während pseudo-2D-Systeme ein trianguläres Blasenmuster zeigen [4], treten in zylindrischen 3D-Betten, abhängig von Frequenz und Amplitude, eine Vielzahl an unterschiedlichen Mustern auf.

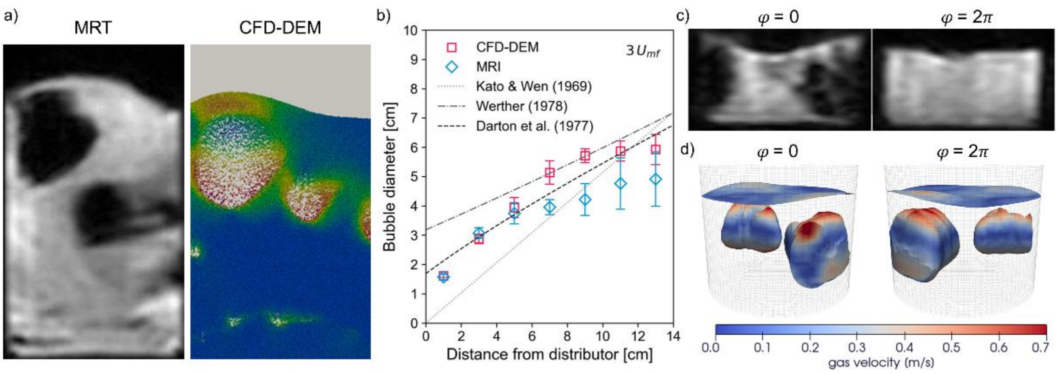

Abbildung 1: a) (links) MRT-Aufnahme eines zentralen vertikalen Schnitts durch die Wirbelschicht mit Geldart-D-Partikeln. (rechts) CFD-DEM-Simulation des gleichen Systems. b) Blasendurchmesser als Funktion der Höhe von MRT-Messungen, CFD-DEM-Simulationen und Korrelationen aus der Literatur. Strukturierte Blasenbildung in der 3D-Wirbelschicht in c) MRT-Messungen und d) CFD-DEM-Simulationen zu zwei Zeitpunkten im Abstand einer Vibrationsperiode.

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Keywords: Wirbelschicht, CFD-DEM, MRT, Vibration

Realization of online monitoring of morphological properties of agglomerates from two-dimensional images

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The morphological characteristics of agglomerates reveal the spatial structures and distribution of particle clusters. These morphological indices also provide valuable insights for improving and optimizing agglomeration processes. Previous studies have investigated the correlation between the two-dimensional ($2D$) and three-dimensional ($3D$) fractal dimensions (D_f) of agglomerates. However, real-time, online monitoring of agglomerate morphology remains a major challenge, mainly due to the difficulty of acquiring accurate $3D$ optical parameters during dynamic processes. To address this limitation, the present study aims to develop a simplified $2D$ image-based approach capable of estimating the key morphological descriptors of agglomerates with sufficient accuracy for online applications. In this study, to mimic the optical effects of online imaging systems, the outer contours of agglomerates were intentionally blurred through a newly developed image-processing algorithm. The analysis was performed based on images captured at the maximum projection angle, from which the maximum contour length (L), projected area (A), and perimeter (P) were extracted. The $2D$ box-counting method ($D_{f,BC,2D}$), which was further correlated with the $3D$ fractal dimension $D_{f,PL,3D}$ obtained from the power law relationship. The modified polydisperse tunable sequential agglomeration model was applied to generate simulated aggregates for correlation establishment. Both the ideal (non-blurred) and blurred image analyses exhibited high accuracy, with coefficients of determination of R^2 = 0.9903 and R^2 = 0.9858, respectively. Furthermore, since online measurements may not always be captured at the maximum projection angle, additional simulations were conducted to determine how many randomly captured $2D$ images are required to achieve comparable accuracy to the maximum angle case. The proposed framework provides a simplified and robust approach for real-time estimation of agglomerate morphology from two-dimensional optical images, bridging the gap between $2D$ and $3D$ structural analyses.

Keywords: agglomerate, fractal dimension, image analysis; power law, real-time monitoring, box-counting method.

Microstructural Fracture Analysis of Multicomponent Agglomerates Using In-Situ µCT and Digital Volume Correlation

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Understanding the fracture behavior of agglomerates is critical for predicting the performance of particulate materials in granulation, powder processing and handling, and other breakage-dominated operations. In this study, the deformation and failure mechanisms of bi- and multicomponent agglomerates composed of spherical soda-lime glass and polystyrene particles bonded with a hydroxypropylmethylcellulose binder are examined. A controlled extrusion-based fabrication route is employed to ensure uniform specimen geometry and reproducible compositions spanning 25 vol.% of each component up to single-component systems.

The internal deformation behavior is characterized through in-situ compression tests within X-ray microcomputed tomography (µCT) combined with Digital Volume Correlation (DVC) [1]. The image-processing workflow, including intensity normalization, morphological filtering, threshold segmentation, DBSCAN-based clustering, and watershed labeling, yields particle-resolved structural data suitable for correlation analysis. Full-field three-dimensional displacement and strain fields are computed using the SPAM DVC framework [2], enabling quantitative assessment of strain localization, interfacial debonding, and microstructural damage evolution during stepwise compression. Complementary ex-situ compression tests performed at matched loading rates provide macroscopic failure metrics across the full range of agglomerate compositions. The combined micro- and macroscale analysis reveals distinct fracture pathways governed by the relative stiffness contrast, interparticle bonding, and volumetric fraction of each material. Overall, the results demonstrate that DVC-enhanced in-situ µCT offers unique capabilities for resolving particle-scale deformation mechanisms in heterogeneous agglomerates and establishes a robust methodological foundation for future investigations of complex particulate materials.

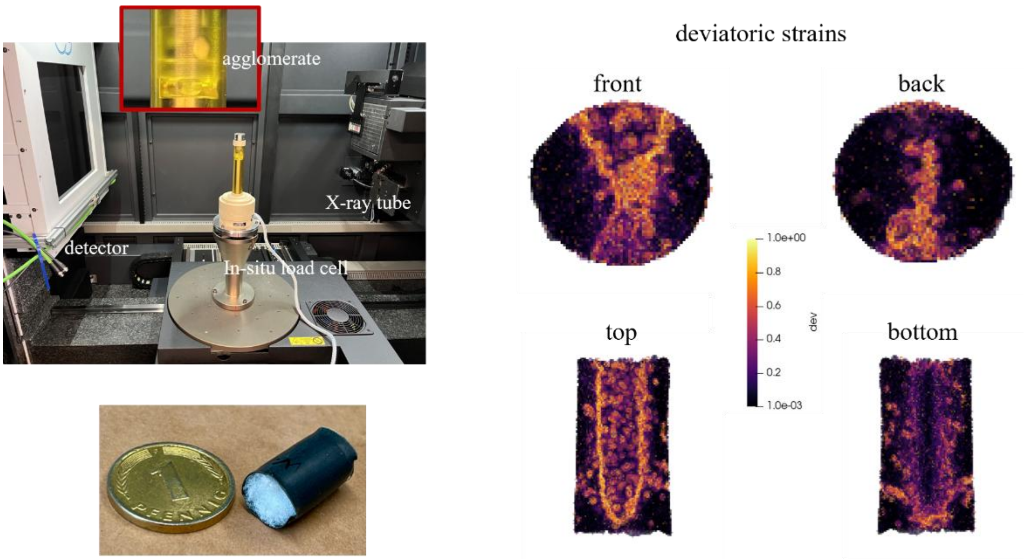

Figure 1: Illustration of the measurement setup during in-situ fracture analysis (left) and illustration of the deviatoric strain fields as a result of DVC analysis (right).

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Keywords: Multicomponent Agglomerates, In-situ X-ray tomography, Digital Volume Correlation (DVC).

Identification of the mechanical parameters of frozen particle fluid systems using adaptive AI-based surrogate modelling

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The Bonded Particle Model (BPM) extends the Discrete Element Method (DEM) by connecting primary particles through virtual bonds, enabling the simulation of particle-reinforced composites and agglomerates [1]. Despite its effectiveness in capturing complex mechanical behavior, determining accurate BPM parameters remains challenging [2]. Bond properties exist at a mesoscale that is neither accessible through macroscopic testing nor direct microscopic measurement. Traditional calibration relies on computationally expensive trial-and-error procedures that often yield non-unique solutions.

This research presents two calibration approaches: (1) a systematic inverse identification framework that combines multiple mechanical tests and can be regarded as a gradient-descent-based method for parameter identification, and (2) a machine-learning-based surrogate modeling approach that efficiently calibrates BPM parameters. The key innovation lies in integrating information from three complementary test configurations, namely uniaxial compression, three-point bending, and direct shear test, to constrain the parameter space more effectively than single-test approaches. By leveraging Principal Component Analysis (PCA) and Bayesian optimization, the framework shows how different loading scenarios collectively narrow the feasible solution space, enabling physically consistent and computationally efficient parameter identification.

Three granular materials, namely sand, glass beads, and γ-alumina, were characterized at both low and high strain rates. From each configuration, key performance indicators (KPIs) were extracted, including maximum strength, stiffness, and fracture toughness for compression and bending, as well as analogous metrics for shear, yielding nine KPIs per material. A Taguchi-based Design of Experiments (DOE) was first used to screen model parameters and identify the most influential bond properties: Young's modulus, normal and tangential bond strengths, and the creep parameters A and m of a power-law creep model. A more extensive Latin Hypercube Sampling was then employed to generate a simulation database using the open-source MUSEN framework, with 300 simulations for each test and strain-rate combination and 1800 simulations per material (5400 in total).

Gaussian Process Regression surrogate models were trained to map BPM parameters to KPIs, providing fast and accurate approximations of the computationally intensive DEM simulations. Bayesian optimization, formulated as a multi-objective problem, was used to minimize the discrepancy between simulated and experimental KPIs across all tests simultaneously, balancing exploration of uncertain regions with exploitation of promising parameter combinations.

Principal Component Analysis of the simulation database showed that integrating information from compression, bending, and shear tests significantly reduced the non-uniqueness of the calibration problem by strongly constraining the feasible parameter space. The resulting surrogate models achieved $R^2 > 0.95$ while reducing computational effort by more than 80% compared with direct simulation-based search. The proposed framework therefore offers a robust, data-driven strategy for BPM parameter identification, enabling physically consistent and computationally efficient calibration of granular materials subjected to diverse loading conditions.

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Keywords: "Bonded particle model", "Discrete element method", "Granular materials", "Surrogate modeling", "Bayesian optimization", "Inverse parameter identification".

Werden wir im Alter wirklich steifer? Untersuchung und Modellierung der Biomechanik von Biozellagglomeraten in Abhängigkeit von Größe und Alter

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Biozellagglomerate, auch Sphäroide genannt, sind 3D-Zellkulturen, die aufgrund ihrer räumlichen Organisation die physiologischen Bedingungen von Geweben deutlich besser nachbilden als herkömmliche 2D-Zellkulturen. Da Sphäroide aus verschiedenen Zelltypen aufgebaut werden können, sind sie insbesondere in der Medikamenten- und Tumorforschung sowie im Tissue Engineering von großer Bedeutung. Über die Zeit verkleinern sich die Sphäroide [1] und die Expression von Genen im Kontext der zellulären Biomechanik sowie die Bildung und Zusammensetzung der extrazellulären Matrix können sich ändern, was zu einer Variation der Biomechanik führen kann. Trotz ihrer zunehmenden Verwendung in unterschiedlichen biomedizinischen Anwendungen ist über die biomechanischen Eigenschaften von Sphäroiden bislang nur wenig bekannt.

In diesem Beitrag werden biomechanische Untersuchungen an lebenden Sphäroiden vorgestellt, die aus Normal Human Dermal Fibroblasts (NHDF) generiert wurden [1]. Hierfür wurden mittels der Liquid Overlay Technik (LOT) Sphäroide mit drei unterschiedlichen Zellanzahlen (5 000, 10 000 und 50 000 Zellen) hergestellt. Es ist bekannt, dass die LOT die Herstellung von Sphäroiden definierter Größen mit sehr geringer Streuung ermöglicht [2]. Die biomechanischen Eigenschaften, sowie die Genexpression wurden an den Tagen zwei, vier und sieben nach der Sphäroidherstellung anhand von Kompressionsversuchen bestimmt. Zu diesem Zweck wurde ein Nanoindenter (TIPremier, Bruker), ausgestattet mit einer beheizbaren Flüssigkeitsstage und einem Kamerasystem, eingesetzt und Relaxationsversuche mit Kompressionen im Bereich von 15-40 % durchgeführt.

Aus den ermittelten Kraft-Weg-Zeit-Kurven konnten mithilfe eines elastisch-plastischen Kontaktmodells [3], das um viskosen Maxwell-Termen erweitert wurde, die biomechanischen Eigenschaften der Sphäroide abgeleitet werden (siehe Abbildung 1). Durch die Modellierung ließen sich die Parameter E-Modul, Steifigkeit, Fließdruck, plastische Deformation und Viskoelastizität in Abhängigkeit von Sphäroidgröße und -alter bestimmen.

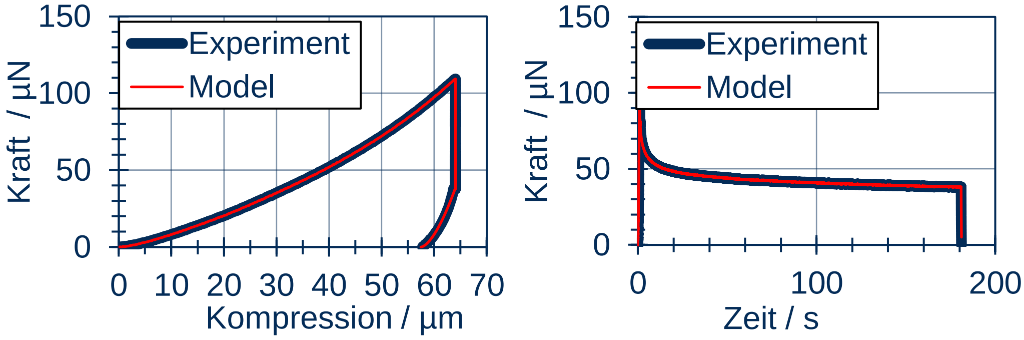

Abbildung 1: Vergleich zwischen Experiment und Modell eines Relaxationstest mit einem 50k NHDF-Sphäroiden am Tag 2 nach Aussaat.

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Keywords: Sphäroide, Zellagglomerate, Biomechanik, Viskoelastizität, Modellierung, Alterung

A DoE-based population balance model for fluidized bed spray heteroagglomeration

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Process modeling has made significant progress in recent decades, but the design and optimization of particulate processes are still often based on empirical knowledge and trial-and-error. This is particularly the case for fluidized bed agglomeration, where several interacting mechanisms occur simultaneously and are difficult to describe mechanistically. While many modeling approaches focus on systems consisting of a single solid component, industrial formulations frequently involve mixtures. In such cases, heteroagglomeration becomes important.

Despite its practical relevance, heteroagglomeration is still insufficiently represented in most population balance models (PBMs). Conventional PBMs often assume a homogeneous bed material and therefore cannot capture how two distinct solids combine into mixed. This creates a gap between experimental observations and mechanistic predictions, especially for pharmaceutical systems, consisting of several different excipients and API.

To address this, an experimentally driven PBM was developed to describe binary heteroagglomeration in a fluidized bed top-spray process. A pharmaceutical model material system consisting of Avicel PH101 (microcrystalline cellulose) as excipient, sodium chloride as a placebo material, and a 10% Pharmacoat 603 (HPMC) binder solution was used. All experiments were carried out in a lab-scale fluidized bed (GF3, Glatt Ingenieurtechnik GmbH) and structured using a Design of Experiment (DoE) approach. For each experiment, particle size distribution (PSD), residual moisture and bulk density were measured throughout the spraying and drying phases. The model is based on a mass-tracer fixed pivot PBM, which tracks both the number of particles in each size class and the evolving mass fraction of the two materials. Agglomeration is described using a flexible, size-dependent kernel with a small set of adjustable parameters characterizing collision rate and agglomeration efficiency.

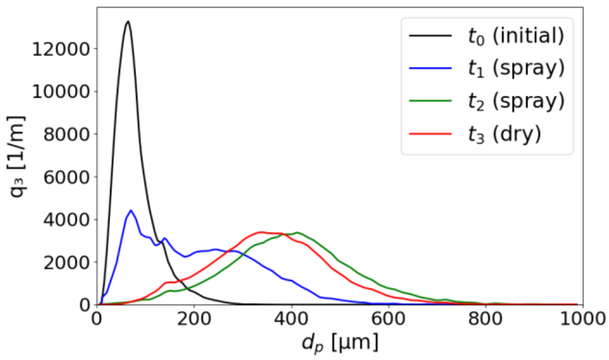

Figure 1: Change of particle size distribution (PSD) during an experiment.

For each experiment, an agglomeration rate ($ß_0$) is estimated directly from PSD data. Using the full DoE dataset, the agglomeration rate ($ß_0$) is modeled as function of the process conditions - fluidization air temperature, air flow, spray rate and nozzle pressure - providing a predictive relationship between operating conditions and agglomeration behavior across the entire design space.

The framework is modular and can be extended further, for example by incorporating drying-related shrinkage or thermodynamic effects. It is also suitable for integration into flowsheet simulation tools such as Dyssol [1], where it may support parameter studies, process design, and optimization at industrial scale.

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Keywords: Fluidized bed, heteroagglomeration, modeling, population balance.

Experimentelle und numerische Untersuchungen zur Strukturbildung von SiO_2-PS-Heteroagglomeraten in gasgetragener Strömung

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Keywords: Heteroagglomeration; Strukturbildung; CFD-DEM-Simulation; Partikelwechselwirkungen; Kalibrierung; Charakterisierung

Die Entwicklung maßgeschneiderter partikulärer Produkte mit zusätzlich integrierten Funktionen basiert auf dem mechanistischen Verständnis partikulärer Prozesse. Eine Möglichkeit, bestehende Partikeleigenschaften zu kombinieren oder durch deren Kombination neue Funktionen zu erzeugen, ist die Heteroagglomeration über Gasphasenprozesse. Der Einsatz solcher Heteroagglomerate kann insbesondere in den Bereichen Energieumwandlung und -speicherung relevant sein, beispielsweise in der Katalyse oder in der Batterietechnologie. Angesichts des großen Potenzials dieser partikulären Verbindungen ist eine detaillierte Analyse der Agglomerationsmechanismen von großer Bedeutung, um die zugrunde liegenden Prozesse zu verstehen und die resultierenden Struktureigenschaften gezielt nutzbar zu machen. Der vorgestellte Forschungsansatz kombiniert experimentelle Untersuchungen und numerische Methoden, um die Bildung und Entwicklung von Siliziumdioxid-Polystyrol-Heteroagglomeraten (SiO_2-PS) als Modellsystem zu untersuchen und die grundlegenden Mechanismen der Strukturbildung aufzuklären.

Zur experimentellen Herstellung der Heteroagglomerate werden zunächst Siliziumdioxid- und Polystyrol-Primäraggregate mithilfe zweier entgegengesetzt gerichteter Sprühtrockner separat erzeugt. Anschließend werden diese in einer definierten Agglomerationszone zusammengeführt, um Heteroagglomerate zu bilden. Durch diese Anordnung kann der Einfluss einzelner Prozessparameter auf die Strukturbildung gezielt untersucht werden. Entlang der Agglomerationsstrecke können Proben an verschiedenen Positionen entnommen werden, deren rasterelektronenmikroskopische Analyse Aufschluss über die sukzessive Bildung und Entwicklung der Agglomeratstrukturen gibt.

Da experimentelle Methoden nur begrenzte Einblicke in die zwischen den Partikeln wirkenden Kräfte ermöglichen, werden ergänzend numerische Simulationen eingesetzt, die eine differenzierte Analyse spezifischer partikulärer Wechselwirkungen während der Agglomeration erlauben. Die experimentellen Ergebnisse dienen als Grundlage für die Kalibrierung und spätere Validierung der numerischen Simulation. Zur Beschreibung der Strömungsbedingungen in der Agglomerationszone wird zunächst eine Strömungssimulation (CFD) durchgeführt. Im Rahmen der Analyse werden unterschiedliche Strömungsarten (laminar, turbulent) untersucht, um das Strömungsverhalten unter variierenden Prozessbedingungen zu ermitteln. Zur Kalibrierung der CFD werden experimentelle Messungen durchgeführt. Im Anschluss erfolgt eine Optimierung der Rechenzeit, die durch eine Verkleinerung der Simulationsdomäne auf den Hauptbereich der Agglomeration realisiert wird. Die Validität der verkleinerten Geometrie wird durch den Vergleich charakteristischer Strömungsgrößen zwischen der vollständigen und der reduzierten Simulation evaluiert.

Des Weiteren erfolgt die Erstellung einer Partikelsimulation (DEM), um die partikulären Wechselwirkungen zu charakterisieren. Die Simulation berücksichtigt Wechselwirkungen auf Basis der DLVO-Theorie. Für die Kalibrierung der DEM werden zunächst die charakteristischen Materialparameter experimentell bestimmt. Hierzu werden die Haftkräfte zwischen den Kontaktmöglichkeiten der SiO_2- und PS-Primäraggregate mithilfe der Rasterkraftmikroskopie quantifiziert. Zusätzlich werden Mikrokompressionsversuche durchgeführt, um den Elastizitätsmodul und den Restitutionskoeffizienten der porösen Primäraggregate zu bestimmen. Die so gewonnenen Materialparameter werden anschließend in die DEM implementiert, um die partikulären Wechselwirkungen realitätsnah abbilden zu können.

Die anschließende Ein-Wege-Kopplung von CFD und DEM ermöglicht die Untersuchung des Agglomerationsverhaltens unter verschiedenen Strömungsbedingungen und erlaubt eine detailliertere Erfassung der maßgeblichen Mechanismen der Strukturbildung. Der Einsatz dieser gekoppelten Methoden bietet zudem die Möglichkeit, die Heteroagglomerationsprozesse submikroner Partikel systematisch in Abhängigkeit von Prozessparametern, Partikeleigenschaften und Wechselwirkungen zu untersuchen. Hinsichtlich der Strukturentwicklung können Parameter wie Koordinationszahl, Anzahl der Heterokontakte und radiale Dichteverteilung der Agglomerate ausgewertet werden.

Die Ergebnisse der Studie stellen einen wichtigen Schritt zum Verständnis der Mechanismen der Heteroagglomeration in gasgetragenen Systemen dar. Das entwickelte und kalibrierte CFD-DEM-Setup bildet dabei die Grundlage für weiterführende Untersuchungen, mit denen die Einflüsse einzelner Prozessparameter systematisch analysiert und optimierte Bedingungen für die gezielte Struktur- und Funktionsausbildung abgeleitet werden können. Das daraus gewonnene Wissen ist entscheidend, um nicht nur die Herstellung des betrachteten Modellsystems zu optimieren, sondern auch auf andere Materialsysteme zu übertragen. Damit schafft die Arbeit eine wesentliche Basis für das mechanistische Verständnis und die gezielte Herstellung maßgeschneiderter partikulärer Produkte.

Lattice-Monte-Carlo-Modellierung der Zerkleinerung von Hetero-Aggregaten mit kontrollierter innerer Struktur

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1. Motivation

Die innere Struktur von Hetero-Aggregaten – insbesondere die Materialverteilung und die daraus resultierende Anisotropie – beeinflusst maßgeblich deren mechanische Stabilität und Zerkleinerungsverhalten. Für viele verfahrenstechnische Prozesse ist daher ein Verständnis der Mikrostrukturwirkung auf die Entwicklung der Partikelgrößenverteilung (PSD) entscheidend. Experimentelle Untersuchungen zeigen (2024, Macromolecules [1]), dass Form und Mischungsgrad die Bruchmechanik signifikant verändern. Bestehende Modellierungsansätze können jedoch komplexe interne Strukturen oft nicht adäquat berücksichtigen. Ziel dieser Arbeit ist die Entwicklung eines effizienten numerischen Frameworks zur Simulation der Zerkleinerung von Hetero-Aggregaten mit realitätsnahen inneren Strukturen.

2. Methodik

Das entwickelte Lattice-Monte-Carlo-(LMC)-Modell beschreibt Partikel als zweidimensionales Gitter, dessen Zellen unterschiedliche Materialien repräsentieren. Materialbindungen zwischen Zellen definieren lokale Festigkeiten, während Rissinitiierung und -ausbreitung durch einen Monte-Carlo-Prozess gesteuert werden. Zur Erzeugung geeigneter Eingangsgitter wurde ein 2D-Aggregatgenerator entwickelt, der auf einem modifizierten Particle Transport and Sticking Algorithm (MPTSA [2]) basiert und über eine vorgegebene Fraktaldimension die Aggregatform steuert. Eine nachgeschaltete Potts-Modell-Umverteilung erzeugt Zielmuster des Mischungsgrades.

Zur Abbildung der Systemdynamik wird das LMC-Modell mit einem Monte-Carlo-Population-Balance-Solver (MCPBE) gekoppelt, der die PSD-Entwicklung effizient simuliert. Die Modellparameter werden mittels eines bereits validierten Optimierungsframeworks (2025, Digital Chemical Engineering [3]) bestimmt, das experimentelle PSD-Daten einliest und hochperformante Sampling-Algorithmen zur parallelen Berechnung nutzt.

3. Zusammenfassung

Das integrierte LMC-MCPBE-Framework ermöglicht eine schnelle und physikalisch konsistente Simulation der Zerkleinerung von Hetero-Aggregaten mit vorgegebenen inneren Strukturen. Durch die Kombination aus strukturbasierter Gittergenerierung, stochastischer Bruchmodellierung und populationsbilanzieller Dynamik erlaubt der Ansatz sowohl die Modellkalibrierung anhand experimenteller Daten als auch systematische Studien zum Einfluss von Mischungsgrad und Form auf die Zerkleinerungskinetik.

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Keywords: Hetero-Aggregate, Mikrostrukturbasierte Zerkleinerung, Lattice-Monte-Carlo-Modell, Population-Balance-Modellierung, Materialverteilung und Mischgüte.

Dry particle coating of carbon black on NMC cathode materials using Mechano-fusion

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The development of electronically conductive and functionalized cathode materials remains a key challenge in lithium-ion battery manufacturing, particularly regarding scalable and solvent-free processing routes. The mechano-fusion (MF) process enables the formation of hetero-aggregates by attaching smaller guest particles to larger host particles, thereby improving interparticle contact and, in turn, modifying the surface functionality of the host material [1]. This work investigates the dry coating of carbon black (CB), used as a conductive additive, onto lithium nickel manganese cobalt oxide (NMC) particles, a common cathode active material in lithium-ion batteries, under systematically varied MF process parameters. Enhancing the electronic contact through CB deposition is expected to improve the electrochemical performance of the resulting cathode composites [2].

MF experiments are conducted using the Picoline machine from Hosokawa Alpine (Augsburg, Germany) with the Picobond module, which features a stator-rotor assembly. The influence of key MF process parameters, such as rotational speed, process time and CB concentration, is studied to understand their impact on the resulting coating structures. Variation of these parameters enables the establishment of process–structure relationships, revealing how they affect coating uniformity and the guest–host interaction during the formation of hetero-aggregates. Dry coating experiments are performed using different CB concentrations and the resulting coated powders are characterized concerning its particle size distribution, specific surface area (BET theory) and density. Techniques like scanning electron microscopy (SEM) and atomic force microscopy (AFM) are explored to understand the surface characteristics of coated structures. A comparative analysis with pristine materials provides insights into the influence of MF process parameters on coating quality.

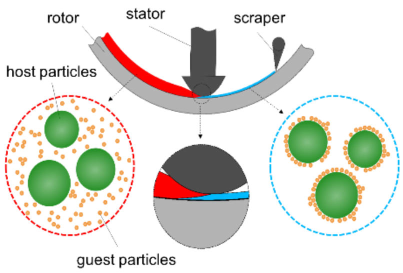

Figure 1: Scheme of MF process [3]

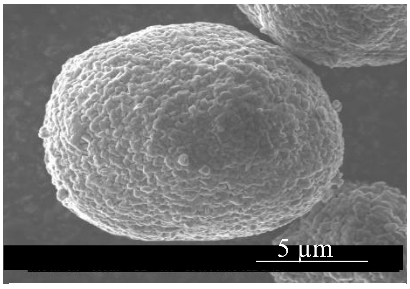

Figure 2: Pristine NMC 622 before coating

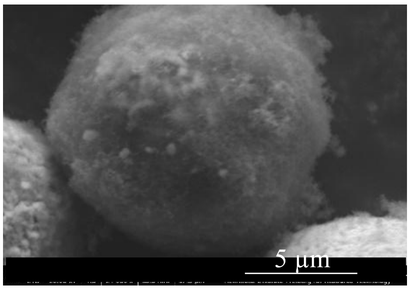

Figure 3: Pristine NMC 622 after coating

The results indicate that MF promotes modification of pristine NMC surfaces, producing smoother and more spheronized particle morphology. Successful CB deposition is confirmed by an increase in BET surface area, while the reduction in density indicates incorporation of low-density CB on the NMC surface. SEM analysis further reveals that higher CB concentrations results in locally thick, non-uniform coating regions, whereas lower CB concentrations yield a thinner, more finely dispersed CB layer across the NMC particles. Overall, the study demonstrates that coating effectiveness depends strongly on both CB concentration and MF operating conditions, highlighting the potential of MF as a solvent-free route for preparing advanced cathode materials for lithium-ion batteries and underscoring the importance of structural characterization for understanding and optimizing dry coating mechanisms.

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Keywords: Dry particle coating, Mechano-fusion, Li-ion batteries, NMC particles, Atomic Force Microscopy

In-situ Investigation of binary powder mixing with Microfocus X-Ray Computed Tomography

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This work studies Powder Mixing and Segregation using Microfocus X-Ray Computed Tomography (micro-CT). Additionally, we study the process numerically. It is part of the Helmholtz project FINEST which addresses challenges in the fields of circular economy, recycling and sustainable resources. Part of this involves the mixing of fine particles to recycle those materials, which cannot be separated further. Due to varying material streams, analysis of the mixing process becomes increasingly important.

Mixing investigation using Microfocus X-Ray Computer Tomography

Micro-CT scans provide insight into the composition of powder mixtures at any point in space and allow analysis of the powder distribution. We developed a 3D analysis method, which describes the quality of mixtures by a variance measure.

We now use this method to study the influence of different particle properties causing segregation. In the context of FINEST, it is their different density, because the particles range from plastics to metals. Multiple combinations of particles from 150 – 250 µm with densities between 0.5 – 5 g/cm³ are mixed in a cylindrical bladed mixer. We give a full range of parameters, such as mixing speed, density ratio and mixing duration, that lead to segregation and the dependency of Mixing Index on those.

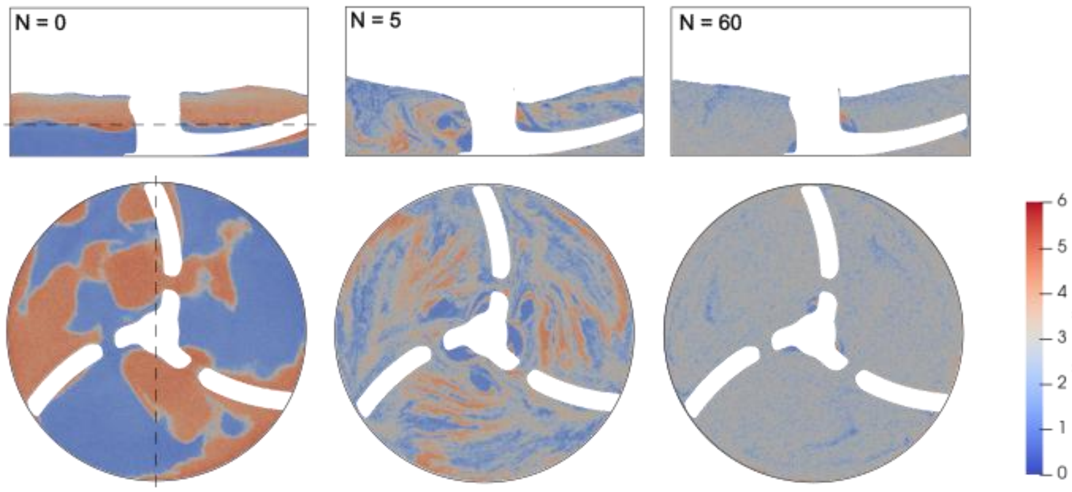

Figure 1 Vertical and horizontal slices through the bed for increasing number of impeller rotations (N) at Fr = 1. Dashed lines in far-left view show the slice positions.

Numerical investigation of segregation in density different mixtures

We simulate the mixing in OpenFOAM using multiphase Euler solvers. We implemented µ(I)-rheology and mixing and segregation effects by a drag model approach. We are currently validating it against the experimental results. Overall, this is a continuum model for bladed mixer for both size and density segregation, adaptable to other geometries. The CFD model allows us to estimate flow distributions, that are difficult to obtain with µCT, and hence complement the present experimental study.

Acknowledgement

The project FINEST is funded by the Initiative and Networking Fund of the Helmholtz Association of German Research Centres (HGF) under grant agreement no. KA2-HSC-10.

Keywords: Microfocus Tomography, Powder Mixing, Continuum Model, Granular Flow

Materialanhaftungen an der Walzenoberfläche in der Kalikompaktierung

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Das Kompaktier-Granulierverfahren zur Herstellung von Düngemittelgranulaten kommt unter anderem in der Kaliindustrie zur Anwendung. Im Wesentlichen setzt sich das Verfahren aus den Makroprozessen Pressagglomeration, Zerkleinern, Mischen und Klassieren zusammen. Im ersten Schritt wird fein-disperses Rohsalzkonzentrat in einer Walzenpresse mit profilierter Oberfläche zu festen, plattigen Agglomeraten, den sogenannten Schülpen, kompaktiert. Im Anschluss werden die Schülpen zerkleinert und auf die Zielgranulatgröße abgesiebt.

Bei dem preissensiblen Produkt ist die Optimierung des Herstellungsprozesses hinsichtlich hoher Produktmassenströme und einem geringen Energiebedarf enorm wichtig. Dabei auftretende unerwünschte Betriebszustände müssen erkannt, untersucht und abgestellt werden. Einer dieser Zustände ist die Bildung einer Materialschicht auf den Walzenoberflächen der Presse, welche zu Verminderungen der Produktionskapazität bis hin zu Anlagenausfällen führen kann.

Im Rahmen dieses Beitrags wird aufbauend auf einer kurzen Übersicht über das Kompaktier-Granulierverfahren und der Beschreibung der Auswirkungen solcher Materialanhaftungen ein Einblick in die Untersuchung der zugrundeliegenden Einflussfaktoren gegeben. Weiterhin wurden die experimentell gewonnenen Ergebnisse genutzt, um auf Basis eines Softsensors eine Regelstrategie zu entwickeln, welche nun in einer Industrieanlage zur Erkennung und Verminderung dieser Anhaftungen verwendet wird.

Keywords: Walzenpressen, Kompaktier-Granulierung, Kalisalz, Aufschmelzungen, Softsensor

Characterization of powder compaction behaviour

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Powder compaction is a key step in many industrial processes, where the applied mechanical stresses can cause plastic particle deformation and increase particle adhesion, which influences the packing behaviour and thus the mechanical strength of the bulk material. A monomodal packing of identical particles is subjected to homogeneous loading. In practice, particulate products consist of particles that are distributed not only by size but also by mechanical properties, for example in a pharmaceutical formulation. This results in a loading situation that strongly depends on concentration, packing arrangement, and local properties. Such complex stress conditions remain insufficiently explored and therefore require further systematic investigation.

In this work, the compaction behaviour of particles with elastic-plastic deformation is investigated experimentally and numerically to improve the predictions of compressibility and the packing structure during the compaction process (Figure 1). The particles are compacted under different normal stresses in an in-situ micro-computed tomography (µCT) compaction cell in a cylindrical die. The µCT imaging allows local analysis of the packing structure, particle displacements, and contact development during compaction [1]. The experiments are used to validate simulations with the Discrete Element Method (DEM) incorporating our previous developed elastic-plastic contact model [2]. This model enables the analysis of plastic deformation and the forces acting on individual particles using measurable mechanical properties of particles. This enables direct comparison of the porosity and stress development in the particle bed for different particle sizes between experiment and simulation at different compaction stresses.

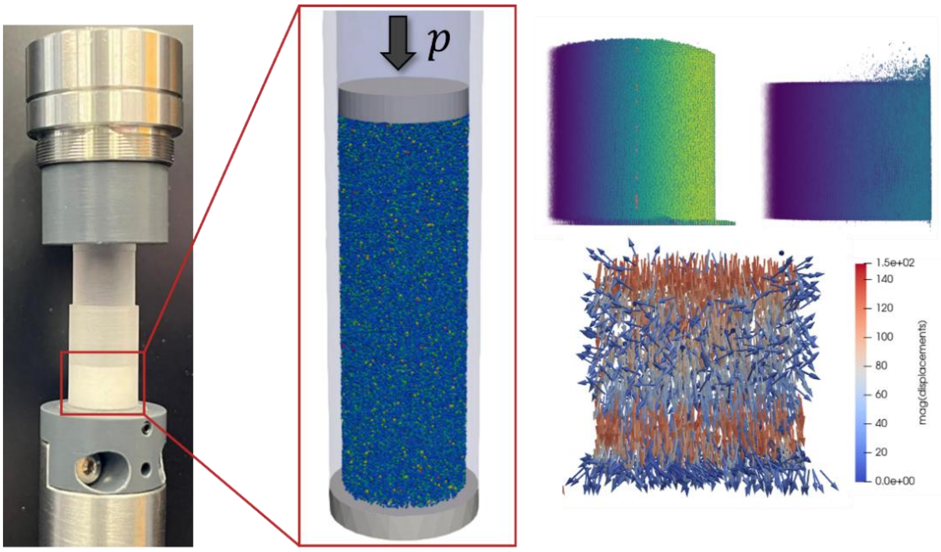

Figure 1: Left: Experimental in-situ setup and its DEM simulation. Right: µCT analysis of particle displacement

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Keywords: Powder compaction, Elastic-plastic deformation, Discrete Element Method, Micro-computed tomography

Optimizing Magnesium Tablet Formulations:

Overcoming Processing Challenges of Trimagnesium Citrate

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Magnesium supplements are widely used and available in various forms: tablets, capsules, powders, and liquids - either as single ingredients or combined with vitamins, minerals, or botanicals. Among magnesium salts, magnesium citrate, magnesium oxide, and magnesium carbonate are most common, with magnesium citrate being the only organic salt [1]. High mineral content is essential for minimizing tablet size; trimagnesium citrate anhydrous (TMC) offers the highest mineral content (16%) among organic salts, making it a preferred choice for tablet formulations. However, its fine powder form presents processing challenges, including dust formation and excessive fines during tableting, and its concentration in formulations is limited to maintain tensile strength.

The tableting properties of different TMC grades were evaluated using a single-punch tablet press (FlexiTab®, Roeltgen). Tensile strength was selected as the primary performance parameter. To enhance mechanical stability, TMC was functionalized through agglomeration, granulation, and coating techniques. Functionality was assessed in a base formulation containing 28.9% microcrystalline cellulose (MCC 102), 4% croscarmellose sodium, and 1.1% magnesium stearate.

Functionalized TMC grades demonstrated improved flowability and reduced dust formation compared to the untreated fine powder. Granulated grades yielded tablets with higher tensile strength and fewer fines during compression, without compromising mineral content. The optimized formulation achieved stable tablets with acceptable mechanical integrity while maintaining a high magnesium load.

Functionalization of trimagnesium citrate anhydrous significantly improves its tableting performance, addressing key processing challenges such as dust formation and tensile strength limitations. Granulation techniques offer practical solutions for producing magnesium tablets with high mineral content and robust mechanical properties, supporting efficient manufacturing and consistent product quality.

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Keywords: Magnesium supplements, trimagnesium citrate, tablet formulation

Formulierung und Optimierung von Tabletten für carbon capture im Festbett

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Carbon capture ist ein Verfahren zur Abtrennung von CO2 aus Industrieabgasen, wie sie z.B. in der Zementproduktion anfallen. Es gibt verschiedene Ansätze für carbon capture Verfahren, dazu gehören die Amin-Wäsche, Membranverfahren oder „amine-grafted“ Feststoffe. Das binden von Aminen auf einem Feststoff verspricht Energieeinsparungen gegenüber der Amin-Wäsche, die sehr energieintensiv ist. In dieser Arbeit wird näher auf die Formulierung geeigneter Grundkörper, basierend auf pyrogener Kieselsäure, für das „amine-grafting“ eingegangen. Dabei wird zum einen die Bruchstabilität der Grundkörper betrachtet, welche wichtig ist, um eine möglichst hohe Langlebigkeit während wechselnden Adsorptions- und Desorptionszyklen sicherzustellen. Zum anderen wird die Porosität über die BET-Oberfläche bestimmt, von der die Adsorptionskinetik sowie die CO2 Kapazität, die aufgenommen wird, abhängt. Das verwendete Ausgangsmaterial ist pyrogene Kieselsäure im nm Größenbereich. Diese wurde im ersten Schritt mit Wasser in einem Labor-Intensivmischer voragglomeriert, um die Partikelgröße von ca. 2 nm auf ca. 2 µm zu vergrößern. Anschließend wurde dieses Material gesiebt und tablettiert. Die Tabletten wurden danach getrocknet und gesintert um deren Stabilität zu erhöhen. Die Bruchkraft wurde mit einem Texture Analyzer gemessen und die Oberfläche wurde über die Stickstoffadsorption in einem BET-System gemessen.

Der Einfluss verschiedener Parameter auf die Bruchfestigkeit und Oberfläche der Tabletten wurde untersucht. Die verwendeten Tabletten haben einen Durchmesser von 4 mm und eine Dicke von 1,6 mm bis zu 2,6 mm bei einer Fülltiefe der Matrize von 10 mm. Die Kompression wirkt sich bei konstanter Masse auf die Tablettendicke aus. Der Wasseranteil in der Voragglomeration, das Trocknungsverfahren und die Temperatur und Zeit im anschließenden Sintervorgang wurden variiert. Das voragglomerierte Material wurde klassiert und die unterschiedlichen Fraktionen auf Tablettierbarkeit getestet. Große Partikel über 0,8 mm wurden verworfen, da sie die Tablettenpresse verstopfen. Abbildung 1a zeigt die BET Oberfläche, abhängig von der Fraktion des voragglomerierten Materials. Abbildung 1 b zeigt die Bruchspannung in Abhängigkeit der Agglomeratgröße. Nach dem Trocknen und Sintern hatten die Tabletten ein Gewicht von 12,15 ± 1,06 mg. Der Wassergehalt des voragglomerierten Materials hat ein Minimum bei der Fraktion 0,125 bis 0,25 mm, das im Versuch die Tabletten mit der höchsten Bruchkraft erzeugte. Ein höherer Wassergehalt in den voragglomerierten Partikeln führt zu einer höheren Dichte von den getrockneten und gesinterten Tabletten. Eine weitere Versuchsreihe mit unterschiedlichen Wassermengen zeigte, dass das Tablettengewicht nach dem trocknen und sintern proportional zum Wasseranteil ansteigt, wenn dieser für die Voragglomeration erhöht wird. Dies legt nahe, dass das Wasser einen Einfluss auf die Anordnung der Silica Partikel im Agglomerat hat und ein dichtes packen begünstigt. Nach dem Trocknen der Tabletten hinterlässt dieses Wasser eine Poröse Struktur, die die BET-Oberfläche vergrößert, sich jedoch negativ auf die Tablettenbruchkraft auswirkt.

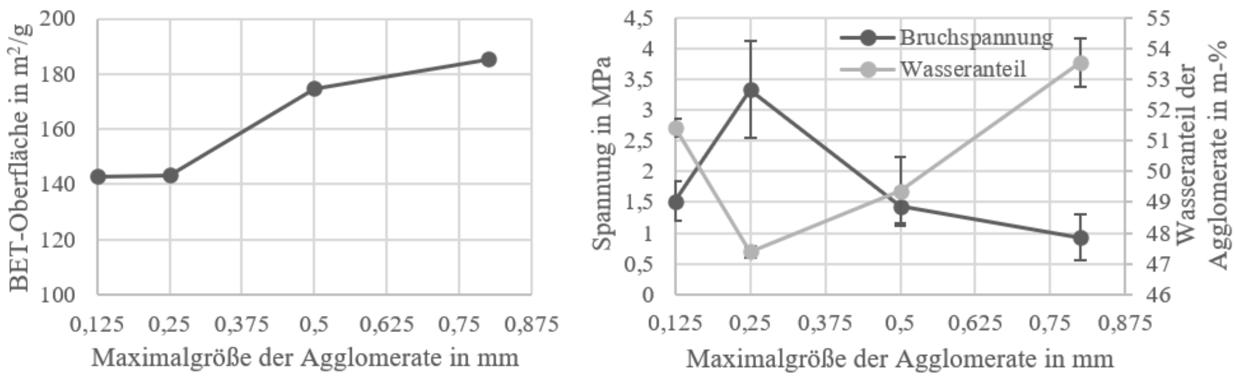

Abbildung 1 a: die BET-Oberfläche der Tabletten; b: deren benötigte Bruchkraft sowie die Feuchtigkeit des voragglomerierten Materials; es ergab sich ein unterschiedlicher Wassergehalt bei unterschiedlichen Agglomeratgrößen

Die Versuche zeigen, dass die Oberflächengröße sowie die Porosität der Tabletten beeinflusst werden können. Tabletten mit einer hohen Porosität haben jedoch eine geringere Stabilität. Daher ist es notwendig einen Mittelweg zwischen einer möglichst hohen Oberfläche und einer akzeptablen Stabilität zu finden. Außerdem müssen die Diffusionswege für das CO2 klein gehalten werden, was kleine Tabletten oder hohle Grundkörper wie z.B. extrudierte Hohlpellets begünstigt.

Keywords: Silica Tablettierung, Bruchfestigkeit, Porosität, Oberfläche

Parameterabhängige Spannungsverteilungen und ihre Einflüsse auf die Eigenschaften von Mantelkerntabletten

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Mantelkerntabletten (MKT) sind eine moderne Darreichungsform mit Vorteilen gegenüber herkömmlichen Tabletten. Negative Einflüsse durch Flüssigkeits- und Hitzeeinwirkung, die bei Nassbeschichtungsverfahren von Tabletten zur Beschädigung oder Inaktivierung von Wirkstoffen führen können, werden durch den Vorgang der trockenen Pressbeschichtung umgangen. Über die besondere Struktur von Mantelkerntabletten kann die Freisetzungskinetik aus dem Kern meist über die Manteleigenschaften gesteuert werden. Der Herstellungsprozess ist jedoch komplex und die mechanischen Eigenschaften der Formulierungen von Kern und Mantel können zu Herausforderungen hinsichtlich der mechanischen Stabilität der pressbeschichteten Tabletten und ihrer Freisetzung führen [1–3]. Besonders im Hinblick auf die mechanischen Eigenschaften der Tablette, den Einfluss des Kerns und die Prozessparameter lässt sich durch gezielte Untersuchungen ein besseres Verständnis über die Spannungszustände während und nach der Herstellung der MKT gewinnen. Um diese Spannungsverteilung genauer zu charakterisieren, wurden unterschiedliche Kerndurchmesser sowie variierte Kern- und Mantelkompressionsspannungen zur Herstellung der MKT verwendet. Als Materialkombination wurden zwei Materialen mit stark unterschiedlichen Deformationsverhalten gewählt: der Kern bestand aus sprödbrüchigem Dicalciumphosphat und der Mantel aus plastisch deformierender Mikrokristalliner Cellulose. Die MKT wurden hinsichtlich ihrer Zugfestigkeit, Porosität und der elastischen Rückdehnung untersucht, um sich die Gesamteigenschaften (Kompaktibilität, etc.) der MKT mit denen der Monotabletten zu vergleichen. Um gezielte Rückschlüsse auf die Spannungsverteilung während der Mantelkompression schließen zu können, wurde die MKT in verschiedene Kompartimente unterteilt (siehe Abb.1). Dabei sind vor allem die ermittelten Porositäten im Mantel interessant, um die dort wirkenden Spannungen einzuordnen (Abb.1 rechts). Die Ergebnisse liefern ein besseres Verständnis über den anisotropen Spannungszustand, der sich auch auf die bereits vorverdichteten Kerne auswirkt (Abb.1 links). Die Geometrieänderungen der Kerne sowie ihrer Zugfestigkeit wurden systematisch untersucht. Hierzu diente ebenfalls Gummimehl als Referenzmaterial für eine komplett elastische Manteldeformation ohne Festigkeitsaufbau im Mantel, um die Auswirkung dieses Extremfalls beschreiben zu können. Um die prozessparameterspezifischen Effekte auf Kern- und Mantelstruktur mit den Prozesszuständen korrelieren zu können, wurde die während der Kompression wirkende radiale Wandspannung analysiert. Diese verdeutlichen die anisotropen Zustände während der Kompression von MKT und erklären die Ergebnisse der Porositätsverteilungen im Mantel und werden abschließend genutzt, um die verschiedenen Versagensmuster bei der Tablettentestung zu erklären.

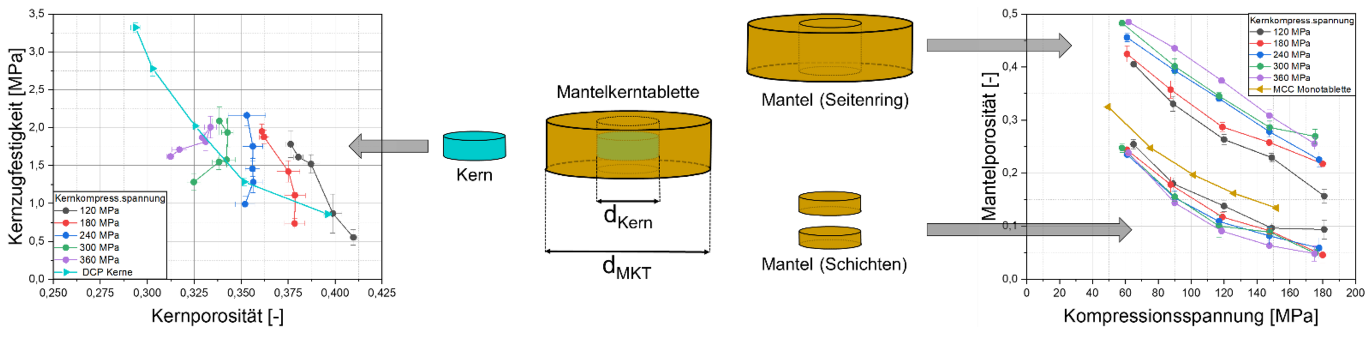

Abbildung 1: Aufbau einer Mantelkerntablette und ihre Unterteilung in verschiedene Kompartimente;
links: Kompaktibilitäten der Kerne; rechts: Porositäten der Mantelkompartimente

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Keywords: Mantelkerntabletten, Spannungsverteilung, Tabletteneigenschaften, Prozessparameter

Hin zur autonomen Tablettierung: in-line Überwachung physikalischer Tabletteneigenschaften

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Einleitung

Die Tablettierung auf einer Rundläufertablettenpresse ist ein trockenes Granulationsverfahren, das typischerweise in eine mehrstufige Produktionslinie integriert ist, bei der ein Wirkstoff, Schmiermittel und anderen Hilfsstoffen zu Tabletten verpresst werden. In der Regel erfolgt die Prozesskontrolle mittels manueller ex-situ Probenahme und off-line Probenanalyse, die anfälliger für Fehler ist und somit inhärent die Produktqualität mindern kann. Folglich ist das übergeordnete Ziel dieses Projektes die Entwicklung und Erprobung eines autonomen Prozesskontrollsystems. Für die Selbstanpassung ist hierbei ein Prozesskontrollsystem notwendig, das die Prozessparameter anpasst auf Grundlage einer Echtzeitüberwachung der Produktspezifikationen sowie eines Kontrollmodells, das die gewünschten Spezifikationen mit Prozessparametern und Materialeigenschaften verknüpft. In diesem Zusammenhang liegt der Fokus dieser Studie auf der Echtzeitquantifizierung physikalischer Tabletteneigenschaften. Die Schritte dafür umfassen die In-line-Implementierung der UV-Vis-Spektroskopie in der Rundläufertablettenpresse, die Korrelation der physikalischen Tabletteneigenschaften mit dem Messsignal, und die Validierung der Messmethode.

Methoden

In diesem Projekt wurde die Pulververdichtung auf einer Rundläufertablettenpresse (Fette 102i, Fette Compacting, Schwarzenbeck, Deutschland) untersucht. Die Formulierungen bestanden aus Theophyllin (10 Gew.%, Alfa Aesar, Haverhill, USA), mikrokristalliner Cellulose (MCC) (89,5 oder 99,5 Gew.%, JRS Pharma, Rosenberg, Deutschland), aus einer feinen oder groben Laktose (89,5 oder 99,5 wt.%, Meggle, Wasserburg am Inn, Germany) und aus Magnesiumstearat (0,5 wt.%, Ligamed MF-2-V, Peter Greven, Bad Münstereifel, Deutschland). Die Partikelgröße wurde mittels Laserbeugung bestimmt (Mastersizer 3000, Malvern Panalytical, Malvern, UK) und die Tabletteneigenschaften (Bruchkraft, Dichte) mit einem Tablettentester (ST50, Sotax, Aesch, Schweiz). Für die in-situ Überwachung von Porosität und Zugfestigkeit wurde UV-Vis-Spektroskopie (Inspectro X, ColVisTec, Berlin, Germany) eingesetzt und die Rohspektren in das Polarkoordinatensystem des CIELAB-Farbraums überführt [1].

Ergebnisse und Diskussion

Zum einen wurde die Anwendbarkeit der UV-Vis Spektroskopie für die Echtzeitbestimmung der Tablettenporosität untersucht (Abbildung 1). Der C*-Wert repräsentiert die Farbsättigung in Polarkoordinaten und wurde hier für MCC (plastisch) und Laktose (spröde) bestimmt, die mit variierenden Kompressionskräften erstellt wurden [1]. Dabei nimmt der C*-Wert mit steigender Porosität ab, weil bei den zugehörigen niedrigeren Kompressionskräfte zu raueren Oberflächen und somit mehr Lichtstreuung führen. Durch ein vermehrtes Fragmentieren und die Bildung glatterer Oberflächen, zeigen brüchige Formulierungen (L_{fine}, L_{coarse}, LT) höheren C*-Werte als plastische. Bezogen auf Laktose, haben Porositätsänderungen bei groben Fraktionen kleinere Auswirkungen auf den C*-Wert als bei feineren, zu erklären durch andere Porositäts- und Oberflächenbeschaffenheiten. Zum anderen wurde in dieser Studie das in-Iine-Monitoring der Tablettenporosität und die Eignung der UV-Vis Spektroskopie als analytische Methode untersucht und dazu am Beispiel einer MCC-Formulierung die Kompressionskraft systematisch über die Zeit variiert und die in-line identifizierte Korrelation der Porosität mit den off-line analysierten Proben verglichen. Die Ergebnisse zeigten eine hohe Übereinstimmung zwischen beiden Datensätzen, weshalb die UV-Vis Spektroskopie für die ausgewählten Porositätsbereiche eine zuverlässige und zerstörungsfreie Messung mit hoher Frequenz ermöglicht. Zusammenfassend wurde die Anwendbarkeit der UV-Vis-Spektroskopie als PAT-Tool zur Echtzeitquantifizierung der Tablettenporosität validiert. Der nächste Schritt in diesem Projekt umfasst die Verbesserung des Messsignals durch Optimierung der Implementierung.

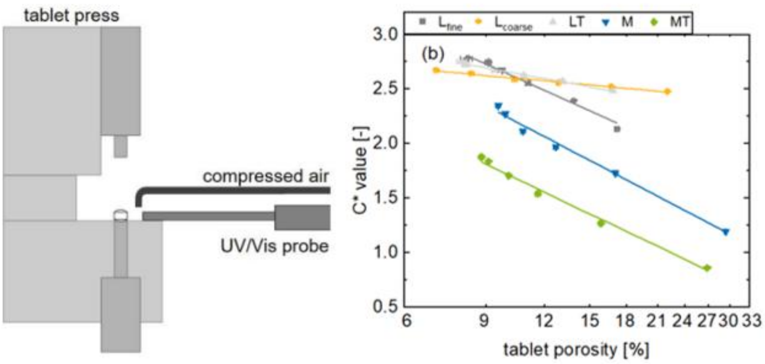

Abbildung 1. Implementierung der UV-Vis Spektroskopie; Korrelation C-Wert & off-line quantifizierte Porosität in logarithmierter Form nach [1]*

Anerkennung

Dieses Projekt wurde durch die Deutsche Forschungsgemeinschaft (DFG, Projekt: TH 1817/8-1) gefördert.

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Keywords: Autonome Prozesskontrolle, Tablettierung, Prozessanalysetechnik (PAT)

Hetero-aggregation of nanoparticles

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Hetero-aggregates of nanoparticles exhibit superior sensing, electrical, optical, and catalytic properties owing to the formation of hetero-contacts between dissimilar materials, making them valuable for applications in electronic, solar, and energy devices [1]. In the gas phase, nanoparticles inherently form homo-aggregates due to strong cohesive forces such as Van der Waals interactions. To achieve effective mixing of different nanoparticle types, these homo-aggregates must first be disintegrated into individual particles or small clusters. However, upon dispersion, nanoparticles tend to reaggregate, during which hetero-contacts can form, leading to hetero-aggregate formation.

The ProCell spouted bed is a promising apparatus for generating hetero-aggregates, as its high inlet jet velocity facilitates the breakup of homo-aggregates while the expansion chamber maintains a low superficial gas velocity, enabling controlled reaggregation [2]. Our previous studies demonstrated that the current ProCell setup could operate at an inlet velocity of 113 m/s (corresponding to 80 m^3/h) with acceptable elutriation. However, higher velocities resulted in excessive particle elutriation. To overcome this limitation, the base plate of the spouted bed was raised to reduce the inlet gap, allowing higher jet velocities to be achieved at the same flow rate. This modification significantly minimized elutriation and improved mixing intensity, enabling operation at jet velocities up to 320 m/s for the same bottom flow rate (80 m^3/h). Additionally, four top milli-nozzles were integrated to stabilize the spouting behavior.

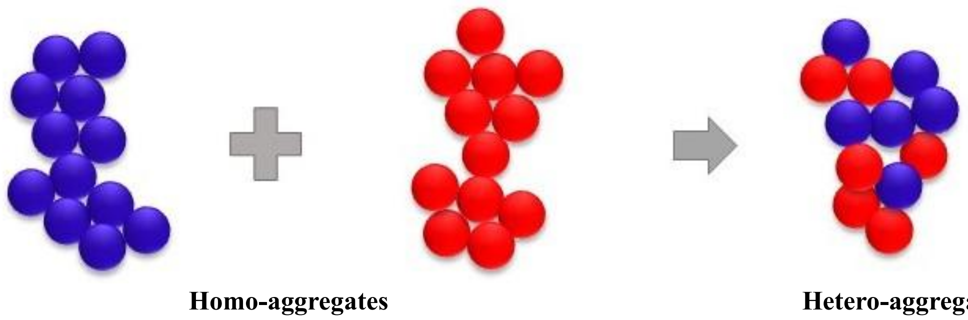

Figure 1: Illustration of nanoparticles mixing (blue and red are primary particles of different materials).

In the modified system, two different nanopowders (Al_2O_3 and TiO_2) will be co-processed to produce hetero-aggregates. The effects of bottom flow rate, top air velocity, and inlet gap on the mixing quality and aggregate structure will be systematically investigated. Scanning Electron Microscopy (SEM) combined with Energy Dispersive X-ray Spectroscopy (EDX) will be employed to characterize the morphology, elemental distribution, and degree of mixing within the hetero-aggregates. The study aims to establish optimized operating conditions for producing high-quality hetero-aggregates with controlled microstructural properties suitable for advanced material applications.

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Keywords: Hetero-aggregates, nanoparticles, mixing, spouted bed.

Upscaling of Batch Fluidized Bed Processes

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Fluidized bed coating and agglomeration are very common processes in pharmaceutical as well as in food and chemical industries. Specifically, in the manufacture of pharmaceutical products, batch processes are widely applied from small lab-scale (i.e., batch sizes of a few grams) to large commercial scale of several hundred kilograms per batch.

During the development of a new pharmaceutical product, commonly three to five upscaling steps are conducted between feasibility studies and commercial manufacture. It is crucial to maintain the intended product quality throughout every step. A reliable upscaling concept is therefore essential for smooth and efficient process development and commercial manufacture.

Glatt has developed and established such an upscaling concept for fluidized bed processes with Wurster configuration. It is suitable for coating and agglomeration processes alike. The concept is based on basic thermodynamical and fluid mechanical principles, resulting in reliable scaleup factors. Thus, extensive calculations or simulations are avoided. Furthermore, it allows a good estimation of the resulting process time. The concept is of course applicable for downscaling as well.

The batch size is scaled while it is key to maintain the same product humidity and temperature to maintain product quality. Fluidization behavior, droplet size and drying capacity in the system must therefore be considered. Underlying assumptions are the availability of fluidized bed equipment that suits the upscaling concept e.g., highly similar geometric shape of the process chambers and that required process parameters such as inlet air volume flow can be realized.

The details of the scaleup concept will be introduced and discussed in this contribution. Prove of the concept will be given by examples.

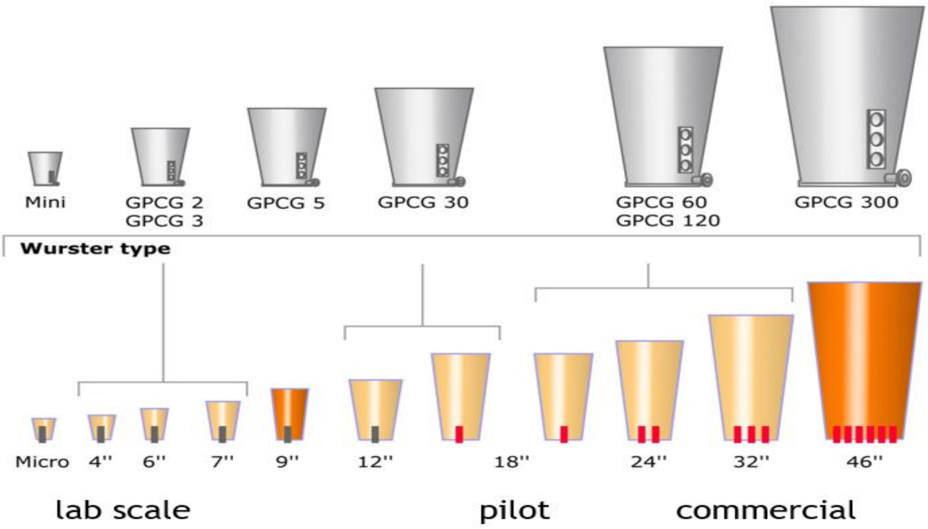

Figure 1: Different sizes of Wurster fluidized beds, with batch sizes ranging from a few grams in the "Mini" to several hundreds of kilograms in “GPCG 300”. GPCG = Glatt Particle Coater and Granulator

Keywords: Scale-up, Fluid Bed, Agglomeration, Coating, Batch Process

Incipient agglomeration at the border to coating vs. breakage: Experimental investigation of the influence of spray flow rate on the growth mechanism

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Agglomeration and coating are key particle enlargement processes in numerous industries. Both rely on spraying binder or coating solutions onto a fluidized bed of particles with simultaneous drying. In agglomeration, wet particle collisions form liquid bridges that solidify and turn into bigger agglomerates with raspberry-like structures. Coating instead deposits successive layers of solution onto particle surfaces, producing onion-like structures. Although the steps of droplet atomization and particle wetting are common, the processes diverge through operating conditions. They may overlap to a certain extent, but depending on the application of the product, only one of the two complementary size enlargement processes should be dominant.

A recent study introduced an optical particle counting method (OPCM) to better observe the early stage of formation of dimers from primary particles. Using high-resolution imaging to detect and classify single particles, dimers, and larger clusters, OPCM allowed direct and accurate tracking of these different particle classes. Results showed that standard Camsizer measurements overestimated dimer formation by about 17% and larger agglomerates by 44%. This highlights the need for detailed experimental data to improve predictive models such as Monte Carlo simulations. In this work, OPCM is used to study how changes in binder flow rate affect the early stage of dimer formation and breakage near the coating regime in spray fluidized beds.

As it can be seen in the Figure 1, increasing the binder spray rate from 7.20 to 8.40 g/min markedly enhanced net agglomeration, reflected by a steeper depletion of primary particles (from -0.01128 to -0.03017 min^{-1}) and higher formation rates of dimers and bigger agglomerates (dimers: 0.00710 to 0.01536 min^{-1}; larger agglomerates: 0.00419 to 0.01481 min^{-1}). Enhanced binder availability increased wetting and collision efficiency, consistent with spray-to-surface ratio effects. Post-spray breakage analysis showed that higher spray rates generated faster apparent breakage (dimers: -0.0416 to -0.0530 min^{-1}), attributed to the larger population of agglomerates available to breakage. Once normalized to initial class fractions, breakage trends inverted ($r_{B,D}$: -0.3524 to -0.2852 min^{-1}), indicating that higher binder spray rates produced stronger bridges and more breakage-resistant structures. Experiments stopping spraying after 5 min confirmed that shorter spraying yields weaker agglomerates with higher normalized breakage ($r_{B,D}$= -0.5431) compared to 10 min (-0.2852), demonstrating reinforcement by continued layering. Overall, binder spray rate strongly governs the balance between aggregation and breakage near the coating boundary.

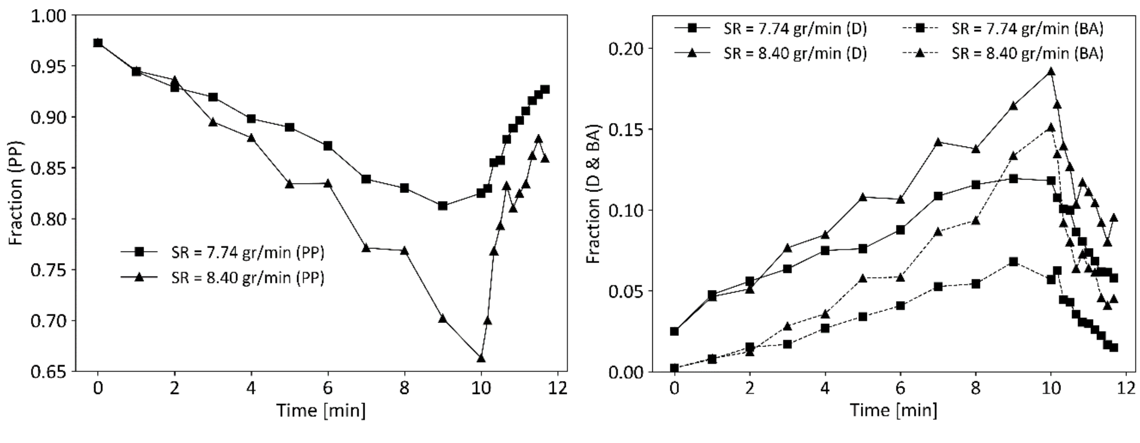

Figure 1: Influence of change in binder flow rate on the net agglomeration rate and breakage of primary particles (left figure), dimers (right figure, solid lines) and bigger agglomerates (right figure, dashed lines).

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Keywords: Spray Fluidized Bed, Agglomeration, Coating, Particle Characterization.

Anhaftungsverhalten trockener feiner Pulver in fluidisierten Systemen

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Feine Pulver neigen stark zur Anhaftungs- und Klumpenbildung. Selbst bei streng kontrollierten Umgebungsbedingungen und minimalen mechanischen Belastungen tritt dieses Problem weiterhin auf. Besonders ausgeprägt ist das Phänomen bei Partikeln kleiner als 100 µm, für die die Schwerkraft praktisch keine Rolle mehr spielt [1]. Wechselwirkungen zwischen Partikeln sowie zwischen Partikeln und Wandoberflächen führen zu Ablagerungen, die die Qualität und Sicherheit des Endprodukts beeinträchtigen und im Zeitverlauf Produktionsausfälle verursachen können [2 – 4]. Ein Beispiel für Caking in einem gasdurchströmten System zeigt Abb. 1 anhand einer Laborspiralstrahlmühle.

Abb. 1.: Caking von Lactose an unterschiedlichen Komponenten einer Laborspiralstrahlmühle.

Im Projekt „Fluid-Cake“ wird das Caking-Phänomen an fluidisierten Systemen untersucht. Für die praktische und schnelle Untersuchung des Anhaftungsverhaltens unterschiedlicher Pulver wurde ein Pulverversuchsstand konstruiert, in dem verschiedene Produkte direkt getestet werden können. Der Versuchsstand bietet den Vorteil, dass unterschiedliche Einflussfaktoren – wie Pulver- und Partikeleigenschaften, Wahl der Prozessparameter und Wandmaterialien – gemeinsam bewertet werden können. Während bisherige Untersuchungen die Abhängigkeit des Adhäsionsverhaltens von Wandmaterialien, Pulverbeladungen und gewählten Gasgeschwindigkeiten gezeigt haben, werden in aktuellen Studien zusätzlich der Einfluss von Pulvereintreffwinkeln, Beschichtungs-stoffen und Reinigungsansätzen sowie die Modifikation des Kohäsionsverhaltens durch den Einsatz flüssiger Additive untersucht. Parallel werden die Pulver- und Partikeleigenschaften charakterisiert und die relevanten Fluidisierungssysteme mittels CFD nachgebildet. Diese vielseitige Herangehensweise ermöglicht eine umfassende Analyse der Faktoren, die das Caking-Phänomen beeinflussen, und liefert praxisrelevante Empfehlungen für die Auswahl geeigneter Pulver und Prozessparameter bereits in der Planungsphase.

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Keywords: Pulver, Anhaftung, Caking, Wandmaterialien, Eintreffwinkeln, Additive.

Online characterization of structure of spray fluidized bed agglomerates

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Agglomeration is a fundamental industrial process for producing bulk materials from individual particles, fox examples in fine chemicals and foods. Spray fluidized bed agglomeration is a versatile technique Spray fluidized bed agglomeration is a versatile technique in which a liquid binding agent is sprayed onto fluidized particles to form agglomerates. The effective properties of products made from bulk materials depend heavily on the agglomerates' morphologies, e.g., the number of neighboring particles (agglomerate strength) or fractal dimension as a measure of accessible surface area (such as for later dissolution of the aggregated material in liquids). Thus, accurately characterizing and controlling these morphologies is essential to ensure high and consistent product quality.

Herein, we present a method of online characterization of spray agglomerate in a real-time environment. We established and quantified the workflow for online determination of spray agglomerates. The workflow is based on dynamic image analysis (DIA) of high speed image sequences. Characterization of the identified agglomerates was performed according to two sets of morphological descriptors, one set contained all information like area, area equivalent diameter, circularity, roundness, solidity and eccentricity to characterize size and shape of the object, leading to access of the multi-dimensional property distribution of spray agglomerates. Another set is one key morphological indicator describing the internal structure, 3D fractal dimension. It influences many usage properties such as mechanical strength or rehydration behavior through formation of specific intra-agglomerate pore space. A model based approach to inferentially obtaining information about 3D fractal dimension of agglomerates is presented [1]. This model utilizes high-detail but scarce offline information from X-ray microcomputed tomography for establishing and training an inferential relationship with online information that is easy and fast to obtain. Experiment studies were performed in a continuously operated pilot-scale spray fluidized bed. The process setup and experimental conditions for spray agglomeration are described in Ajalova et al. [2]. The results show clear observation of the rapid temporal evolution of agglomerate morphology under different process conditions with increasing time, which help to optimize the process operation, allow process control and will yield defined products.

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Keywords: agglomeration, image analysis, morphology, structure

Multiscale consistency for carbon nanostructures: bridging molecular mechanics and continuum modeling of solid materials

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Reliable modeling of the processes of dispersion of carbon nanotubes and their nanoaggregates in polymer resins, on which the strength and reliability of nanocomposites depend, is primarily determined by the correct choice of models for determining the properties of both the nanotubes themselves and the properties of representative continuum volumes of C-C covalent bonds. This work addresses the challenge of consistently transferring atomistic parameters of the covalent C–C bond into phenomenological material properties within the framework of continuum mechanics. The study focuses on determining the effective transverse diameter of the covalent C–C bond in carbon nanostructures. Classical models of the representative volume of a C–C bond based on the Euler–Bernoulli hypothesis exhibit violations of thermodynamic stability, manifested by non-physical values of the Poisson's ratio ($\nu > 0.5$). Thiese inconsistencies arise from neglecting shear deformation. The main attention in this work devoted to analyzing the dependence of the obtained parameter on the Poisson's ratio, as well as on the influence of interatomic stiffness constants. To overcome the limitations of classical models, an approach based on Timoshenko beam theory is introduced, which accounts for both bending and shear effects. This framework establishes energetically equivalent states between the phenomenologically defined representative volume and the corresponding atomic-scale C–C bond model. As a result, a sixth-order algebraic equation is derived, relating the effective bond diameter d, Poisson's ratio ν, and the force constants of molecular mechanics. The solution of this equation reveals the existence of a specific range of feasible values for the effective diameter and the corresponding range of Poisson's ratios, within which thermodynamic stability is maintained. Within this stability domain, macroscopic material parameters can be directly expressed in terms of atomistic force characteristics. It is shown that for Poisson's ratios lying within this range, the C–C bond diameter varies between d = 0.0839268 nm at ν = 0 and d = 0.0847 nm at ν = 0.5. Notably, these values are consistent with electron-density-based estimates of the C–C bond diameter, which vary from approximately 0.08 nm to 0.09 nm (Fig. 1). Therefore, the actual cross-sectional area is determined not by the atomic radius or tabulated parameters, but by the distribution of electron density that ensures the strength and stiffness of the bond. The proposed approach provides a rigorous and physically consistent basis for multiscale modeling of carbon nanostructures such as carbon nanotubes, graphene, and components made of nanomodified materials. Comparison of the obtained results with data reported by other authors demonstrates good agreement. Thus, for engineering calculations of nanostructures, such as nanotubes, it is recommended to use the effective C–C bond diameter d =0.0844 nm, which corresponds to a Poisson's ratio of ν=0.32.

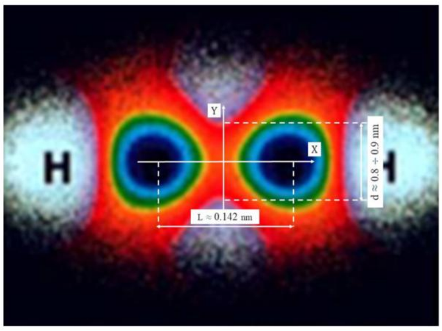

Figure 1. Two-dimensional moiré cross sections of the electron density distribution for the C_2H_2 molecule (extended Huckel method) [1]

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Keywords: carbon, covalent bond, electron density, molecular mechanics, structural mechanics.

Modelling of textiles in a rotating drum

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Textiles as part of a washing process performing motion as part of a rotating drum can be considered as a special and complex form of a bulk solid. Contrary to regular bulk solids, textiles are characterized by a planar geometry. Additionally, they are deformable and depending on the state of the washing process they are also part of a complex multiphase flow. These characteristics make process description of textiles in a rotating drum as part of e.g. a washing process difficult to address, which is different to other processes involving more regular bulk solids as part of e.g. granulation [1] or drying [2], where a much more sophisticated process understanding for drums prevails.

The aim of a recently started project is therefore to gain this understanding through a combined experimental and numerical approach. Textiles are firstly simulated in a drum rotating around a horizontal axis at different process conditions. Particular attention is paid to the realistic movement of the textiles and their interaction with water. The fluids air and water are modelled using the volume-of-fluid method (VOF) to represent a continuous flow field in which both phases move. The simulation is performed in ANSYS Fluent, which allows coupling with the institute's available DEM code.

The VOF method according to [3] is used to track the phase boundary, while curvature and capillary surface tension forces are calculated using the continuum surface force (CSF) model by [4]. Textiles prevailing in the drum are represented using a bonded particle model (BPM) within the discrete element method (DEM). Mechanical textile parameters are determined experimentally and then used to simulate the textile properties in the DEM. The characterization of textiles is based on the Kawabata Evaluation System for Fabrics (KES-F), which measures bending stiffness, shear strength and compressibility [5].

The contact forces between particles thus textiles are calculated using suitable DEM contact models. Alternative contact models commonly used in textile DEM simulations are also evaluated to improve the representation of interactions between textiles and between textiles and liquids. For the coupling of liquids and particles, especially in highly deformable or porous structures such as textiles, the extended CFD-DEM framework described by [6] is used. This framework improves the treatment of hydrodynamic forces, porosity effects and local resistance, thereby increasing the stability of multiphase simulations.

The simulation results are later validated using experimental data. Open questions concern the permeability and soaking behavior of textiles, the CFD-DEM coupling strategy, friction modelling in wet textiles, and the deformation of textiles under rotation.

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Keywords: Computational fluid dynamics (CFD), textiles, volume of fluid method (VOF), discrete element method (DEM)

Heißbrikettierung von direktreduziertem Eisen in Abhängigkeit des Kohlenstoffgehaltes und Metallisierungsgrads

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Die Stahlindustrie steht im Hinblick auf die Umsetzung der Ziele des Green Deal der Europäischen Union vor der Aufgabe einer massiven Einsparung der Treibhausgasemissionen. Im Jahr 2050 wird beabsichtigt, Stahl zu 100 % auf Basis von grünem Wasserstoff zu produzieren. Als Alternative zur Roheisengewinnung über die Hochofenroute gilt das Verfahren der Direktreduktion des Eisenerzes mit Wasserstoff. Dieses Verfahren stellt jedoch unter den derzeitigen Bedingungen hohe Anforderungen an die Qualität des eigesetzten Eisenerzes, was das überwiegend zur Verfügung stehende Eisenerz allerdings nur bedingt erfüllt. Zudem ist auch die Umstellung der Direktreduktion des Eisenerzes vom Reduktionsmittel Erdgas auf Wasserstoff mit einer Änderung des Kohlenstoffgehaltes im reduzierten Eisen verbunden.

Im Rahmen des durch den Research Fund for Coal and Steel (RFCS) der EU geförderten Projektes „HBI C-flex“ (Grant Agreement no. 101112479) forscht ein breites Konsortium aus Industrieunternehmen und zwei Universitäten, unter welchen Bedingungen auch aus Erzen minderer Qualität Eisen mit flexiblen Kohlenstoffgehalten von bis zu 0 % herstellbar ist. Neben der eigentlichen Direktreduktion kommt hierbei der Heißbrikettierung des direktreduzierten Eisens (DRI) in Form von DRI-Pellets eine entscheidende Bedeutung zu, um die Porosität der DRI-Pellets zu reduzieren und eine unkontrollierte Re-Oxidation, z. B. bei Lagerung und Transport, zu unterbinden. Nach der erfolgreichen Inbetriebnahme des Versuchsaufbaus zur Verarbeitung der Proben unter Stickstoffatmosphäre wurden im Projektrahmen DRI-Proben mit variablem Kohlenstoffgehalt und Metallisierungsgrad auf einer hydraulischen Laborstempelpresse bei Temperaturen von 600 °C bis 900 °C und Pressdrücken von 150 MPa bis 300 MPa brikettiert und damit die Versuchsdatenbasis kontinuierlich erweitert.

Durch die Steigerung des Pressdrucks und der Presstemperatur kann die Brikettqualität erwartungsgemäß gesteigert werden. Allerdings beeinflussen der Kohlenstoffgehalt und der Metallisierungsgrad maßgeblich die Brikettqualität: So führen eine höhere Metallisierung und ein höherer Kohlenstoffgehalt in der Regel zu einer höheren Brikettqualität. Anhand der vorliegenden Versuche wurde ein Regressionsmodell zur Beschreibung dieser Zusammenhänge aufgestellt. Parallel hierzu wurden Kraft-Weg-Daten zur Beschreibung des Verdichtungsverlaufes aufgenommen. In der Auswertung werden diese mit den Einflussgrößen des Agglomerationsprozesses und den Kennwerten der Brikettqualität in einen mathematischen Zusammenhang gebracht.

Schlagworte: Heißbrikettierung, Pressagglomeration, direktreduziertes Eisen
(**Keywords:** hot briquetting, press agglomeration, direct reduced iron)

Vom Batch- zum Kontiprozess: Gekühlte Ultraschalldispergierung von CNT verstärkten Epoxidharzen mit sensorischer Dispergiergradbewertung

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Die Dispergierung von Carbon Nanotubes (CNT) in hochviskosen Polymermatrizen stellt aufgrund starker Agglomerationstendenzen und der gleichzeitigen Empfindlichkeit der Polymermatrix gegenüber hohen mechanischen und thermischen Belastungen eine besondere verfahrenstechnische Herausforderung dar. Insbesondere ultraschallbasierte Dispergierverfahren ermöglichen einen hohen Energieeintrag, welche jedoch häufig zu einer Degradation der Polymermatrix führt [1].

Im Rahmen eines DFG-Forschungsprojekts wird ein neuartiger gekühlter Batch-Ultraschalldispergierungsprozess mit integrierter Durchflusszelle entwickelt, der eine intensive Dispergierung bei gleichzeitig kontrollierter thermischer Belastung erlaubt.

Das entwickelte Anlagendesign kombiniert eine ultraschallbasierte Dispergierung mit einer gezielten Kühlung der Dispergierzone. In Blindversuchen wurde das Epoxidharz mit spezifischen Energieeinträgen von bis zu 5 kJ/g belastet, ohne dass in mechanischen Zugversuchen an ausgehärteten Proben eine messbare Schädigung der Polymermatrix, bzw. eine Absenkung der Probenfestigkeit nachgewiesen werden konnte. Zur Bewertung des Dispergiergrads wird ein angepasster Inline-Sensor auf Basis der statistischen Extinktion (SE) eingesetzt.

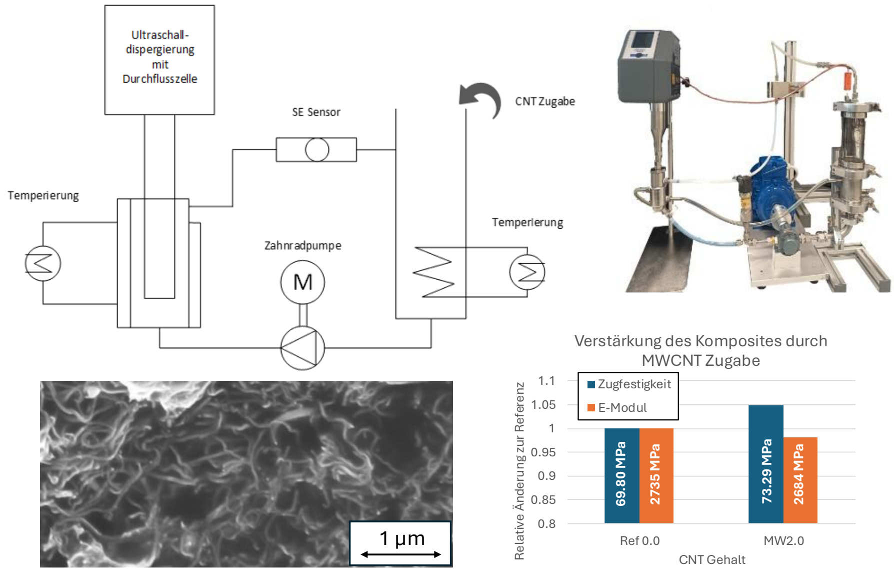

Abb. 1: Anlagendesign, REM-Aufnahme einer disperg. Probe und ermittelte Zugfestigkeit.

Zur Einordnung und Validierung der sensorisch erfassten Dispergiergrade werden ergänzend rheologische Untersuchungen durchgeführt, um den Zusammenhang zwischen Dispergierzustand und Fließverhalten der CNT-Epoxidharz-Suspensionen zu analysieren. Auf Basis rheologischer Kennwerte wie Scherverdünnung und Fließgrenze wird ein Abgleich mit dem mittels statistischer Extinktion bestimmten Dispergiergrad angestrebt, wie er auch in der Literatur zur Charakterisierung von CNT-Dispersionen beschrieben wird [2]. Darüber hinaus wird der Zusammenhang zwischen Dispergierzustand und den mechanischen Endfestigkeiten ausgehärteter CNT-Epoxidharz-Proben untersucht.

Die experimentellen Untersuchungen werden durch numerische Modellierungen zur Schädigung von CNT-verstärkten Kompositen auf der Mikroskala in einer weiteren Arbeit von O. Hondliakh ergänzt [3]. Aufbauend auf den gewonnenen Erkenntnissen ist es das Ziel, das vorgestellte Batch-Ultraschalldispergierverfahren perspektivisch zu einem kontinuierlichen Prozess weiterzuentwickeln.

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Keywords: Ultraschalldispergierung, Kohlenstoffnanoröhrchen-Komposite, Anlagendesign, Rheologie, Statistische Extinktion

Influence of compression kinetics on data quality for material deformation characterization

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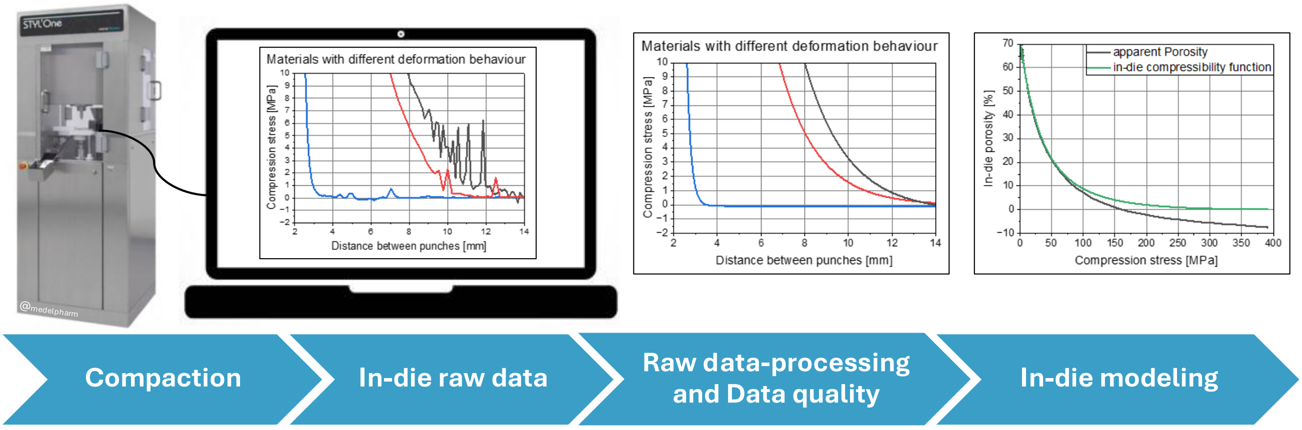
In the manufacturing of pharmaceutical tablets, it is fundamental to precisely meet critical quality attributes, such as tablet strength, disintegration time and release kinetics, which are often influenced by process parameters like the compression stress or compression speed. An increased compression speed affects the material-process-property relationship. The speed of loading and unloading as well as the duration of maximum loading, also referred to as 'dwell time', may influence the deformation behaviour of pharmaceutical materials based on their physicochemical nature. Such compression kinetics-dependent deformation properties may be introduced to the formulation by a kinetics-sensitive active pharmaceutical ingredient and create a conflict of objectives with economic production on rotary presses. As a result, high compression speeds may lead to impaired product quality or destructive defects like capping and delamination.

In this study, materials with different kinetic dependence were compressed on a compaction simulator emulating a production press at different compression speeds. Increasing compression kinetics can result in artefacts due to the construction of the compaction simulator and can disturb and distort the measurement signals. It is therefore advantageous to identify the extent and origin of the artefacts and to develop a method for optimization of the analytical quality of the characteristic material deformation parameter. The focus of this study is on the advancement of in-die compression data of the compaction simulator. The aim is to systematically evaluate the resulting deformation behaviour of different pharmaceutical materials, as well as the occurrence of signal noise and artefacts. For this purpose, different pharmaceutical materials are processed with different compression parameters to acquire in-die compression raw data. The raw data is analyzed for signal noise and artefacts, and optimized with some post-processing procedures. This in-die compression data is further modeled according to the in-die compression function [1] for the compression and decompression phase, finally, to obtain the characteristic in-die compression parameters, e.g. specific tablet energy, in-die elastic recovery, with improved analytical quality.



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Keywords: Powder compaction, compression speed, deformation behaviour, signal noise, compressibility modeling

Dyssol: A tool for dynamic flowsheet simulation for complex solids processes

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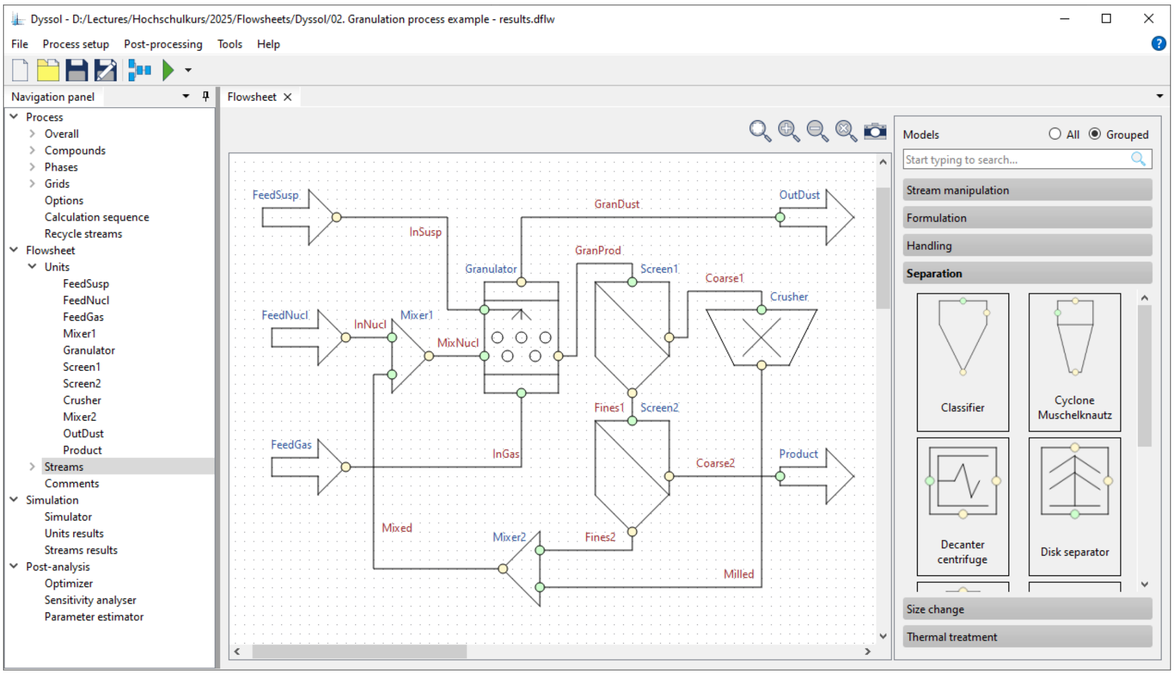
Dynamic modeling of interconnected solids processes is an important yet still underrepresented topic in process engineering. Traditional approaches often struggle to capture the complex dynamics of solids processing, as they must account for distributed material properties such as particle size, porosity, and moisture content, all of which are critical for industrial applications. Dyssol [1], an open-source environment for dynamic flowsheet modeling, was developed to address these challenges. It integrates advanced algorithms and numerical methods to enable the simulation of granular solids and their dynamic behavior.

Dyssol's unique capabilities include support for both dynamic and steady-state models, multidimensional distributed solid properties, and an extensible library of unit-operation models. To ensure maximum flexibility and applicability, the framework employs a sequential-modular calculation approach. This allows users to integrate new heterogeneous models of virtually any complexity and to combine a variety of algorithms and numerical methods – from differential equations to data-driven techniques [2]. As a result, the simulation environment has proven applicable to a wide range of processes, including agglomeration, granulation, crystallization, drying [3], chemical looping combustion, battery recycling, minerals grinding, ceramic-tile production [4], and zeolite synthesis [2].



Modeling the granulation process in DyssolPro

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Keywords: Flowsheet simulation, Distributed parameters, Dyssol.

Einfluss der Rührflügelgeometrie auf die Matrizenfüllung in Rundlauftablettenpressen

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Die Matrizenfüllung ist einer der entscheidenden Prozessschritte bei der Tablettierung, da sie unmittelbar die Tablettenmasse und damit zentrale Qualitätsmerkmale wie Wirkstoffgehalt und Festigkeit bestimmt. Für die Pulverbereitstellung im Füllschuh sind die Rührflügel verantwortlich, deren Bewegung und Geometrie maßgeblich beeinflussen, wie das Pulver oberhalb der Matrizenfüllung verteilt und transportiert wird. Die Geometrie der Rührflügel kann bzgl. mehrerer Parameter variiert werden, beispielsweise in der Speichenhöhe, dem Anstellwinkel oder durch das Anbringen einer Fase an der Unterseite (vgl. Abbildung 1). Diese Konstruktionsmerkmale bestimmen die Art und Intensität der Kräfte, die auf das Pulver einwirken, und beeinflussen dadurch die Ausbildung unterschiedlicher Zonen mit variierender Pulverdichte. Zur Untersuchung dieser geometrischen Einflüsse wurden 3D-gedruckte Rührflügel verwendet, an denen schrittweise die genannten Konstruktionsmerkmale variiert wurden. Es konnte gezeigt werden, dass die Wahl der Rührflügelgeometrie sowohl den absoluten Pulvervolumenstrom in die Matrize beeinflusst als auch dessen Schwankung. Aufbauend auf bestehenden Modellansätzen zur Beschreibung der Volumenströme bei unvollständiger Matrizenfüllung [1, 2, 3] werden die gefundenen Zusammenhänge zwischen Rührflügelgeometrien, Pulvereigenschaften und den resultierenden Füllergebnissen systematisch analysiert. Zusätzlich wird die Tablettenpressen bei verschiedenen Prozessparametern (Matrizentisch- und Rührflügeldrehzahl) untersucht. Neben den Volumenströmen wird auch der Einfluss der Rührflügelgeometrie auf die Schwankungen der Tablettenmassen untersucht, da diese direkt mit einer gleichbleibenden Produktqualität verknüpft sind. Ziel der Untersuchungen ist ebenfalls eine modellhafte Beschreibung der Einflüsse der Rührflügelgeometrien. Dabei ist vor allem die Entwicklung der Schwankungen mit variierenden Prozessparametern interessant, um Aussagen über die Robustheit eines Setups gegenüber Änderungen in der Produktionsgeschwindigkeit und der zu verpressenden Formulierung zu treffen. Die Ergebnisse liefern ein besseres Verständnis der geometrischen Einflussgrößen auf die auf das Pulver ausgeübten Kräfte sowie die resultierende Matrizenfüllung und tragen dazu bei, Rührflügel gezielter auszulegen und Füllprozesse stabiler zu gestalten. Die Integration von konstruktiven Parametern in bestehende Modellansätze bietet dabei die Möglichkeit, für eine bestimmte Kombination aus Rührflügelgeometrie, Tablettiermasse und Produktionsgeschwindigkeit ein erwartbares Füllergebnis zu berechnen. Dadurch kann der Schritt der Matrizenfüllung besser kontrolliert und Tablettierprozesse effizienter ausgelegt werden.

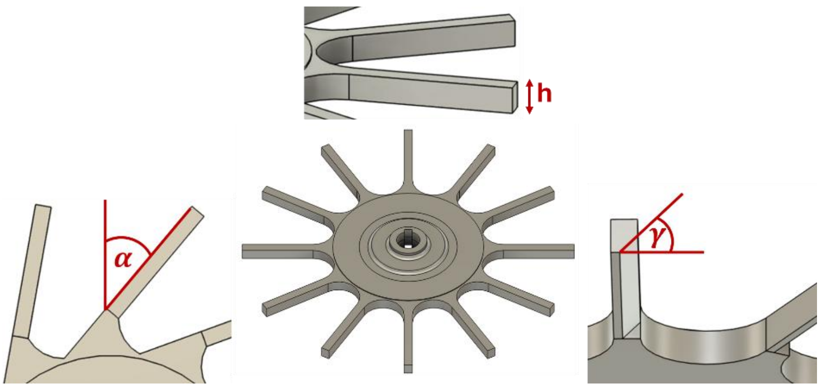

Abbildung 1: Untersuchte Variationen der Rührflügelgeometrie

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Keywords: Rührflügelgeometrie, Matrizenfüllung, Massenschwankungen, Pulverbewegung

Data-Driven Densification Modelling of Aluminosilicate Powder Mixtures

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Sintering of ceramic powders is a key operation in bulk solids processing, in which the governing of coupled evolution of microstructure, reaction kinetics as well as thermal and mass transport take place in the same time-scale. Since the sintering for white-tile and aluminosilicate part manufacturing process is necessary at temperatures near the on-set temperatures of the least melting component, they belong to one of the most energy and CO_2-intensive operations in their processing lines. Therefore, it's important to accurately model the process at various length-scales. Although there has been a breakthrough in simulating its macroscopic process, the nature of its microscale effects and densification activation has not been studied in-depth [1]. While recent in-situ studies have revealed sintering phenomena in heterogeneous powder mixtures, they remain descriptive and do not deliver transferable densification laws suitable for process design [2].

In this contribution, a data-driven approach is presented that derives densification laws directly from quantifiable in-situ experimental data. Environmental scanning electron microscopy (ESEM) sintering micrographs are analyzed to extract quantitative descriptors of neck growth, particle rearrangement and pore closure, which are synchronized with coupled mass spectrometry (MS) and ex-situ differential scanning calorimetry and thermogravimetry (DSC-TGA) signals to capture thermally activated events and gas-evolution processes at different heat-up and isothermal protocols. This work demonstrates a tentative pathway to propose new simulation-ready densification models forming for future multi-stage simulations of liquid phase sintering.

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Keywords: Liquid Phase sintering; Densification modelling; Machine learning; In-situ characterization; Bulk solids processing

Simulation-guided segregation reduction in a pharmaceutical batch powder blending process

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Achieving homogeneous blends of active pharmaceutical ingredients (APIs) and excipients is critical in tablet manufacturing to ensure consistent dosage and robust powder processability. Traditionally, the development and scale-up of powder blending operations rely on expensive, labor-intensive experimental trials that provide limited insight into blending dynamics. Discrete Element Method (DEM) simulations offer deeper process understanding and can significantly reduce experimental effort and cost.

In this study, DEM simulations were used to investigate the blending dynamics of two APIs and various excipients in an industrial-scale bin blender. Powder components were experimentally characterized using dynamic angle of repose tests, and the results were used to calibrate DEM parameters for three modeled powder components. Simulations of a 25-minute blending operation, comprising a 20-minute pre-blending stage and a 5-minute final blending step, revealed axial concentration gradients of the APIs. Experimental validation through targeted sampling and HPLC analyses confirmed these simulation predictions.

The DEM model was then applied to evaluate strategies to mitigate these API gradients. A 90° reorientation of the blending container around the vertical axis prior to the final blending step notably improved axial homogeneity. This approach effectively reduced inhomogeneity with minimal engineering modifications and could be further refined to substantially decrease overall blending time.

These findings demonstrate the effectiveness of calibrated DEM simulations as tools for the design and optimization of pharmaceutical blending processes. The simulation-based methodology provides a robust framework for identifying process risks and evaluating mitigation strategies, enabling faster, more efficient process development while reducing reliance on costly experimental work.

Keywords: discrete element method, powder blending, powder characterization, segregation risk

Fachgruppe Computational Fluid Dynamics:

Vorträge und Poster

Modellierung der Strömungsvorgänge in Rotor-Stator Mischern mit Physics-Informed Neural Networks (PINNs) ohne Verwendung von Trainingsdaten

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Inline-Mehrstufen-Rotor-Stator-Mischer (RSMs) haben sich als industrielle Lösung etabliert, um hochviskose Flüssigkeiten schnell und effizient zu mischen und gleichzeitig den Temperaturanstieg während des Prozesses zu minimieren. Im Gegensatz zu herkömmlichen Chargenmischern, die in diskreten Batches arbeiten, ermöglichen RSMs einen kontinuierlichen Betrieb, was zu verbesserten Produktionsraten und Mischeffizienzen führt. Die Herausforderung beim Mischen hochviskoser Flüssigkeiten liegt in ihrer Neigung, laminare Strömungsregime beizubehalten, was die Mischrate zusätzlich begrenzt. Die Mehrheit der bisherigen Studien verwendet zur Modellierung der Phasenverteilung und des Mischprozesses Computational Fluid Dynamics (CFD) Verfahren, die jedoch anfällig für numerische Diffusion sind. Dies kann zu einer Überschätzung der Mischeffizienz führen. Deshalb wird ein Modell vorgestellt, das auf Physics Informed Neural Networks (PINNs) [1] basiert und als alternative Lösung zu herkömmlichen Computational Fluid-Dynamics (CFD) Methoden vorgeschlagen wird. Das einzigartige Merkmal von PINNs im Vergleich zu anderen maschinellen Lernansätzen liegt in ihrer Fähigkeit, physikalische Gleichungen – wie die Navier-Stokes-Gleichungen – direkt in ihre Verlustfunktionen zu integrieren und somit auf die Verwendung von Testdaten verzichtet werden kann. Im Vergleich zu herkömmlichen CFD-Methoden, wie der Finite-Volumen-Methode, verwenden PINNs netzfreie Approximationen mit kontinuierlichen Funktionen. Dadurch entfällt die Notwendigkeit iterativer Lösungen auf diskretisierten Gittern, und numerische Diffusion wird vermieden. Ein trainiertes PINN-Modell wird verwendet, um die Strömung durch einen Standard-Rotor-Stator-Mischer zu simulieren. Die PINN-Vorhersagen zeigen eine gute Übereinstimmung hinsichtlich Druckverlust- und Drehmomentberechnung mit Literaturdaten [2] und werden im Detail diskutiert. (siehe Abb. 1).

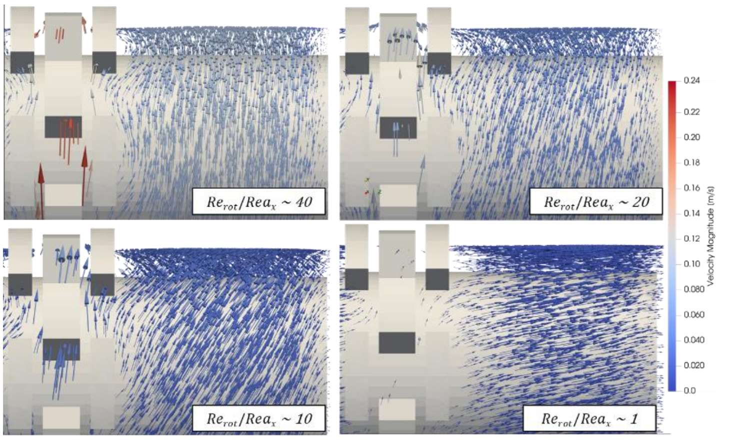

Abb. 1: Effekt der Reynolds-Zahlen für die axiale und rotatorische Bewegung auf das Strömungsfeld

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Keywords: Rotor-Stator Mischer, Physics Informed Neural Networks (PINN), Machine Learning (ML)

An octree-based sampling algorithm for processing big simulation data

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Increasing computational resources led to a wide spread of applying machine learning (ML) techniques in computational fluid dynamics (CFD), e.g., for data analysis or optimization [1]. However, ML techniques require typically pre-processing of the fluid flow data, which is memory-intensive when dealing with scale-resolved simulations and sequences of flow fields. While most pre-processing techniques involve an interpolation step of the flow data onto a structured grid [2], this approach is associated with a lower achievable compression ratio, and might fail to capture essential flow physics. The present work introduces an improved Sparse Spatial Sampling (S^3) algorithm [3] for data reduction in flow simulations. S^3 iteratively generates an octree grid based on a user-defined metric field, efficiently down-sampling the data while preserving key features of the metric. The sampled grid enables efficient post-processing and memory-intensive tasks, such as the singular value decomposition of snapshot matrices. The enhanced S^3 is evaluated on scale-resolving simulations of transonic flow past tandem airfoils, incompressible flow past a circular cylinder, and flow around an aircraft half-model. In all cases, S^3 substantially reduces cell count while preserving the dominant flow dynamics. The S^3 source code and examples are publicly available on GitHub [4].

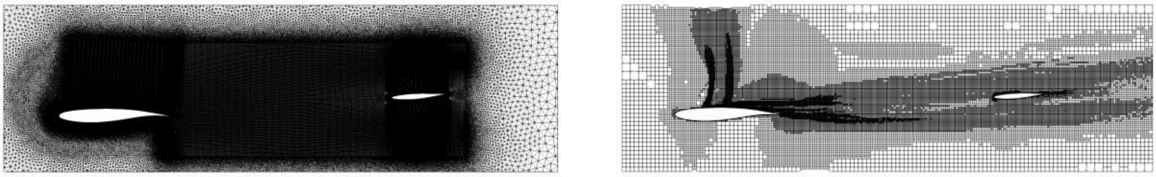

Figure 1: The left figure depicts the original grid from the simulation conducted by [4]. The right figure shows the grid generated by S^3. The grid was created based on the temporal standard deviation of the local Mach number field from CFD and captures 75% of the metric, while reducing the mesh size by 76.2% compared to the original grid.

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Keywords: big simulation data, mesh sampling, post-processing, modal analysis

ML-assisted CFD of compressible multiphase phase-change flows

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Modelling thermal phase change in multiphase flows is inherently challenging due to the strong coupling of heat and mass transfer, the nonlinear behaviour of phase transition, pressure- and temperature-dependent thermophysical properties, and the complex dynamic evolution of the liquid–vapor interface. Thermal phase-change simulations in OpenFOAM are commonly performed using *interThermalPhaseChangeFoam*, a two-phase VOF solver. However, this solver assumes constant material properties and accounts for compressibility only through phase change. These simplifications limit the predictive capability for heat-transfer rates in condensing and boiling flows, especially across wide thermodynamic ranges where variations in material properties strongly influence interfacial dynamics and phase-change characteristics.

To overcome these limitations and accurately capture heat and mass transfer in compressible boiling and condensing flows, we extend the capabilities of *compressibleInterFoam* to model thermal phase change with fully variable thermophysical properties, removing the need for an explicit equation-of-state closure. Temperature- and pressure-dependent polynomial expressions for specific heat, density, and viscosity are developed using data from the CoolProp library, an open-source thermophysical database. An enthalpy-based formulation of the energy equation is employed to improve model robustness; however, iteratively computing temperature from enthalpy using Newton's method becomes computationally expensive when properties vary with both temperature and pressure. To alleviate this bottleneck, we develop a machine-learning-based temperature prediction framework using artificial neural networks trained on extensive CoolProp thermodynamic datasets.

The neural network models are developed and trained in PyTorch. The model uses enthalpy, phase fraction, and pressure from the conservation-equation fields as inputs to predict temperature with a target accuracy of ±1 °C. The number of hidden layers and neurons is determined using a random search algorithm. Mean-square error is used as the loss function during training and validation, while maximum absolute error is adopted as the performance criterion for selecting the deployment model. The trained networks are integrated into OpenFOAM using ONNX Runtime, an open-source, cross-platform inference engine that enables fast and efficient data exchange during simulations. Figure 1 illustrates the overall framework. This study demonstrates a hybrid data-driven and physics-based modelling approach in OpenFOAM by leveraging machine learning to achieve accurate temperature-field prediction in thermally driven phase-change processes in compressible multiphase flows.

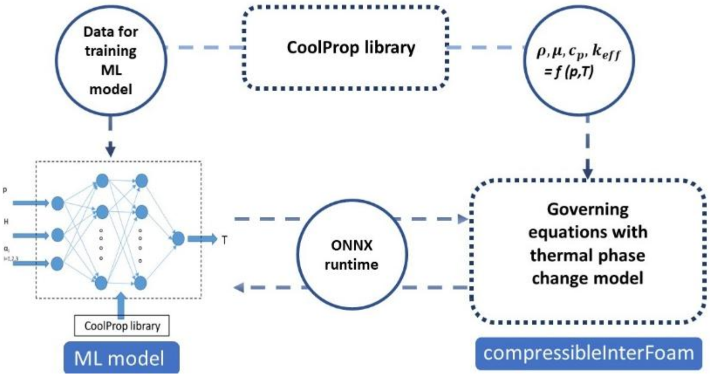

Figure 1: Newly developed framework for modelling compressible multiphase flows with phase change

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Keywords: CFD, Phase change, multiphase, machine learning, compressible flows.

Optimization of VoF-LPT coupling parameters

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The Volume-of-Fluid (VoF) method is a well-established and widely accepted approach for the simulation of primary atomization and liquid breakup processes. In particular, VoF-based simulations are indispensable for resolving the early stages of breakup, where complex interfacial dynamics, ligament formation, and droplet detachment govern the resulting spray characteristics. However, as the liquid structures fragment into increasingly smaller droplets and ligaments, the computational cost of VoF simulations rises dramatically. Performing fully resolved VoF simulations of an entire spray is therefore prohibitively expensive for most practical, industrially relevant applications.

A promising strategy to alleviate this limitation is the coupling of VoF with a Lagrangian Particle Tracking (LPT) approach. In such VoF-LPT frameworks, small, nearly spherical liquid structures that are expensive to resolve in VoF are converted into Lagrangian droplets, which can be modeled at significantly lower computational cost. One of the foundational contributions in this area is the work by Heinrich & Schwarze [1], where the coupling decision is based on droplet size and sphericity criteria. This framework has since been successfully applied in other industrially relevant applications, such as a swirl atomizer [2]. In practice, coupling parameters are usually chosen based on user experience and case-specific considerations, leading to frequent hyperparameter optimization and poor generalization.

The objective of this work is twofold: first, to systematically quantify the benefit of VoF-LPT simulations in comparison to fully resolved VoF reference simulations; and second, to establish a more rigorous and transferable methodology for determining VoF–LPT coupling parameters. To this end, a pure VoF simulation is used as a high-fidelity reference. Building upon this baseline, Bayesian optimization (similar to [3]) is employed to explore and quantify the trade-off between simulation accuracy and computational cost in VoF-LPT simulations. The proposed approach aims to provide objective guidance for coupling parameter selection and to enable more efficient spray simulations without compromising predictive accuracy.

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Keywords: Optimization, Volume of Fluid, Lagrangian Particle Tracking, seamless VOF-LPT Coupling

Echtzeit-Vorhersage von Suspensionszuständen in gerührten Reaktoren mittels eines datengetriebenen, CFD-basierten Reduced Order Model

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Die präzise Kenntnis und Kontrolle von Suspensionszuständen sind in vielen chemischen und pharmazeutischen Prozessen entscheidend für Produktqualität, Effizienz und Betriebssicherheit. Angesichts der inhärenten Komplexität mehrphasiger Strömungen in Reaktoren sind konventionelle Echtzeit-Überwachungsmethoden oft unzureichend. Diese Arbeit stellt einen innovativen, datengetriebenen Ansatz zur Echtzeit-Vorhersage von Suspensionszuständen vor.

Umfassende, hochauflösende Upfront-CFD-Simulationen wurden durchgeführt, um die komplexen Strömungs- und Suspensionsdynamiken über einen breiten Bereich relevanter Betriebsparameter (z.B. Rührergeschwindigkeit, Feststoffanteil, Fluideigenschaften) detailliert zu erfassen. Die daraus generierten Daten bildeten die Grundlage für die Entwicklung eines Reduced Order Models (ROM). Dieses ROM wurde darauf trainiert, Suspensionszustände akkurat aus minimalen Sensordaten, insbesondere einzelnen Drucksignalen aus dem Reaktor, vorherzusagen.

Das entwickelte ROM zeigte eine hohe Vorhersagegenauigkeit über den gesamten untersuchten Parameterraum. Seine Robustheit und Zuverlässigkeit wurden durch eine umfassende Validierung mit experimentellen Daten bestätigt. Dank der geringen Rechenkosten ermöglicht das ROM den effizienten Einsatz auf Edge-Geräten, wodurch eine kontinuierliche und präzise Überwachung des Suspensionszustands im laufenden Betrieb realisiert wird. Dieser Ansatz bietet ein leistungsstarkes Werkzeug zur Optimierung der Prozessführung, zur frühzeitigen Erkennung von Abweichungen und zur Erhöhung der Betriebssicherheit in der chemischen Verfahrenstechnik. Die Integration von CFD, ROM und Edge Computing ebnet somit den Weg für intelligentere und autonomere Prozessüberwachung in der Industrie.

Keywords: Feststoffsuspension, CFD, ROM, gerührtes System,

How Coarse Graining Affects Mixing and Segregation in Granular Flows:

A Systematic CFD–DEM Study

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Mixing and segregation phenomena play a crucial role in a wide range of process engineering applications, and accurate predictions of these mechanisms are essential for reliable reactor design. CFD combined with DEM is a well-established approach to model granular systems, since it resolves particle level contact dynamics as well as fluid-particle interaction. However, the computational cost of CFD-DEM simulations is extremely high, which restricts their application to laboratory scale reactors with a limited number of particles. To overcome this limitation, coarse-grain CFD-DEM methods have become increasingly popular [1]. In these approaches, groups of physical particles are represented by larger so-called grains, which significantly reduces the computational effort and allows the investigation of industrial scale systems within practical time frames. The coarse grain procedure, however, changes important physical mechanisms such as particle inertia, collision frequency and gas-solid coupling. This creates an open question regarding the accuracy of predicted mixing and segregation behavior.

The present study provides a systematic evaluation of coarse-grain CFD-DEM for different classes of granular systems [2]. In the first part, a bidisperse mechanically agitated system is examined to assess the representation of mixing and segregation in a contact dominated system. In the second part, a bidisperse fluidized bed is analyzed with varying particle size ratios and gas velocities in order to study gas-driven mixing and segregation phenomena. In the final part, a large-scale polydisperse fluidized bed is investigated by comparing a monodisperse coarse-grain representation with a polydisperse coarse-grain representation. Two widely used coarse grain procedures are evaluated across all systems and complemented by system specific fine-tuning strategies.

Across all investigated systems, the results reveal clear limits and characteristic trends of the coarse-grain approach. In the mechanically agitated system, the predicted segregation depends strongly on the chosen strategy. Scaling with a constant coarse-grain factor amplifies the upward motion of large particles and strengthens the Brazil Nut effect, whereas scaling with a fixed grain diameter results in weaker segregation. In the bidisperse fluidized bed, the suitability of each strategy is closely linked to the particle size ratio and gas velocity. At low diameter ratios, scaling with a constant grain diameter reproduces mixing and segregation more accurately, while the differences between strategies diminish as particle sizes become more similar. In the large scale polydisperse fluidized bed, the coarse-grain procedure affects overall particle dynamics, and the simulations show that additional system specific adjustments are required to maintain realistic behavior. Overall, the study identifies the main error sources introduced by coarse graining and provides practical guidance on how coarse-grain CFD-DEM can be applied reliably to predict mixing and segregation in granular systems.

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Keywords: Coarse-grained CFD-DEM, Granular mixing, Segregation, Fluidized beds, Multiphase flow

A Morphology-adaptive Euler-Euler method: Recent developments and applications

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Industrial gas-liquid flows are characterized by a wide range of spatial and temporal scales, making their simulation particularly challenging. Traditionally, specific flow regimes are modeled using dedicated methods, each defined by how interfaces are represented and resolved. However, industrial-scale simulations demand a unified framework capable of flexibly switching between these methods to accurately capture the cross-scale nature of multiphase flows. To address this, a morphology-adaptive Euler-Euler model - *MultiMorph* - has been developed at HZDR. This hybrid approach enables the simultaneous treatment of different flow morphologies, with a dedicated phase for each morphology associated to a physical phase, and transfer models accounting for interactions and transitions between them. For instance, dispersed bubbles can coalesce, grow, or enter refined mesh regions, triggering a transition to a continuous representation. Conversely, when mesh coarsening occurs or large structures fragment into smaller, unresolved structures, a transition from a continuous to a dispersed representation takes place. The model also incorporates a class-method-based approach for tracking large numbers of dispersed bubbles or droplets, providing detailed information on size distributions. Recent advancements have refined the treatment of under-resolved structures, improved the mechanisms for morphology transitions, and demonstrated the feasibility of including a two-dimensional morphology.

The number of impressive applications of *MultiMorph* is increasing, e.g., rotating packed beds modelled by TU Berlin, or the gas separator region of an ebullated bed hydroprocessor by the University of Ottawa. Our recent developments are focused on the simulation of stirred tanks, which are common in the chemical and mineral industries. Achieving a reliable simulation is challenging due to the complexity of rotating flows and gas-liquid interactions. Within the Helmholtz-funded HPC-Gateway initiative, a semi-implicit phase-transport method was implemented by the core developers at OpenFOAM Foundation, allowing stable simulation at large Courant numbers. *MultiMorph* ensures a consistent free-surface behavior and adaptive morphology transitions, e.g., the formation of gas pockets in impeller wakes. Additionally, *MultiMorph* is implemented within the OpenFOAM Foundation's software, emphasizing sustainable research and modern IT practices. Both the source code, [1] and a comprehensive suite of validation and application cases, [2] are publicly available. The proposed contribution will give a comprehensive overview about *MultiMorph*, recent developments and applications.

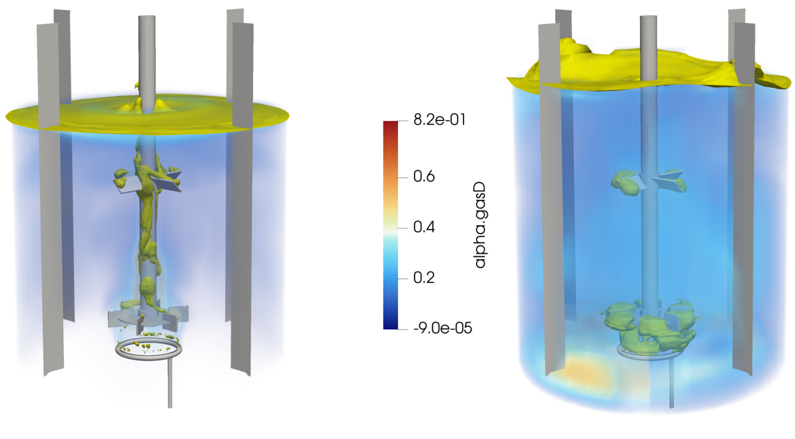

Figure 1: Simulation of an aerated stirred tank operating in the flooding (left) and full recirculation (right) regime.

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Keywords: Numerical Simulation, Multiphase Flow, Morphology Transitions, Industrial Application

Berechnung von Feststoff-Gas-Strömungen mit CFD- und CFD-DEM gekoppelten Simulationen in Wirbelschicht und pneumatischer Förderung

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Die numerische Analyse von Feststoff-Gas-Mehrphasenströmungen stellt eine zentrale Herausforderung in zahlreichen verfahrenstechnischen Anwendungen dar, da das dynamische Verhalten dispergierter Partikel stark von komplexen Wechselwirkungen zwischen Feststoffphase und umgebender Gasströmung geprägt ist [1]. Feststoff-Gas-Strömungen können numerisch entweder vollständig kontinuierlich mittels Euler-Euler-Methodik oder als partikelaufgelöste Systeme in gekoppelten CFD-DEM-Simulationen beschrieben werden. Während die Kontinuumsmodellierung große Anlagen effizient abbildet [2], ermöglicht die CFD-DEM-Kopplung eine detaillierte Erfassung der partikelinduzierten Mikrostruktur und Kontaktmechanik [3].

Im Rahmen dieser Arbeit wurden unterschiedliche Methoden der Simulation von Feststoff-Gas-Strömungen untersucht und miteinander verglichen. Dabei wurden ein kontinuierlicher und ein diskreter Ansatz für die feste Phase betrachtet. Beim diskreten Ansatz kann die Kopplung der DEM Simulation an die CFD-Software (siehe Abbildung 1) entweder so gestaltet werden, dass innerhalb der CFD-Software eine Einphasenströmung oder eine Zweiphasenströmung gelöst wird [4]. Diese Varianten wurden für die CFD-DEM Kopplung mit dem open source Strömungslöser OpenFOAM und dem kommerziellen Strömungslöser Ansys Fluent umgesetzt. Als technische Anwendungsbeispiele wurden eine Wirbelschicht und eine pneumatische Förderung betrachtet, wobei die Simulationsergebnisse jeweils mit experimentellen Ergebnissen aus der Literatur verglichen wurden.

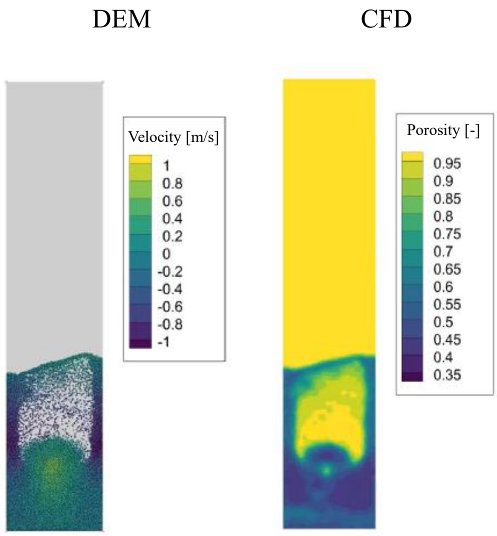

Abbildung 1: Kopplung der diskreten Partikelphase mit der kontinuierlichen Gasphase bei einer Wirbelschicht

Bei beiden Anwendungsfällen werden die Druckverluste im System im zeitlichen Verlauf und zeitlichen Mittel ausgewertet. Die mittlere Partikelhöhe innerhalb einer Wirbelschicht ist ein wichtiges Maß für die Fluidisierung des Feststoffs. Aus diesem Grund werden bei den Wirbelschichtsimulationen auch die mittleren Partikelhöhen ausgewertet. Die Ergebnisse zeigen Unterschiede und Gemeinsamkeiten der Kopplungsmethoden sowie den Einfluss der verwendeten CFD-Software. Damit kann analysiert werden, ob die Verwendung einer lizenzfrei verfügbaren CFD-Software eine vergleichbare Alternative zu kommerziellen Codes für die Berechnung von Feststoff-Gas-Strömungen darstellt oder diese kommerzielle Software sogar übertreffen kann.

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Keywords: Gas-Feststoff-Strömung, CFD-DEM, Kopplungsmethoden, Wirbelschicht, pneumatische Förderung

Consistency and Convergence in Two-Way Coupled Euler–Lagrange Frameworks

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Euler–Lagrange (EL) and CFD/DEM simulations have become indispensable tools for predicting particle-laden flows across a wide range of industrial and environmental applications. Their popularity stems from the ability to track millions of particles at a manageable computational cost, while coupling them to a continuum description of the carrier phase. However, despite decades of development and widespread use, there is growing evidence that two-way and four-way coupled EL simulations suffer from a fundamental lack of numerical consistency, most notably a strong dependence on the underlying fluid mesh resolution. In many practically relevant regimes, this mesh dependence leads to systematic errors in the predicted hydrodynamic forces and particle dynamics, even when widely accepted best-practice guidelines are followed [1,2].

Recent work has demonstrated that the root cause of this problem lies in the way momentum exchange between particles and fluid is modeled [1]. In classical particle-source-in-cell (PSIC) formulations, hydrodynamic forces are evaluated using the locally available (disturbed) fluid velocity field and subsequently fed back to the fluid as singular or weakly regularised source terms. As a consequence, particles interact with a flow field that already contains their own self-induced disturbance. This error grows with the ratio of particle diameter to mesh spacing and does not vanish under mesh refinement in the conventional sense, rendering the method formally non-convergent. Even for particle sizes an order of magnitude smaller than the grid spacing, errors in drag prediction of order 10% have been shown to persist across a wide range of Reynolds numbers [2]. These findings imply that many existing two-way and four-way coupled EL and CFD/DEM simulations may yield qualitatively plausible but quantitatively incorrect predictions, particularly in regimes where particle feedback plays a dominant role. The presentation argues that incremental fixes, such as ad-hoc smoothing, kernel spreading, or simple undisturbed-velocity reconstruction, are insufficient to resolve the issue at its core.

Instead, two consistent pathways forward are proposed. The first pathway is to adopt a fully volume-filtered Euler–Lagrange framework, in which the governing equations are derived by filtering the Navier–Stokes equations from the outset. In this setting, hydrodynamic force closures, such as drag, are formulated in terms of filtered fluid quantities and an explicit filter length scale, rather than mesh-dependent local velocities. This approach removes the ambiguity associated with undisturbed velocity estimation and yields force models that are independent of the fluid grid resolution [3].

The second pathway builds on a microstructure-informed force framework, in which particle–particle arrangements are explicitly accounted for through descriptors derived from Voronoi tessellations and related measures. Force models derived from particle-resolved DNS demonstrate that both the ensemble-averaged drag and its fluctuations depend strongly on local microstructure, an effect that cannot be captured by conventional isotropic drag closures. Incorporating this information provides a route towards mesh-independent and physically grounded force models suitable for dense and moderately dense flows [4].

Together, these approaches suggest a necessary paradigm shift: away from mesh-dependent point-force formulations, and towards filtered and microstructure-aware EL frameworks that restore physical consistency and predictive reliability in particle-laden flow simulations.

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Keywords: Euler–Lagrange simulations, CFD–DEM coupling, Particle-source-in-cell (PSIC), Volume-filtered Euler–Lagrange framework, Filtered drag models, Microstructure-informed force models

Eisen als Energieträger – CFD-Simulationen der Eisenpulververbrennung

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In den letzten Jahren sind Metallpulver als alternative Energieträger mehr und mehr in den Fokus gerückt. Metalle können verbrannt werden, um Wärme zu erzeugen, und die daraus entstehende Metalloxide können mit erneuerbarer Energie, in Form von grünem Wasserstoff, zurück in Metalle umgewandelt werden. Dieser metallischer Brennstoffzyklus öffnet neue Möglichkeiten für die Energieversorgung Deutschlands, wovon wir eine konkret verfolgen, und zwar die Umrüstung von Kohlekraftwerken auf Eisenpulververbrennung. Um dieses Ziel zu erreichen, müssen zunächst CFD-Simulationen der turbulenten Eisenpulververbrennung durchgeführt werden, wofür zunächst wiederum CFD-Simulationen der laminaren Eisenpulververbrennung durchgeführt werden müssen, um das grundlegende Modell zu bilden. Letztere sind Gegenstand dieser Arbeit.

Experimentelle Grundlage unserer Simulationen ist ein laminarer Bunsenbrenner, der mit Eisen betrieben wurde [1]. Dieser Brenner wurde mit zwei unterschiedlichen Modellierungsansätzen untersucht: Einphasige Simulationen nach dem „dusty gas model“ wurden mit OpenFOAM v11 [2] durchgeführt. Die Besonderheit dieser Simulationen ist die Verwendung eines Sektionalen Ansatzes, um die Partikelgrößenverteilung des Eisenpulvers zu modellieren. Somit können Simulationen hochskaliert werden vom Laborbrenner bis hin zu Industriebrennkammer, ohne die Fähigkeiten heutiger HPC-Architekturen zu überschreiten. Mehrphasensimulationen hingegen wurden mit MFiX [3] durchgeführt: Ein CFD-Solver nach der Euler-Euler-Methode, der speziell für Schüttgüter entwickelt wurde. Hier wurden nicht nur die gekoppelte Navier-Stokes-Gleichungen beider Phasen gelöst, sondern auch Gleichungen für die granulare Temperatur des Pulvers. Somit wird das physikalische Verhalten des Eisenpulvers genau dargestellt, was bei einphasigen Simulationen nicht der Fall ist. Die Ergebnisse beider Simulationsmethoden werden vorgestellt und sowohl miteinander als auch mit experimentellen Ergebnissen verglichen. Anschließend werden wir einen Ausblick auf unseren turbulenten Simulationen geben, die ebenfalls uns darin unterstützen werden, unser Ziel zu erreichen: Simulationen der Verbrennung von Eisenpulver in industriellen Brennkammern.

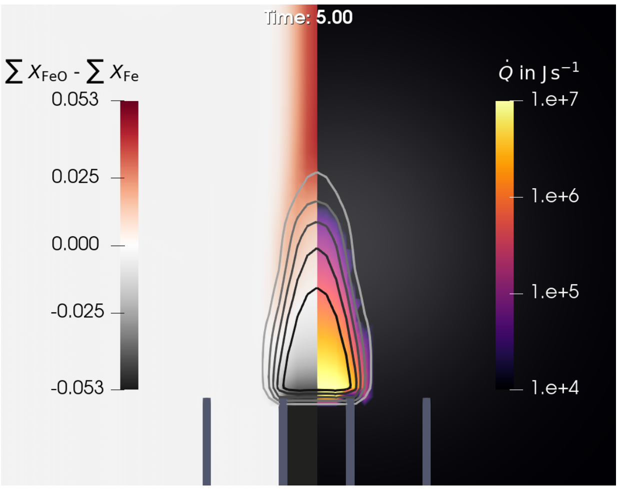

Abb. 1: Der Eisenoxidüberschuss (links), die Wärmefreisetzungsrate (rechts) und Temperaturkonturlinien von 600 K (außen, hellgrau) bis 1800 K (innen, schwarz) einer Eisenflamme (OpenFOAM-Simulation).

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Keywords: Metallische Energieträger, Eisenverbrennung, Euler-Euler-Simulationen, Sektionaler Ansatz.

Numerical Study on Turbulence-Chemistry Interactions Models at High Pressure Gasification Conditions

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The high-pressure partial oxidation (HPPOX) is a key technology for syngas production in industrial applications. Accurate and scalable simulation models are essential to ensure reliable predictions across different reactor scales, from laboratory experiments to pilot plants and ultimately to full-scale industrial reactors. In this work, we perform a comprehensive computational fluid dynamics (CFD) study focused on the evaluation of two turbulence-chemistry interaction models: the Eddy Dissipation Concept (EDC) [1] and the Partially Stirred Reactor (PaSR) [2] model. The investigation begins with a detailed analysis of the non-catalytic natural gas reforming in a small-scale 41 L reactor using different burner concepts [3]. Pressures up to 60 bar and temperatures up to 1450 °C are considered. Both models are evaluated based on their treatment of turbulent mixing and chemical reaction time scales. The results highlight distinct differences in how each model captures the flame structure and reaction zones, particularly in chemistry dominated regions (post combustion zones). Subsequently, the models are applied to simulate a series of pilot-scale experiments in a 455 L reactor at pressures between 50-70 bar and syngas temperatures in the range of 1200 to 1400 °C [4]. For both setups, the flame structure was validated against optical measurements. The PaSR model demonstrates superior performance in terms of capturing the main reaction regimes, being able to accurately model both the fast combustion reactions and the slow gasification reactions without the need of model's parameter fitting. The model predictions show good agreement with available plant data, confirming its robustness and scalability for large-scale applications. This study illustrates the critical role of selecting appropriate turbulence-chemistry interaction models for scalable and predictive CFD simulations, and provides practical insights for the design and optimization of industrial HPPOX processes.

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Keywords: CFD, Gasification, Combustion, Scaleup, Turbulence-Chemistry

Lagrangian Analysis of Reactive Flows Inside Porous Media using CFD

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Triply periodic minimal surfaces (TPMS) exhibit great potential as catalyst carriers due to their high specific surface area, which provides abundant active sites. Furthermore, the highly interconnected channel networks promote homogeneous reactant distribution, enhanced mixing, and efficient heat and mass transfer [1]. Indeed, first results indicate the efficiency of TPMS as a support structure in heterogeneous catalysis by effectively increasing the activity and mitigating stagnant dead zones [2].

To evaluate the potential of TPMS structures as catalyst carriers, reactive flows are simulated using the finite volume method. The investigated reactive system is based on the urea-urease reaction scheme, in which the enzymatic catalyst is immobilised on the TPMS structure (Figure 1). Numerical tracer particles are initialized to analyse possible correlations between yield, selectivity, and the underlying fluid-dynamic state by means of Lagrangian measures. As the reaction kinetics are strongly sensitive to local conditions such as temperature and pH, reproducing the reactive system without substantial assumptions is complex, which renders validation equally challenging [3]. In contrast, velocity fields inside these periodic structures can be measured non-invasively by Magnetic Resonance Imaging (MRI), facilitating validation of the characteristic tracer particle advection behaviour [4]. In particular, the contact rate of particles, the exit-age distribution, and the local age distribution are considered to assess the effectiveness of TPMS structures for heterogeneously catalysed processes.

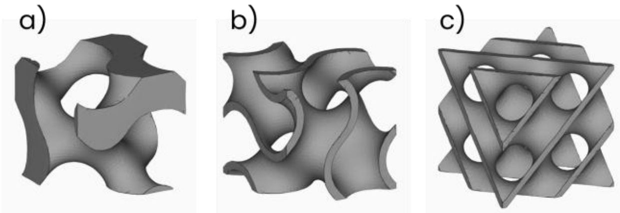

Figure 1: Renderings of lattice structures based on TPMS, (a) Gyroid TPnS, (b) Gyroid TPSf, (c) Diamond TPSf.

Within the Collaborative Research Centre CRC1615, structured "SMART Reactors" are developed, which are able to adapt quickly to changing raw materials, energy supply and reaction conditions. As a part of that, self-adapting structures are designed to control reactions regarding the operating conditions, i.e., temperature, pressure drop or pH-value. This works builds the foundation for further design guidelines of self-adapting structures with high specific surface area to improve the reaction with respect to yield and selectivity, and thus the entire process.

Acknowledgments

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Keywords: TPMS, CFD, Heterogeneous Catalysis, Lagrangian Analysis, Reactive Mixing

CFD Based Kinetic Parameter Estimation Method for Arbitrary Reactor Geometries

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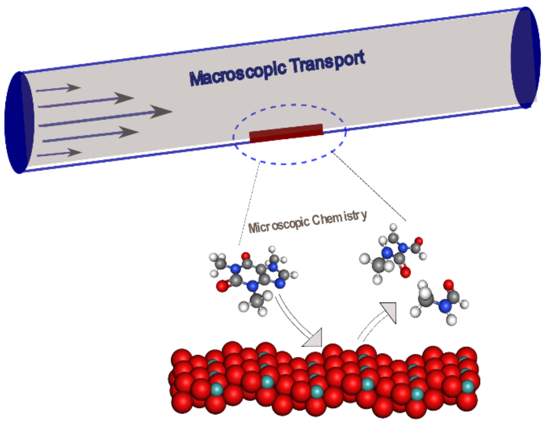
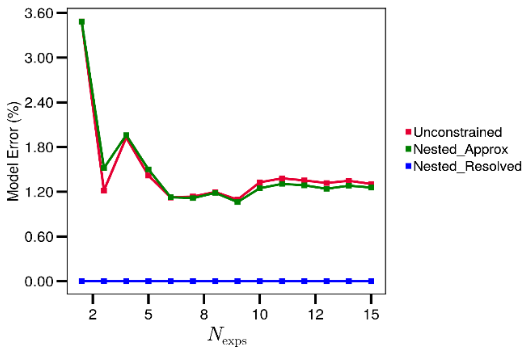
To estimate the kinetic parameters of surface catalytic reactions, ubiquitously ideal reactor models like the CSTR, stagnation point flow, or the plug flow are used. This allows the system to be governed by either an analytical or a simple ODE based solution. However, modern in-situ atomic scale surface characterization experiments seldom allow such flow geometries, e.g. by installing devices like probes and pumps in the vicinity of the catalyst. In such scenarios, the coupling of transport and kinetics can be crucial. This coupling can be described by full scale computational fluid dynamics (CFD) which accounts for complex flows that are described by Navier Stokes equations since simplistic models result in to misleading information about the surface coverage, activity or reaction conditions over the surface of the catalyst. Nevertheless, the concomitant huge computational burden prevents conventional CFD from being a practical tool in these cases beyond a few validation runs, particularly when solving inverse problems for kinetic parameter estimation (KPE).

To address this challenge, we exploited our recently developed reduced order models (ROMs) for heterogeneous catalytic systems[1,2]. The ROMs have two advantages: (1) Their pre-processing or offline part is cheaper than other ROMs and (2) the online part requires only solving non-linear equations (NLEs) rather than a partial differential equation (PDE) system. This enables solving inversely the governing non-linear PDE system with minimal computational effort which is perfectly suited for KPE. In this study we demonstrate different approaches for solving inverse problems for KPE based on previously developed ROMs. The inverse problem can be formulated as either an unconstrained or a nested optimization problem. The unconstrained approach is faster whereas the nested approach is more accurate. Depending on the practitioner's requirement either approach or a combination of both approaches can be opted. We investigate these approaches by estimating kinetic parameters for trivial mass action kinetics as well as more complex methanol formation kinetics.





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Keywords: parameter estimation, CFD, kinetic, catalysis, optimization

CFD-Based Hydrodynamic and Reactive Flow Modeling for Top-Blown Rotary Converter using a Two-Fluid Approach

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The present work studies the complex hydrodynamics and gas-liquid interactions inside a top-blown rotary converter (TBRC) by use of computational fluid dynamics (CFD). TBRCs are widely used in the non-ferrous metals industry for recovering valuable and precious metals such as Au, Ag, PGMs, Te, Se, Pb, Zn and Sn from both primary and secondary resources. With increasing focus on carbon-neutral production, replacing fossil fuels with renewable or low-emission alternatives has become a key challenge. Injecting fuels such as H_2 or NH_3 significantly affects furnace operation and may introduce new safety and design considerations. To evaluate these changes without the need for full-scale trials, a multiphase numerical modeling strategy is applied. In this work we developed a reliable two-fluid model to represent the interaction between molten material, gas jets and rotation-induced motion. To ensure reliability for industrial-scale studies, the hydrodynamic performance of this model is validated against previously published high-resolution Volume of Fluid (VOF)[1] results. The comparison includes key parameters such as void fraction distribution, turbulence kinetic energy, and mixing behavior, confirming that the two-fluid approach can accurately reproduce essential flow characteristics while significantly reducing computational cost. With the hydrodynamic foundation established, the two-fluid model is extended to reactive modeling. A first application examines the effect of introducing 5% hydrogen during the treatment of a cassiterite concentrate and compared against the VOF model under realistic operating conditions. Overall, this work demonstrates the feasibility of the two-fluid model for industrial-scale TBRC simulations and provides insight into both hydrodynamic and reactive phenomena relevant to future low-carbon furnace operation.

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Keywords: CFD, Two-fluid model, VOF, TBRC

CFD–DEM Modelling of Seabed Milling and Hydrocyclone-Based Containment for Sustainable Deep-Sea Mining

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The increasing demand for critical minerals has renewed interest in deep-sea mining of polymetallic sulphide deposits near black smokers at water depths of 3,000–5,000 m. These deposits are rich in copper and zinc, with economically relevant by-products such as gold and silver. A major challenge is the mitigation of sediment resuspension and turbidity plume formation during seabed excavation and material transport. In this work, a coupled Computational Fluid Dynamics–Discrete Element Method (CFD–DEM) framework is developed using Siemens StarCCM+ to simulate the vertical trench cutting, cutting transport, hydrocyclone-based separation and containment process.

A vertical trench cutting method for seabed milling is investigated using counter-rotating milling wheels of 1.25 m diameter operating at 15–25 RPM. The flow is resolved using RANS and URANS and various turbulence models are analysed. The selected cases employ Large-Eddy Simulation (LES) with the WALE model to resolve the fine scale turbulent structures to understand the flow behaviour. Reynolds numbers based on wheel diameter and tip speed range from 1×10^6 to 7×10^6. DEM simulations employ spherical particles with diameters of 1–10 cm and densities of 2,500–3,700 kg m^{-3}, including cohesion and contact forces to represent varying seabed strengths. One-, two-, and four-way coupled CFD–DEM approaches are evaluated to assess particle entrainment, transport, and bond breakage. Different concepts like wheel rotation directions, speeds etc for the extraction of cuttings have been investigated. Upstream of the milling process, a hydrocyclone-based separation and containment unit is analysed using a parametrised geometry. Inlet velocities of up to 6 m s^{-1} correspond to Reynolds numbers between 1×10^6 and 8×10^7. A Design of Experiments (DoE) study with over 100 configurations varies cone angle, cone height, core height, filter height, and domain radius, with pressure drop used as the primary performance metric. The results show that core height, domain radius, and filter height dominate pressure losses, while cone angle has a minor influence. Particle tracking simulations indicate velocity-dependent separation behaviour with cut-off diameters (St ≈ 1) in the range of 1.7–2.5 mm. Overall, the study demonstrates how multiphase CFD–DEM modelling can support the design of sustainable deep-sea mining systems with reduced sediment plume generation.

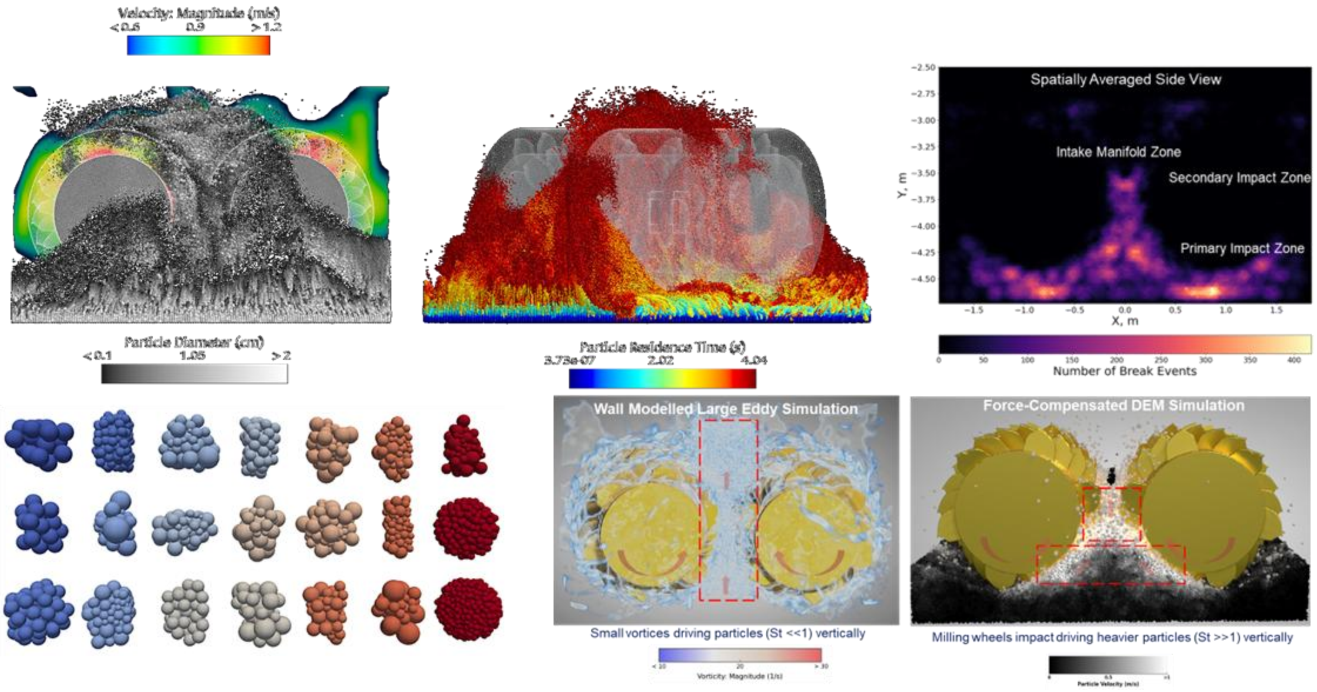

Figure 1 Multiscale CFD–DEM visualisation of trench cutting, particle entrainment, and turbulence-driven transport in deep-sea mining.

Keywords: CFD–DEM coupling, sustainable deep-sea mining, trench cutting, multiphase flow, Large-Eddy Simulation, particle entrainment, hydrocyclone separation, plume mitigation

The influence of non-spherical particles on the performance of gas cyclone separator: Analysis based on the Eulerian-Lagrangian Method

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Efficient particulate matter (PM) separation from syngas is essential for raw gas cleaning in processes like biomass gasification. Cyclone separators, utilizing inertial vortex separation, are a widely adopted, highly effective solution. However, the hydrodynamics of the multiphase flow within these devices are extremely complex, characterized by highly turbulent flow and intricate particle-flow, particle-particle, and particle-wall interactions. Previous numerical studies have commonly employed the Euler/Lagrange approach coupled with Large-Eddy Simulation (LES) for the gas phase and utilized spherical particle models [1]. This approach is often insufficient, as particles in real-world industrial processes are predominantly non-spherical. This study investigates the influence of non-spherical particle morphology on the grade efficiency and internal flow dynamics of gas cyclone separators. The research focuses on incorporating advanced non-spherical particle modeling [2] to accurately assess the resulting deviation in separation performance at the room temperature. Since the forces and torques acting on non-spherical particles differ from those on spherical ones, the standard point-mass particle tracking available in OpenFOAM required modification. In this work, the implementation is structured specifically for ellipsoid particles. The particle orientation is tracked using quaternions, and the forces (drag, lift) and torque (hydrodynamic, pitching) acting on the ellipsoid particles as the starting point are derived from Zstawny et al. [3]. The particle-wall collision model is adopted from Quintero et al. [4] based on the hard-sphere model for non-spherical particles. Stochastic particle-particle collisions [5] are also taken into account to ensure comprehensive modeling of particle interactions. Preliminary results, as demonstrated by the green and brown curves in Figure 1, indicate that reduced particle sphericity leads to a diminished separation efficiency. This highlights the necessity of incorporating realistic particle shapes for accurate predictive modeling of cyclone performance. Furthermore, this study provides crucial guidance for particle random wall collision model.

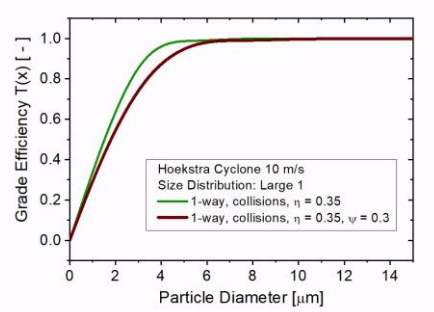

Figure. 1 Grade efficiency curves obtained from simulations using different sphericity (inlet velocity 10 m/s, only one-way coupling, particles Large 1, particle mass loading of 0.35, wall roughness Dg = 10°, inter-particle collisions);

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Acknowledgement: The present research is conducted within the Project Horizon Europe ResMe2E; Project number: 101172988. The financial support by the European Community is gratefully acknowledged.

Keywords: non-spherical particle, gas cyclone, grade efficiency, Euler-Lagrangian method, OpenFOAM.

Flow structure, particle transport and clustering within a T-junction

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Abstract

A T-junction is a flow configuration found in physiological flow systems, small-scale tube fittings, and industrial piping systems. Such a flow system is also quite well known for mixing different fluids or splitting a liquid steam into two streams with identical flow rates. In this study the final objective is related to the analyses of particle transport effects on the erosion of the walls within the device, mostly occurring in the stagnation point region. The idea of using such a flow configuration for defined erosion measurements was originated some years ago by Reis et al. (2023). However, the flow structure in a T-junction is rather complex and associated with the development of vortical structures (Vigoloa et al. 2014) which naturally influence the particle transport and the resulting concentration distribution as well as the wall collision rates. In the present study, a liquid-particle system is considered and the influence of numerical method (RANS or LES) and particle size on the concentration fields and the wall collision frequency pattern is investigated for a T-junction with channels of quadratic cross-section (18 mm x 18 mm).

The numerical computations are conducted using the Euler/Lagrange approach wherefor all required particle transport models are implemented in a custom solver OpenFOAM. The flow field is computed by RANS, URANS and LES, considering both one-way and two-way coupling. The particles are tracked by considering drag, shear and rotational lift as well as gravity and buoyancy (Sommerfeld and Lain 2015). Particle turbulent dispersion was modelled through a stochastic single-step Langevin model. Inter-particle collisions were treated by a stochastic approach and hard-sphere wall collisions were calculated by solving the impulse equations with restitution ratio and wall friction parameters, both depending on impact angle (Sommerfeld and Taborda 2024). Moreover, a stochastic method is used to model the transport of irregular angular particles (Sommerfeld and Lain 2018) and also the irregular particle-wall collision was described in a stochastic way (Quintero et al. 2020). The considered particle sizes were in the range between 20 μm and 200 μm, yielding Stokes numbers between 0.03 and 2.5, similar to experimental studies Reis et al. (2023). A typical result for an inlet Reynolds number of 100,260 using the k-ω-SST turbulence model is shown in Figure 1, depicting the geometry with mesh and particle concentration distribution in different views. The clustering of the particles in the vortical structures is visible.

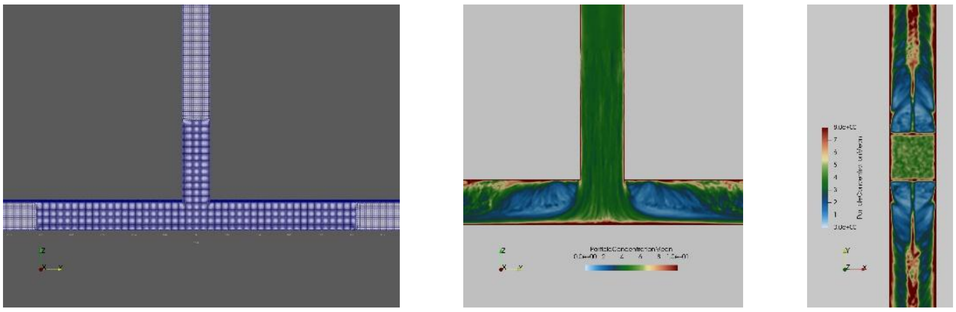

Figure 1: Configuration and mesh of the T-junction (left), side view of the concentration field in the midplane for a particle size distribution, D_{mean} = 100 μm (middle) and top-view of particle concentration field, midplane horizontal channel (right).

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Keywords: T-junction, Euler/Lagrange, concentration distribution, wall collisions, non-spherical particles, clustering.

CFD Modelling of Dry Paper Forming Section for Uniform Web Formation

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In papermaking, approximately 60% of the total energy consumption is attributed to the thermal drying of the wet web. Traditionally, fibres are transported in water at concentrations between 1 and 3 wt% to ensure uniform flocculation. To overcome this energy-intensive step, we are developing a technology demonstrator for dry web formation. One of the key challenges is the controlled transport and deposition of cellulose fibres in an airstream. The process must minimize air consumption while achieving a uniform fibre distribution to ensure consistent sheet formation.

To address this, components of the technology demonstrator are integrated into a CFD model for flow optimization. The demonstrator consists of a forming head that distributes fibres onto a moving wire using a sieve–brush mechanism. Below the wire, a suction unit applies negative pressure to fix fibres onto the belt. A uniform velocity profile across the machine width is essential to avoid basis weight variations. Additionally, the accumulating fibre layer influences the airflow, which should compensate for irregularities in web formation. The CFD model includes the suction box geometry, which can be optimized by adjusting guide plates, and a multiphase simulation of fibres entering the forming head as flocs. Fiber separation is modelled using a rotating brush represented as porous media, followed by a sieve modelled similarly, ensuring even fibre deposition onto the wire. The wire itself is treated as porous for airflow but impermeable to fibres. Figure 1a) illustrates the simulation setup.

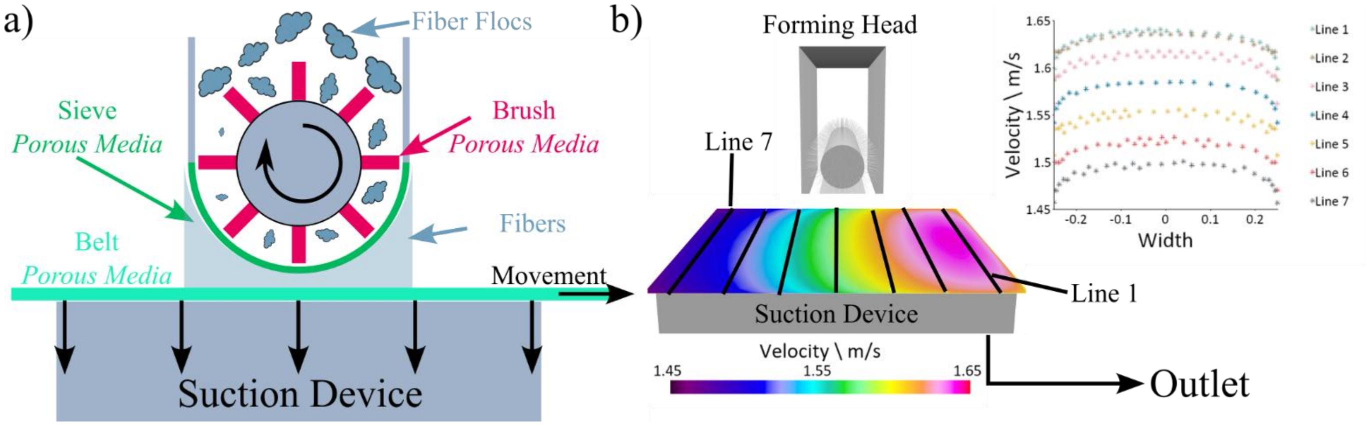

Figure 1: a) Simulation setup showing fibre flocs being combed through different porous media and forming a web on the moving wire. b) Initial airflow simulation in the suction device, illustrating minor velocity variations in the cross-machine direction and a decrease toward the edge zones.

Initial simulations, shown inf Figure 1b), for the suction box geometry considered only airflow. Results indicate that along the cross-machine direction, velocities remain relatively uniform in the central region but decrease toward the edges, while significant fluctuations occur in the machine direction. These are acceptable since the wire movement averages out these variations. The next simulation stage will incorporate guide plates in the suction device and experimentally determined porous media properties for the wire to optimize airflow. Subsequently, the model will be extended to include multiphase simulations of fibre deposition and its impact on flow behaviour. For this purpose, the material constants—permeability and Forchheimer coefficient—of the components represented as porous media (sieve and brush) must also be determined. Given the known geometry, these parameters can be obtained using the Darcy law through an appropriate pressure-drop simulation, which can also account for directional dependence (anisotropy) [1].

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Keywords: “Computational Fluid Dynamics”, “Eulerian-Eulerian Multiphase simulation”, “Fibre Simulation”

A simulation model for oblique flow through a wire screen with application to hydrodynamic cell design optimization of a membraneless electrolyzer

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Metallic screens are used in a variety of engineering applications, e.g. in filters, permeable claddings along façades of buildings, fog harvesters and endovascular stents. These screens can take many different shapes, e.g. perforated plates, expanded metals, honeycombs and wire meshes, for example. In such configurations, fluid flow has a multiscale character, from the scale at the pore size of the screen to the scale of the entire device. Since this scale difference can be several orders of magnitude, fully resolved CFD simulations are commonly avoided for whole systems, so that the effect of a screen needs to be represented by a model instead.

If a case is considered where fluid flow approaches a screen not in perpendicular direction but in an oblique manner, a screen model must capture two relevant physical effects: First, resistance in normal direction leads to a pressure drop. Second, the flow is deflected from its incident direction, generally towards the normal. In the present contribution, a homogenized approach is applied to model steady laminar flow through a woven wire screen, implemented as an additional source term in the momentum equation. To calibrate the model parameters, fully resolved simulations were performed for a representative part of the wire screen with different angles of attack of the incident flow. An exemplary case is illustrated in Fig. 1 together with the homogenized counterpart. On this basis, it is shown that the calibrated model matches pressure drop and flow deviation very well, even for high angles of attack, and hence improves upon the available literature.

As an application of the homogenized screen model, the hydrodynamic optimization of a membraneless electrolyzer employing wire screen electrodes is demonstrated. These electrochemical devices are gaining attention for the production of green hydrogen due to their low cost, robust operation, and simplicity. The lack of a membrane, however, requires an improved hydrodynamic cell design since only the electrolyte flow is responsible for the separation of the gas products, H_2 and O_2. Typical geometries of membraneless flow-through electrolyzers can be classified by a T- and I-shaped cell design. The former features parallel electrodes and a global flow deflection of 90°, whereas the latter has angled electrodes and straight flow channels. However, both cell designs suffer from an inhomogeneous electrochemical reaction over the cross-sectional electrode area due to either poor electrolyte velocity or poor current density distribution. A new Y-shaped membraneless cell design could be recently developed in [1], representing a sweet spot between the established electrolyzer geometries.

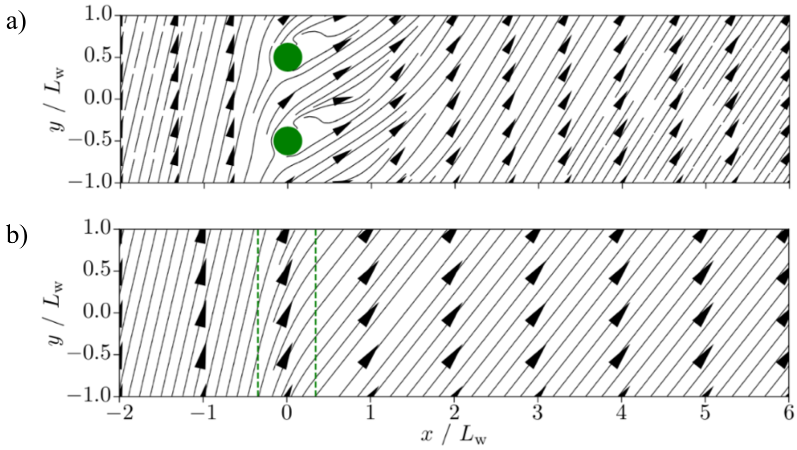

Figure 1: a) Streamlines of fully resolved flow through representative part of woven wire screen. Cuts of wires are indicated with green circles. b) Streamlines of flow through homogenized screen. Region of homogenized screen model indicated with green dashed lines. Only parts of computational domains are shown.

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Keywords: wire screen electrode, homogenization, membraneless electrolyzer.

Modeling the Wetting Behavior on Structured Surfaces Using a Diffuse Interface Approach

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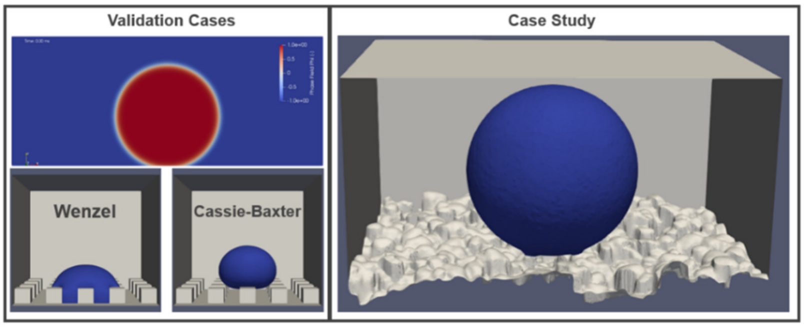
In thermal separation unit operations, such as distillation, structured packings are widely employed. To improve liquid wetting and enhance separation performance, the surfaces often feature micro and macro structures. Understanding the interaction between structured surfaces and liquids in terms of wetting is therefore of utmost importance. Due to greater flexibility than conventional methods additive manufacturing is increasingly used to produce such structured packings. However, the wetting behavior on 3D-printed surfaces remains largely unexplored. This work aims to partially fill this gap using computational fluid dynamics (CFD).

To model the wetting behavior of a two-phase system, we employ a diffuse interface approach. In the model, the infinitely thin interface between gas and liquid is replaced by a transition region of defined thickness. The thermodynamically consistent diffuse interface model consists of a coupling between the incompressible Navier–Stokes equations and the Cahn–Hilliard equations (CHNS model). The model was implemented using the finite element toolbox FEniCS. The resulting nonlinear equation system was solved with PETSc, as described in [1]. In classical sharp interface models, a sharp fluid-fluid interface is assumed and its motion occurs only through convection, driven by the local fluid velocity. This leads to a contradiction if a no-slip boundary condition (i.e., zero velocity at the solid surface) is also assumed. It is commonly referred to as the singularity problem of the contact line. While classical sharp interface models are challenged by the singularity problem, the CHNS model avoids it entirely. The diffuse interface approach allows for topological changes in the interface to be naturally simulated. Our work aims to employ a more natural approach to obtain physically sound insights into the wetting behavior on small scales.



This work consists of two steps: validation and case study. In the first step, we investigated the wetting behavior of a droplet on a smooth and a structured surface. For both cases, a no-slip boundary condition was applied on the solid surface. In the first validation case, we simulated a spreading droplet on a smooth surface with no initial velocity in 2D. The normalized spreading radius as a function of time was compared with the experimental data from [2] and showed good agreement. In the second validation case, with a regular structured surface, the model was decoupled and extended to 3D. We observed the transition from Cassie–Baxter state to Wenzel state for various equilibrium contact angles and pillar spacings. The results were then compared with the transition criterion equation proposed by Jäger et al. [3] and the results again showed strong agreement. In the second step, we will apply the validated model to investigate the wetting behavior of a droplet on a 3D-printed surface. The surface structure is measured by confocal imaging and the postprocess surface structure directly imported into the simulation domain. The simulation results will provide a deeper understanding of the fluid dynamics and the resulting separation performance of structured packings.

We kindly acknowledge that this work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)-ProjectID 533252297

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Keywords: Cahn-Hilliard-Navier-Stokes, Wetting Behavior, Structured Packings.

A Paradigm Shift in Multiphase CFD: Kinetic Theory Meets High-Order Numerics

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Dispersed multiphase flows frequently occur in nature and are central to many process engineering disciplines. However, despite new models, algorithms and enhanced hardware, multiphase computational fluid dynamics (CFD) simulations still rely almost exclusively on Euler–Euler CFD for larger-scale applications (e.g. industrial equipment). In this framework, dispersed phases are treated as interpenetrating continua, so particle properties such as size, shape, composition, and internal state are collapsed into a few averaged fields. Even with extensions like population balances or pseudo-phases, only a small number of size and velocity classes is resolved, and all particles typically share the same temperature and composition. As a consequence, closure laws (e.g., drag, lift) still require extensive case-by-case tuning: the same bubble column configuration simulated about 20 years apart [1,2] needed parameter retuning in both studies to match experiments.

We propose a kinetic-theory-based framework, the **Kinetic Theory of Fluid Particle Flow (KTFPF)** [3], as a more physical yet still tractable alternative. KTFPF introduces a Boltzmann-like description based on a number density function in a joint physical–property space and derives mass-weighted transport equations that consistently couple single-particle dynamics and ensemble behavior. A structured decomposition of the property space into resolved and averaged components yields moment equations in which dispersed-phase mass, species, momentum, and energy depend on space, time, and selected particle properties (cf. Fig 1). This embeds Lagrangian information in an Eulerian description and bridges the gap between Euler–Euler and Euler–Lagrange models.

To solve the resulting high-dimensional equations, we plan to use a discontinuous Galerkin spectral element method (DGSEM). DGSEM offers local conservation, high-order accuracy on complex geometries, straightforward extension to multidimensional property spaces, and efficient matrix-free, tensor-product implementations on GPUs. Although it comes with challenges (implementation complexity, stability control, higher cost per degree of freedom), we believe its advantages are particularly compelling for KTFPF.

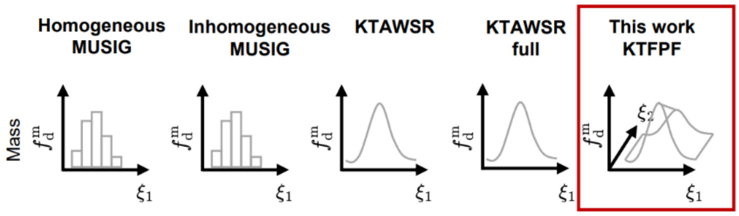

Figure 1: Schematic illustration of the different model approaches. f_d^m *mass density function and* ξ_i *properties. Adapted from [3].*

In the talk, we will outline this KTFPF–DGSEM program, discuss expected benefits and numerical challenges, and invite the community's feedback on its potential for industrial multiphase CFD.

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Keywords: Discontinuous Galerkin Method, Spectral Element Method, Computational Fluid Dynamics, Reactive Multiphase Flow, Kinetic Theory of Fluid Particle Flow.

Improvements in the Dispersion Direction Handling for High-Fidelity CFD Simulations of Liquid-Liquid Dispersion Separation

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The separation of liquid-liquid dispersions, as seen in gravity phase separators, is frequently modelled by rate-based models that compute the interphase force balance and thereby determine the sedimentation velocity. These models require the assignment of one liquid as the dispersed phase and another liquid as the continuous phase. This assignment is referred to as dispersion direction. It will be constant within the dispersion until the sedimenting dispersed phase reaches a boundary, called active interface, where the dispersion direction inverts and the initially dispersed phase becomes continuous and vice versa. [1]

Rate-based one-dimensional approaches to model the settling behaviour are well established [1,2]. However, simulations that resolve the global three-dimensional bulk flow patterns additionally require a CFD-solver. Numerous publications have explored this possibility, but fail to produce a change in dispersion direction [3], assign dispersion directions that contradict classical assumptions [4], or use low-fidelity phase interaction models that do not encompass dispersion direction information [5].

The upcoming presentation will discuss how the treatment of the active interface, particularly the sharp inversion of dispersion direction, represents the key limitation that prevents the successful combination of CFD with dispersion-direction dependent rate-based models. Furthermore, it will introduce a new algorithm and its implementation in the CFD-framework OpenFOAM. This algorithm detects the active interface within the simulation domain during runtime and adjusts the local fluxes to correct for the previously determined limitation. Finally, exemplary simulation results obtained with the new algorithm will be shown, to demonstrate the potential of CFD simulations of liquid-liquid dispersion separation with the new algorithm.

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Keywords: liquid-liquid dispersion, phase separation, Euler-Euler, multiphase CFD

Numerical Investigation of Bubble Collapse Near a Rigid Wall: A Virtual Mass–Based Criterion for Jetting

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The asymmetric collapse of a cavitation bubble near a rigid wall can generate re-entrant liquid jets along with extreme pressure and temperature conditions that are central to cavitation erosion, surface damage, and bubble-induced chemical processes. Using Direct Numerical Simulations (DNS) with an All-Mach compressible multiphase solver in the *Basilisk* framework, we investigate single-bubble collapse near a rigid boundary as a function of the non-dimensional stand-off distance: $\gamma = d_0 / R_0$. By resolving the interface kinematics, we identify the interfacial acceleration gradient defined as the difference in normal acceleration between the wall-facing and distal sides of the bubble as a robust indicator of jet formation. From this quantity, an effective virtual (added) mass coefficient gradient is introduced, $\Delta C_m, eff$, to quantify the wall induced asymmetry in liquid inertia. Strong jetting, characterized by a re-entrant jet that penetrates the opposite bubble interface during collapse, is observed for $\gamma < 3$ when the acceleration gradient exceeds 0.18 $\mu m/\mu s^2$ and $\Delta C_m, eff \geq 0.1$. Weak, non-penetrating jets occur for $0.06 \leq \Delta C_m, eff < 0.1$, while nearly spherical collapse is recovered for $\Delta C_m, eff < 0.06$. In addition, the collapse time, bubble centroid displacement, and peak gas pressure inside the bubble at collapse are found to scale linearly with $\Delta C_m, eff$, demonstrating that virtual mass asymmetry governs both jet dynamics and global collapse intensity. These clearly distinguished jetting regimes provide a predictive framework for controlling bubble-wall interactions and collapse dynamics, with direct relevance to cavitation erosion mitigation, ultrasonic and hydrodynamic cleaning and advanced water-treatment technologies based on cavitation-induced OH radical generation.

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Keywords: Cavitation dynamics, Bubble collapse, Jet formation, Added mass, Rigid wall.

Using quadrature-based moment method to model transport inside mesopores of heterogeneous catalysts

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Throughout the chemical and process industries, heterogeneously catalyzed gas phase reactions are commonly carried out in fixed bed reactors. In highly relevant industrial processes, such as selective oxidation and emission control, transport limitations inside the mesoporous (mean pore diameter $d_{\mathrm{pore}} = 10 - 200$ nm) catalyst strongly influence the reaction at the catalytic active sites. Therefore, optimization of the catalyst geometry (e.g., shape and dimensions) and morphology (e.g., porosity (profiles), pore diameter, location of catalytic active sites) has great potential to improve the performance of such reactors. Spatially resolved modeling of the pore system can significantly contribute to a better understanding of the interplay between surface reaction and transport within catalysts and is a necessary step towards computer-aided catalyst design. However, the commonly used models are based on simplified assumptions concerning the pore characteristics and/or simplify the influence of the pore system on the heat and species mass transport [1].

Recent developments in high-resolution X-ray and electron tomography make it possible to obtain a spatially resolved description of the mesopore system [2]. These tomograms can be used as the underlying geometry for the simulation of energy and species mass transport coupled with surface reaction. However, the biggest challenge in modeling transport inside mesopores is that the small pore diameters result in Knudsen numbers ($Kn_i = \frac{\lambda_i}{d_{\mathrm{pore}}}$ with λ_i: mean free path of molecule i) higher than 0.01. This causes the continuum assumption to break down, rendering the commonly used Navier-Stokes-Fourier equations invalid. Since molecular dynamic simulations are too computationally expensive for such large and complex geometries, a coarse-grained molecular dynamic method is essential to model the transport coupled with the catalytic reaction within the mesoporous catalyst.

In this contribution a novel and general approach to model energy and multicomponent species transport in mesoporous systems for arbitrary Knudsen numbers is presented. The Boltzmann equation is solved for each component of the mixture using the quadrature-based moment method (QBMM) [3]. A robust closure for the unknown moment flux terms is achieved using the recently developed Hyperbolic Quadrature Method of Moments (HyQMOM) [4]. The resulting set of partial differential equations can be solved using the finite volume method. As a first step, the capability of QBMM to describe multicomponent diffusion within the continuum limit is tested. Therefore, a 1D QBMM model with a generalized Bhatnagar-Gross-Krook (BGK) collision operator to describe the interaction between equal and unequal molecules is implemented. As shown in Figure 1, the QBMM results align well with the Maxwell-Stefan diffusion model. This indicates that multicomponent diffusion can be described using QBMM.

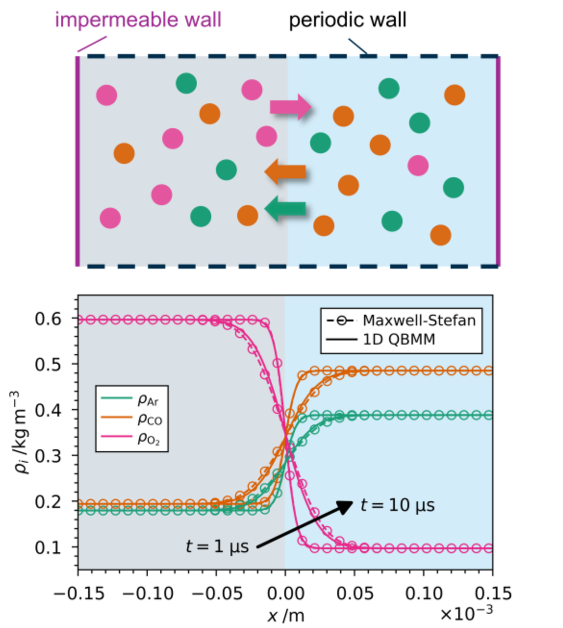

Figure 1: Mixture composition described by partial density calculated with the Maxwell-Stefan diffusion model and 1D QBMM (at $p = 1\ bar, T = 400\ K$).

The presented model serves as the foundation for pore-resolved simulations of mesoporous catalysts. For the first time, the QBMM method has been used to describe multicomponent diffusion within the mesopores of a catalytic system. Future work will extend the concept to 2D and 3D domains and introduce reflecting boundary conditions at the pore walls to model molecule-wall collisions.

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Keywords: quadrature-based moment method, Boltzmann equation, mesoporous catalysts, transport phenomena beyond the continuum limit, multicomponent diffusion.

Modellierung der Partikelpopulation und Vergasung im Zyklonreaktor

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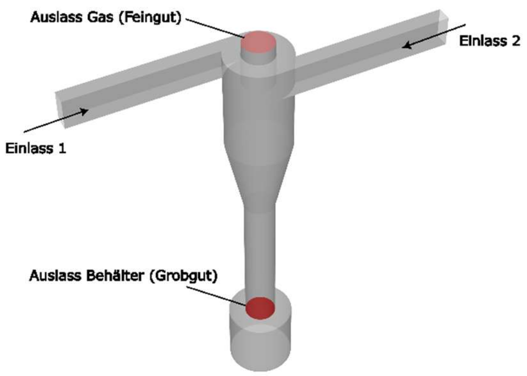
Der untersuchte Zyklon steht im Fokus eines neuartigen Biomasse-Vergasungssystems, in dem die Prozesse der Reaktion und Partikelabscheidung unmittelbar miteinander gekoppelt sind und überlagert ablaufen [1]. Abbildung 1 zeigt den hierzu verwendeten Prototypen. Die Ansaugung der Luft und Zufuhr der Biomasse erfolgt über zwei identisch ausgeführte, gegenüberliegende Einlässe, die für eine gleichmäßige Strömungsführung im Zyklon sorgen [2].

Im Mittelpunkt der Arbeit steht die CFD-Analyse der Größen- und Massenänderung injizierter Biomassepartikel während des Vergasungsprozesses im Zyklon. Das in den Arbeiten von HadiJafari et al. [3] und Chishty et al. [4] vorgestellte numerische reaktionskinetische Modell zur Zyklonvergasung wird hierzu auf ein validiertes zweiphasiges CFD-Modell des Zyklons übertragen. Die thermochemischen Prozesse werden durch die Kombination aus Species-Transport-Modell zur Abbildung der homogenen Gasphasenreaktionen und dem Discrete Phase Model (DPM) zur Beschreibung der Lagrange-basierten Partikeldynamik sowie der heterogenen Biokohle-Reaktionen umgesetzt. Durch Trocknung, Ausgasung und Biokohle-Reaktionen verlieren die Partikel kontinuierlich Masse, wodurch sich auch ihre Größe zeitabhängig verringert. Dieser dynamische „Schrumpfungsprozess" beeinflusst nicht nur die Partikelgrößenverteilung, sondern wirkt sich auch unmittelbar auf Strömung, Verweilzeitverhalten und Trenneffizienz im Zyklon aus.

Ziel der Untersuchung ist es, die zeitliche Entwicklung der Partikelgrößen in Kopplung mit der Verweilzeit zu erfassen und daraus ein Maß für den Reaktionsfortschritt beziehungsweise die Vergasungsvollständigkeit abzuleiten. Hierfür werden Partikeltrajektorien hinsichtlich lokaler Masse, Größe und Temperatur ausgewertet, sodass sich die relative Größenänderung und ein dimensionsloser Umsetzungsgrad bestimmen lassen.

Die Analyse ermöglicht eine quantitative Beantwortung der zentralen Fragestellung: *Wie vollständig wird die Vergasung im Zyklon realisiert?* Auf Basis dieser Informationen können charakteristische Reaktionszeiten und Umsetzungsgrade bestimmt werden, die eine Bewertung der Prozessintensität und potenzielle Optimierungsansätze für den energetischen Betrieb des Zyklonvergasers erlauben. Als erster Meilenstein wird die Implementierung der Reaktionskinetik sowie eine erste Bewertung ihrer Auswirkung auf die Partikelgrößenverteilung erreicht.



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Keywords: Zyklon, Prozessintensivierung, Partikelgrößenverteilung, Biomasse, Thermochemische Konversion

A geometric interpolation scheme for dynamic wetting in 3D VOF simulations

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Wetting phenomena are known to strongly influence the behavior of droplets or bubbles at surfaces, thereby impacting many industrial applications and also daily life. In numerical simulations to predict the behavior, often simplified modeling has been used, neglecting contact angle dynamics and hysteresis. This work presents a three-dimensional framework for simulating dynamic wetting phenomena using the volume of fluid (VOF) method, implemented in Basilisk [1]. A geometric interpolation scheme is developed to obtain an accurate and reliable value of the contact line velocity. To capture realistic wetting dynamics, a dynamic contact angle model is integrated that considers also contact angle hysteresis [2]. Our framework allows for a three-dimensional evolution of the contact line if axial symmetry does not hold true [3]. The approach is validated against various experimental results of droplet spreading and sliding and demonstrates quantitative agreement with the wetting behavior observed. Additionally, a comparative analysis between dynamic and static contact angle models is performed. A validation example of droplet splashing is shown in Fig. 1 [3,4].

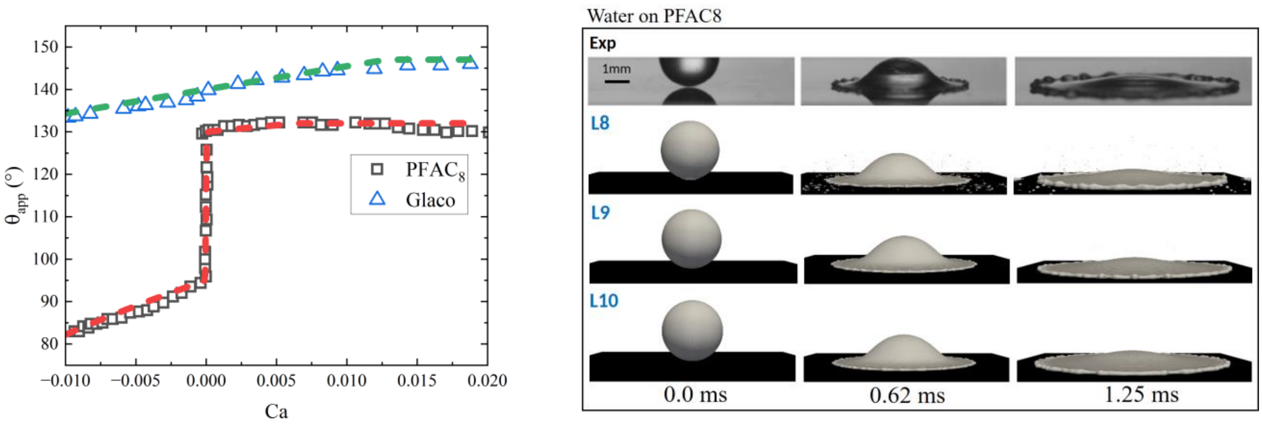

Fig. 1: Droplet impacting a hydrophobic PFAC8 surface. Left – wetting dynamics (Ca is the dimensionless contact line velocity). Right – comparison of experimental [4] (top) and simulation results [3] (below; resolution is increasing downwards).

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Keywords: dynamic wetting, contact line velocity, volume of fluid method, geometric interpolation.

CFD Investigation of porous felts based on CT-Scans

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Papermaking is an energy-intensive process. Even small increases in mechanical dewatering significantly reduce the energy demand for thermal drying. In the press section, the paper web is dewatered by the combination of pressure and press felts of polyamide fibers. The felt accepts water from the paper web under force. Due to the expansion of the felt beyond the pressing region, rewetting reduces the dry content of the paper web. Although several studies have examined the structural properties of press felts, the detailed flow behavior inside their complex, porous structure remains insufficiently understood, limiting further optimization of dewatering efficiency and rewetting control.

In this work, X-ray computed tomography (CT) is used to reconstruct the three-dimensional microstructure of an industrial press felt. After binarization, the geometry can be imported to Simcenter STAR-CCM+ to conduct CFD simulations [1]. As a validation, pressure drop measurements were performed to derive the permeability κ and the Forchheimer coefficient β via Equation 1 [2].

$$\frac{\Delta p}{L} = \frac{\eta}{\kappa} \cdot v + \rho \cdot \beta \cdot v^2 \tag{1}$$

Actual deviations between the simulation and experiments are attributed to binarization limitations of the CT reconstruction. Therefore, additional tests were carried out to identify the most reliable reconstruction algorithm. Since the porosity of the felt differs between the experiment and simulation, the initial results take this difference into account and showing a correlation between the friction factor f_p and the modified Reynolds number Re* (see Figure 1a). Additionally, the streamlines of the dimensionless velocity (v/v_0) indicate the formation of preferred channels in the porous medium, revealing an uneven mass transport across the felt (see Figure 1b).

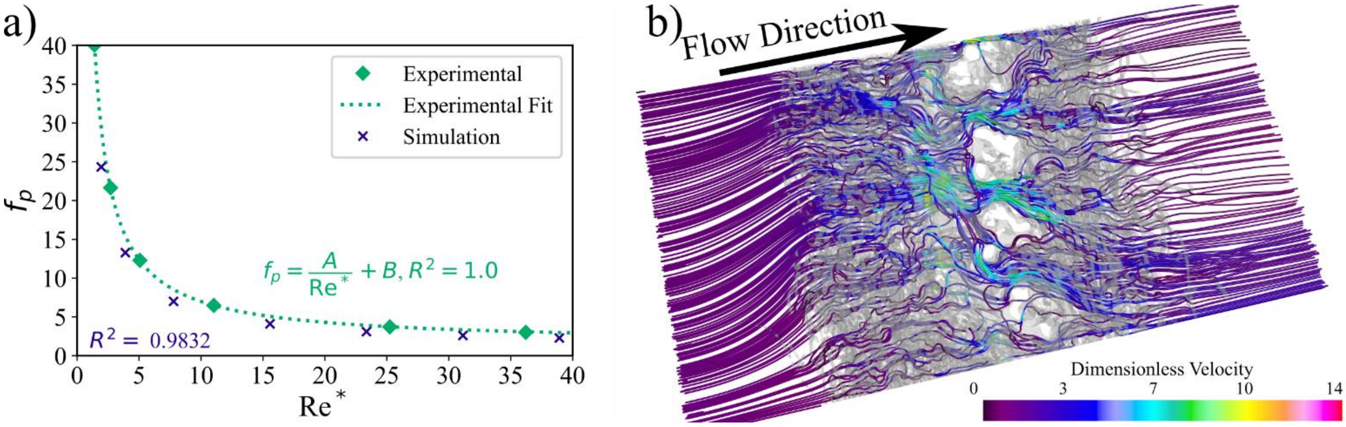

Figure 1: a) Comparison between experimental and simulation values for the friction factor f_p vs. the modified Reynolds number Re* accounting for different porosities b) Streamlines of the dimensionless velocity v/v_0 showing preferred channels in the felt.

Ongoing work involves tomography and pressure drop measurements under compressed conditions. These experiments enable the determination of the permeability κ and the Forchheimer coefficient β as a function of pressure. The CFD model provides insights into dewatering and rewetting on the pore scale and can serve as a basis to develop innovative, more effective press felt designs.

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Keywords: Porous media, permeability, dewatering, pressure drop.

Application of a Morphology-Adaptive Approach to the Gas-Liquid Flow in a Rotating Packed Bed

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The Rotating Packed Bed (RPB) is a device that exploits high-gravity fields to intensify gas-liquid mass transfer and has its use cases in fluid separation processes especially in distillation and absorption. In essence, the RPB consists of a rotating annular rigid bed which produces high centrifugal field. The liquid is fed at the center of the RPB, while the gas flows from the outer casing of the RPB inwards in the counter-current setup. However, despite the promise of intensified transfers, the RPB has not been widely utilized in industrial context in Europe to date. This is due to incomplete knowledge about the device, for example the phase distribution and flow regime of the gas-liquid flow inside the packing are unknown, even though these factors are essential for proper scale-up and design. Recent experimental studies on RPBs have contributed useful data, such as the overall volumetric mass transfer coefficient [1] and liquid holdup in the packing using computed tomography [2]. However, these are still insufficient to provide adequate information for reliable process modeling, for instance the liquid holdup data is limited to aqueous systems. We thus employ computational methodologies to complement existing insights into the device.

The metal foam NCX 1116 by Recemat BV, which is often applied as packing in RPB operations, is reconstructed to finely resolve the gas-liquid-solid interaction in the simulations. We implement a reconstruction procedure for the metal foam and utilize the produced foam surface in the grid generation process [3]. Earlier Volume-of-Fluid (VOF) based multiphase flow simulations reveal that the complex geometry of the metal foam and the interplay of the different forces inside the packing generate flow structures spanning a wide range of length scale, such that the smaller liquid droplet would become under-resolved in the context of VOF.

In principle, adopting a finer discretization should capture the flow structures that are presently under-resolved. However, finer grids would increase the computational effort exponentially and render the simulation infeasible. To address this issue, we applied a morphology adaptive modeling (MultiMorph, [4]) that is able to handle the dispersed as well as resolved interfacial structures. With the MultiMorph model, the VOF method is recovered in the limit of highly resolved interfaces and the Euler-Euler method is recovered in the limit of poorly resolved dispersed interfaces. The MultiMorph model thus allows the resolution of larger flow structures that are possible given a computational grid while maintaining a realistic physical description of the under-resolved dispersed phase.

In our contribution, we present the application of the MultiMorph model for the gas-liquid flow simulations inside the complex geometry of metal foam packing in the RPB. The simulations are compared to the VOF method qualitatively (see e.g. Figure 1) as well as quantitatively in terms of local liquid holdup and specific surface area between gas and liquid in the packing. These quantities are essential in the description of the heat and mass transfer processes inside the device and currently cannot be determined experimentally, which emphasizes the significance of our contribution in the research of RPBs.

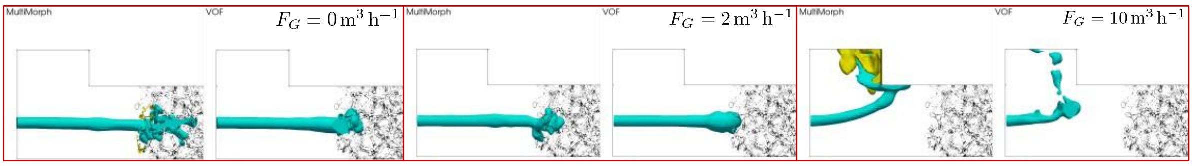

Figure 1 - Comparison of MultiMorph (left) and VOF (right) simulations of the RPB at different gas counter-current flow rate through visualizations of the isoVolume of the liquid phase and feature edges of the domain.

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Keywords: Rotating packed Bed, Metal foams, Virtual reconstruction, Morphology adaptive multifield, VOF, Two-fluid model.

CFD Modeling of Water Desalination Using Nanoporous Membrane Contactors

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Membrane distillation (MD) is a thermally driven desalination process operating at moderate temperatures and suitable for low-grade heat utilization. In direct contact membrane distillation (DCMD), a hydrophobic porous membrane separates a hot saline feed from a cold permeate stream, enabling vapor transport driven by a vapor pressure gradient [1].
In this work, a two-dimensional CFD model of a flat-sheet DCMD module is developed to resolve coupled momentum, heat, and mass transfer in the feed channel, membrane, and permeate channel. The computational domain consists of two channels, each 400 mm long, separated by a 100-µm-thick porous membrane. Vapor transport inside the membrane is described using a combined Knudsen–Poiseuille model to account for transitional flow in the membrane pores. The governing equations are solved using the Galerkin finite-element method with appropriate numerical stabilization schemes. Mesh refinement is applied near the membrane interfaces to accurately capture steep temperature and concentration gradients.
The model predicts velocity, temperature, vapor concentration, and diffusive vapor flux distributions throughout the module. Hot feed water at 333 K and cold permeate water at 293 K flow counter-currently. Evaporation occurs at the feed–membrane interface, followed by vapor diffusion through the membrane pores. Figure 1a–c shows representative temperature, vapor concentration, and diffusive vapor flux distributions. Along the module length, the thermal driving force decreases due to heat transfer and vapor transport.
To quantify polarization effects, the temperature polarization coefficient (TPC) and concentration polarization coefficient (CPC) are evaluated from temperature and vapor-concentration profiles extracted at the module mid-length. Figure 1c illustrates the transverse temperature and concentration profiles for inlet velocities of 0.1 and 1.0 m s^{-1}. Increasing inlet velocity significantly reduces both thermal and concentration polarization [2]. As summarized in Table 1, the TPC increases from 0.31 at 0.1 m s^{-1} to 0.62 at 1.0 m s^{-1}, indicating enhanced convective heat transfer and thinner thermal boundary layers. Similarly, the CPC rises from 0.23 to 0.36 with increasing velocity, reflecting reduced mass-transfer resistance and weaker vapor depletion near the membrane surface. These results demonstrate that inlet velocity is a key operating parameter controlling polarization effects in DCMD. The presented CFD framework provides a valuable tool for analysing transport limitations and supporting the hydrodynamic optimization of membrane distillation modules.

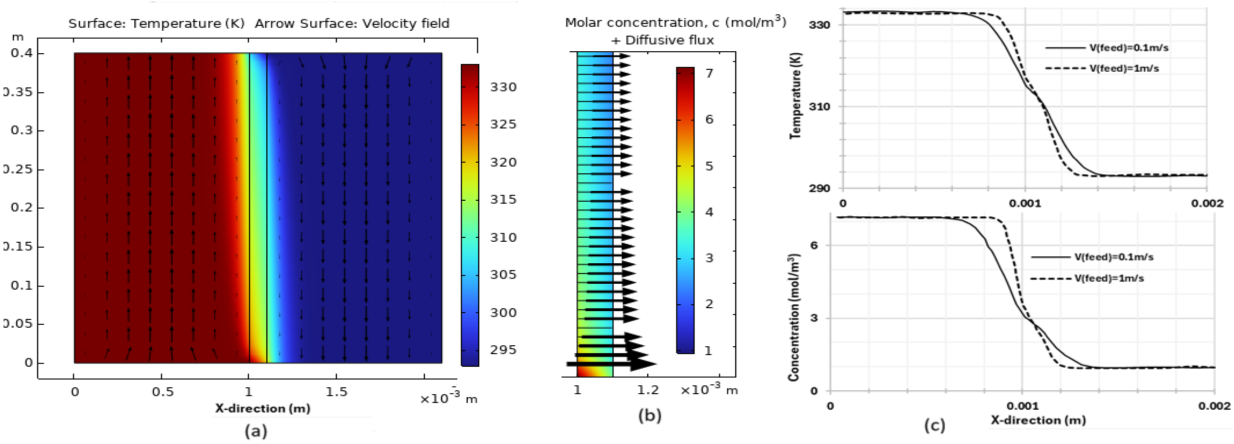

Fig. 1. (a) Temperature and vapor concentration contours, (b) diffusive vapor flux distribution, (c) transverse temperature and concentration profiles.

Table 1. Effect of inlet velocity on temperature and concentration polarization coefficients

Velocity (m s^{-1})	T_{feed} (K)	$T_{permeate}$ (K)	TPC	CPC
0.1	333	293	0.31	0.23
0.5	333	293	0.46	0.28
1.0	333	293	0.62	0.36

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Keywords: CFD simulations; membrane distillation; porous membranes

CFD based Multiphase Analysis of Drying Dynamics in an Industrial Spray Dryer

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Spray drying is a key unit operation in the food, pharmaceutical, and chemical industries, where complex multiphase flow phenomena strongly affect process efficiency and final product quality. Accurate numerical modelling of industrial spray dryers remains challenging due to the wide range of spatial and temporal scales involved, spanning from millimetre-scale nozzle flows to metre-scale drying chambers, and from millisecond droplet breakup to residence times on the order of minutes. In this work, Computational Fluid Dynamics (CFD) is applied to investigate airflow dynamics within a full-scale industrial spray-drying tower with a tower height of 16m and chamber diameter of 6m, with particular emphasis on free and coaxial jet development and swirl-induced flow structures using swirl vanes. A systematic comparison of turbulence modelling approaches is performed, including steady Reynolds-Averaged Navier–Stokes (RANS) using various turbulence models, unsteady RANS, and Large-Eddy Simulation (LES) employing the WALE subgrid-scale model which is further used for multiphase flow initialisation. The flow near the walls nozzles is resolved to 30-40 times Kolmogorov length scale and provides valuable insights into flow recirculation and shedding phenomena. The analysis aims to provide in-depth insights into jet stability, recirculation zones near the top wall, and near-nozzle jet flow behaviour, all of which play a crucial role in industrial dryer performance and mitigation of explosion risks.

To approach realistic drying conditions, multiphase simulations are conducted using an Euler–Lagrange framework coupled with a Reaction Engineering Approach (REA) for droplet evaporation. Various case studies using full-fat milk are used to analyse droplet trajectories, evaporation rates, and particle–wall interactions relevant to understanding wall deposition or fouling. The effects of particle temperature (50–80 °C), drying air temperature (150–220 °C), and inlet air humidity on moisture content, residence time, and wall impingement are systematically investigated. These results aim to establish a foundation for future wall-sticking models and quantitative assessments of fouling risk. Model validation against aerodynamic rake measurements demonstrates strong agreement in free-jet velocity profiles with an average error of 5%, despite the complexity and scale of the industrial geometry. Overall, the study highlights the capability of advanced CFD and multiphase modelling to support the optimisation of air distributor designs and mitigate fouling risks, contributing to safer and more efficient industrial spray drying processes.

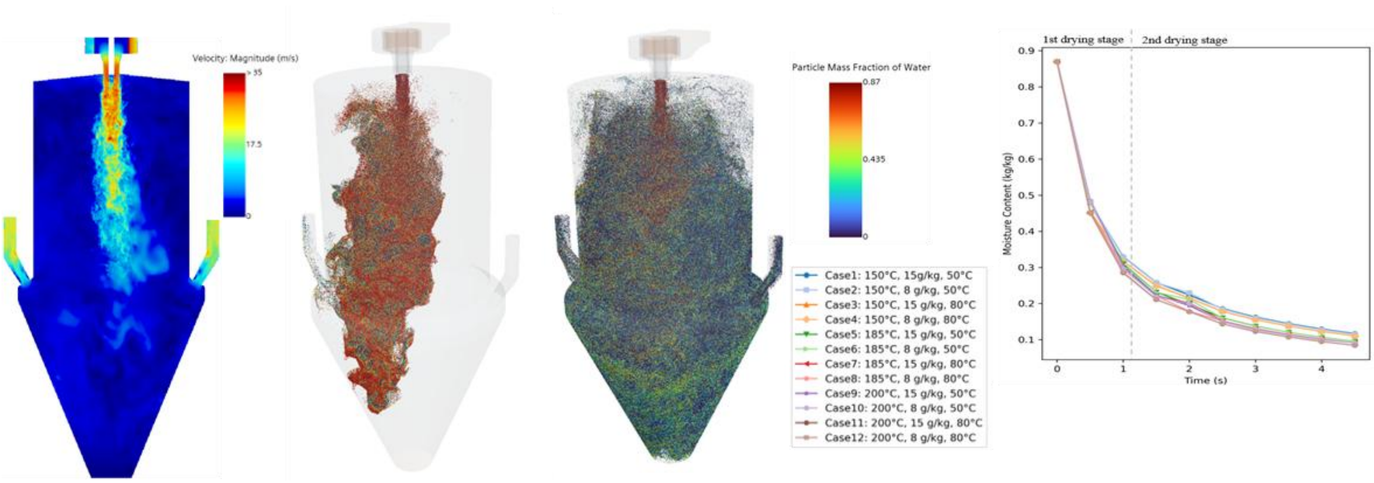

Figure 1 Velocity field, particle evaporation behaviour, and moisture evolution in an industrial spray dryer for different operating conditions.

Keywords: Spray drying, Multiphase CFD, Turbulence modelling, Large-Eddy Simulation (LES), Reaction Engineering Approach, Droplet evaporation.

CFD Modelling of Fibre Suspension in Turbulent Backward-Facing Step Flow

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The flow behaviour of fibre suspensions plays a critical role in paper manufacturing, as achieving a uniform flow is essential for producing a uniform paper structure. Controlled turbulence is therefore employed to prevent fibre flocculation and ensure consistent sheet formation. Particle Image Velocimetry (PIV) is employed to investigate the interaction between fibres and the surrounding flow field, providing high-resolution velocity-vector measurements [1]. While PIV provides detailed velocity-field information for flows that are optically accessible, CFD simulations enable insights into real machine geometries. Moreover, CFD allows rapid modification of boundary conditions and geometrical configurations, facilitating flow optimisation without the time-consuming and costly adjustments required for experimental rigs. Once validated, CFD simulations provide a robust framework to systematically examine different flow regimes, geometric configurations, and fibre characteristics. These insights support the targeted optimisation of paper-machine fluid dynamics, generating the right level of turbulence to suppress flocculation, achieve highly uniform paper, and, where possible, increase operational efficiency under given boundary conditions.

In this work, a CFD model was developed in Simcenter STAR-CCM+ and validated against experimental PIV data from our project partners at the Technical University of Darmstadt. A modified Fibre Floc Evolution (FFE) method, which treats fibres in suspension as an immiscible liquid, was implemented to model flocculation phenomena [2]. A turbulent Eulerian–Eulerian multiphase simulation was conducted. For validation, velocity profiles downstream of the test section were extracted along a reference line in the Y-direction (Figure 1a) and compared with corresponding PIV measurements. The validation is based on an experimental channel equipped with a backward-facing step, intentionally integrated as a turbulence generator to produce the controlled turbulent mixing required to suppress fibre flocculation in paper-forming processes. Additionally, contour plots of the velocity field from both numerical and experimental analyses were compared (Figure 1a), revealing a deviation of maximum velocity of only 8.6 %. As shown in Figure 1b, the simulated and experimental velocity distributions exhibit strong agreement.

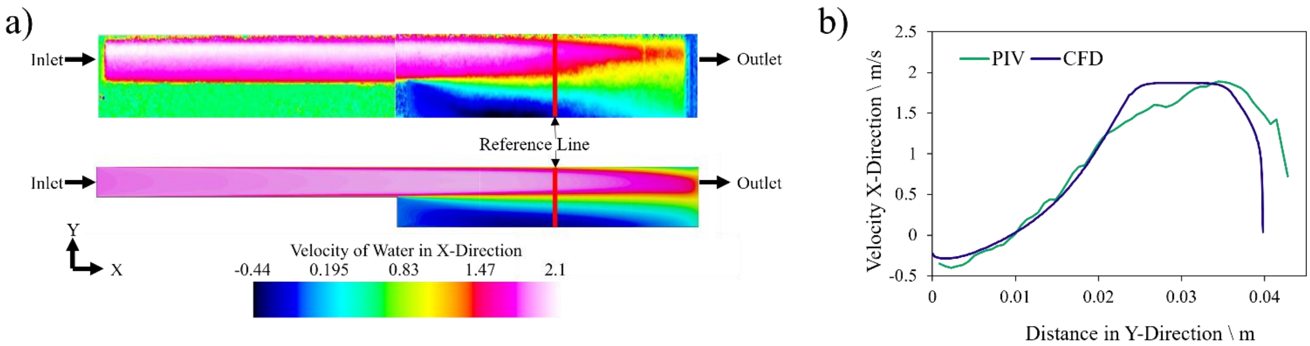

Figure 1 a) Velocity contour obtained from PIV (Top) and CFD (Bottom) b) Velocity in X direction along the reference line

These results demonstrate the capability of the CFD model to reliably capture key flow characteristics of fibre suspensions. Future work will extend the validation by examining additional parameters, including floc diameter, turbulent kinetic energy, and other relevant flow metrics. With this model it is then possible to optimize the geometry of the sheet forming section.

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Keywords: “Computational Fluid Dynamics”, “Eulerian Eulerian Multiphase simulation”, “Suspension Flow Dynamics”

Numerical investigation of additively manufactured internal structures for enhanced heat transfer in fixed bed structures

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Radial heat transport in narrow packed-bed reactors with small bed to particle diameter (1.5<N<5) is a key factor for temperature fields, reaction rates and catalyst stability in strongly exothermic or endothermic gas–solid processes. In such configurations, heat is mainly supplied or removed through the reactor wall, so that wall-adjacent bed morphology, local hydrodynamics and the interplay of conductive, convective and radiative mechanisms jointly govern reactor performance. To control or suppress near-wall channeling and increase heat transfer, a variety of additively manufactured fins, lattices and surface structures are implemented both experimentally and numerically in this project. To study these coupled phenomena, the projects complexity is incrementally increased by starting with morphological investigations of the bed followed by a lab-scale reactor for low temperature thermal inspections and then a further reactor with dry reforming of methane (DRM) as a representative reaction system. These investigations are conducted and closely linked both experimentally (Klaus Hahn, KIT) and numerically through Particle Resolved CFD (PRCFD) (Alexander Nicolai, TU Berlin). A particular focus is on the heat transfer in the near-wall region.

The current and initial stage yields numerical considerations to accelerate the particle-filling of the reactor bed and solely concentrates on morphological aspects. Previous studies have suggested internal structures to enhance the heat transfer [1] or compared the typical Direct Energy Method (DEM) with the rigid body method for the filling procedure [2]. The lack of experimental validation data for both methods is the source of this investigation. Hence, a digital DEM design study of different particle (sphere, cylinder) and reactor shapes (straight or spiral fins, periodic open cellular structures (POCS), wavy reactor walls or manipulated reactor surfaces) will reduce the spectrum of possible reactor configurations. The aim is a densely packed bed, a radial and axial porosity profile and their correlation to the reactor geometry and particle properties. Based on these results, the designs are additively fabricated and experimentally filled with the particles to then be scanned through NMR. A consecutive study compares the computationally highly efficient rigid body method versus the physically appropriate DEM with the scanned topology as its validation data.

The progress and not to mention the workflow of these initial results combined or embedded within the whole project is presented. Future steps include the acceleration of the PRCFD meshing pipeline and fluid dynamical and thermal investigations all the way to the DRM reaction.

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Keywords: CFD-DEM, Rigid Body, Additive Manufacturing, Heat Transfer

Entwicklung eines effizienten Simulationsmodells für die Spanerfassung beim Nutsägen im Gleichlauf

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Eine leistungsfähige Absaugung und damit Erfassung der Späne bei spanender Holzbearbeitung ist nicht nur aus Sicht des Arbeits- und Brandschutzes essenziell, sondern trägt auch maßgeblich zu einer hohen Oberflächengüte der gefertigten Werkstücke bei. Durch geeignete Gestaltung kann der dafür erforderliche Energiebedarf reduziert werden. Das Nutsägen mit scheibenförmigen Werkzeugen im Gleichlauf stellt eine besondere Herausforderung dar, weil ein Teil der entstehenden Späne durch die Nut ausgeworfen und häufig nicht ausreichend erfasst wird, was zu einem geringen Erfassungsgrad führt [1].
Die relevanten physikalischen Prozesse bei diesem Bearbeitungsvorgang reichen von der Zerspanung über Span-Span- und Span-Wand-Kollisionen bis hin zum Flugverhalten und pneumatischen Transport der Späne. Gleichzeitig ist die Industrie an effizienten Berechnungsmethoden, das heißt Methoden mit vertretbarem Berechnungsaufwand und hinreichender Genauigkeit, interessiert, mit deren Hilfe verbesserte Systeme zur Spanerfassung mit reduziertem Versuchsaufwand entwickelt werden können.
Im vorliegenden Beitrag wird eine solche Berechnungsmethode unter Verwendung der Software Simcenter STAR-CCM+ vorgestellt. Die Berechnung der Luftströmung in der Absaughaube mit rotierendem Werkzeug wird dabei mit der Simulation der Spanbewegung gekoppelt. Für die Strömung werden die Reynolds-gemittelten Navier-Stokes-Gleichungen mit k-ω-SST-Turbulenzmodell gelöst. Zur Partikelsimulation kommt die Diskrete-Elemente-Methode zum Einsatz. Ziel ist die realistische Berechnung der Erfassungsgrade von Holzspänen in Abhängigkeit von der Haubengeometrie sowie von Zerspanungs- und Absaugparametern.
Die Strömung um das rotierende Werkzeug und die Durchströmung der Absaughaube beeinflussen sich gegenseitig und können deshalb nicht unabhängig voneinander betrachtet werden. Zur Reduzierung des Berechnungsaufwands werden die wandnahen Grenzschichten weitestgehend nicht aufgelöst, sie haben für die Spanbewegung in diesem Bereich eine untergeordnete Bedeutung. Die Werkzeugbewegung wird als rotierender Bereich mit „sliding mesh interface“ abgebildet. Die Spanfreisetzung wird durch mitbewegte Partikelinjektoren in der Nähe der Werkzeugschneiden modelliert. Auf Grundlage einer optischen Klassifizierung real erzeugter Späne aus Spanplatte [2] wird ein reduziertes Größen- und Formspektrum wie folgt definiert: Das Größenspektrum wird auf die am häufigsten auftretende Größenklasse reduziert. Das Formspektrum dieser Größenklasse wird mithilfe realistischer Verteilungen modellhafter Formparameter, wie Seitenverhältnis und Spherizität, abgebildet. Das Kollisionsverhalten der Späne mit dem Werkzeugkörper und der Absauganlage beeinflussen den weiteren Weg der Partikel maßgeblich. Als Kollisionsmodell wird das Hertz-Mindlin-Modell verwendet, die notwendigen Parameter sind Resultate von Kollisionsexperimente mit realen Spänen. Der Flug der Späne wird maßgeblich durch die Partikelträgheit sowie den Luftwiderstand bestimmt, der mit dem Haider-Levenspiel-Modell für nichtspärische Partikel berechnet wird.
Das Zusammenspiel der Modellierung von Spanfreisetzung, Kollisionsverhalten und Spanflug wird zunächst anhand von Zerspanungsversuchen ohne Absaughaube validiert. Dabei werden die optisch bestimmten Partikeltrajektorien aus Experimenten mit den simulierten Partikeltrajektorien verglichen. Die grundsätzliche Modellkonfiguration baut auf [3] auf. Anwendung findet die Methode schließlich bei der Simulation eines Zerspanungsvorgangs mit Absaughaube. Die dabei ermittelten Werte des Spanerfassungsgrades werden mit experimentell ermittelten Erfassungsgraden verglichen.
Der Beitrag stellt die wesentlichen Modellierungen und Vereinfachungen der Methode zur effizienten Berechnung des Spanerfassung detailliert vor. Durch zahlreiche Vergleiche mit verschiedenen experimentellen Referenzdaten wird die Qualität der Methode beurteilt.

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