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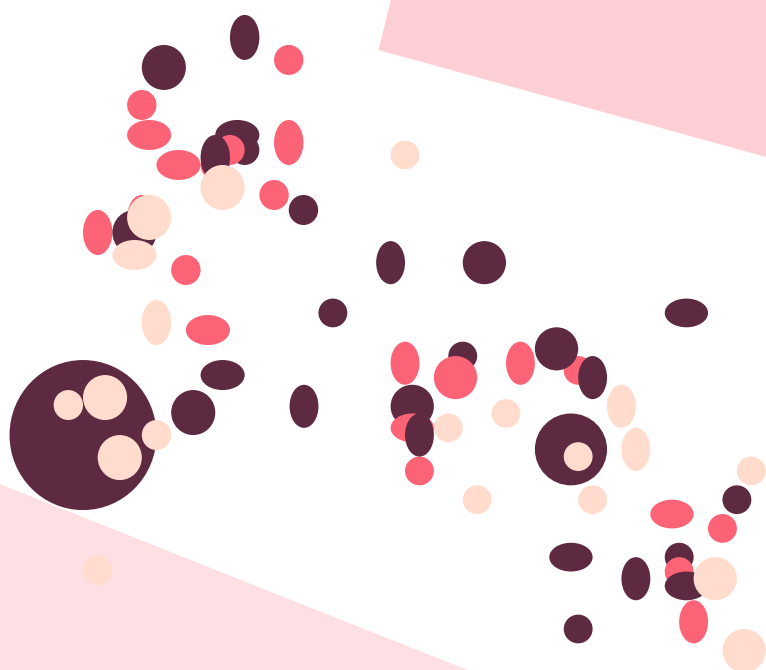
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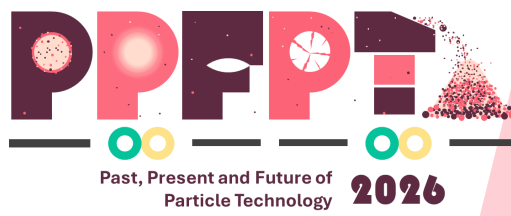
Past, Present and Future of
Particle Technology

2026



Book of Abstracts

30th March – 1st April 2026



Book of Abstracts

Past, Present and Future of Particle Technology Conference 2026

Editors:

Wei Pin Goh

Colin Hare

Mojtaba Ghadiri

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Preface

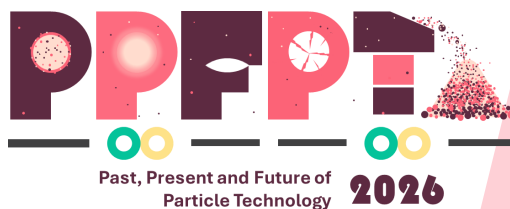
Ever since the EPSRC Specially-Promoted Programme on Particle Technology, coordinated by the late Leslie J. Ford, the UK has maintained a globally leading position in the field. Over the past decades, tremendous progress has been achieved in the design of advanced processes, novel instrumentation for powder characterisation, and the development of robust sensors for online and at-line process monitoring and control.

Recent years have seen the emergence of transformative technologies that are reshaping particle science and engineering. High-resolution imaging (e.g. X-ray computed tomography, focused ion beam SEM), dynamic powder rheometry, and image-based and laser diffraction systems for particle shape and size analyses have greatly enhanced our ability to quantify particle morphology, flowability, spreadability, dispersion, breakability and cohesion under process-relevant conditions. Parallel advances in multi-scale modelling, from discrete element methods (DEM) and computational fluid dynamics (CFD) to population balance modelling (PBM), have deepened our understanding of complex particulate systems across manufacturing scales.

Continuous manufacturing in the pharmaceutical sector and powder-based additive manufacturing (AM) are prime examples of areas that have benefited from these developments. These technologies rely on a much-improved grasp of powder behaviour, flow dynamics, and interparticle interactions, leading to enhanced process robustness and product quality.

Today, however, the field is undergoing a new paradigm shift driven by the exponential growth of Artificial Intelligence (AI) and Machine Learning (ML). Data-centric approaches are increasingly being used to complement traditional experimental and simulation techniques. Machine learning algorithms, ranging from physics-informed neural networks and Gaussian process regression to deep convolutional and graph neural networks, are being applied to predict powder flow, optimise mixing and granulation processes, and identify critical material attributes from high-dimensional datasets. The integration of ML with digital twins and real-time sensor data is enabling intelligent process control, adaptive manufacturing, and predictive maintenance, moving the industry closer to fully autonomous, data-driven particulate processing.

This booklet presents the abstracts from the three-day conference, encompassing plenary and keynote lectures, as well as oral and poster presentations. In support of developing future leaders in the field, half a day is dedicated to early-career researchers (ECRs), offering them a valuable opportunity to present their work, exchange ideas, and engage with established experts. The ECR session is sponsored



by the Particle Technology Special Interest Group of the Institution of Chemical Engineers. The Royal Society of Chemistry Particle Characterisation Interest Group and Formulation Science & Technology Group sponsor the poster presentation award and poster reception, while Malvern Panalytical and Verder Scientific are sponsoring and exhibiting at the conference.

Organising Committee

Wei Pin Goh – University of Leeds

Colin Hare – Newcastle University

Mojtaba Ghadiri – University of Leeds

March 2026, Leeds, United Kingdom

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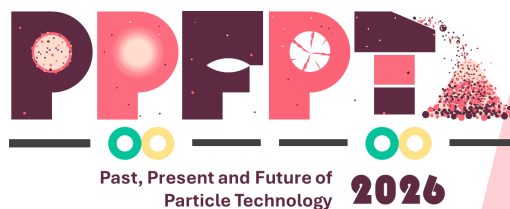
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Past, Present and Future Particle Technology - A Focused Personal Overview (Part 1)

Mojtaba Ghadiri

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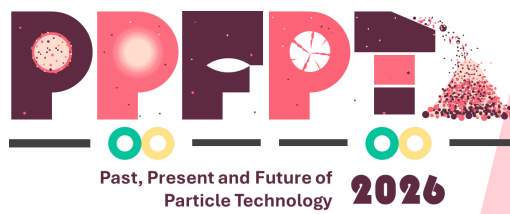


Over the course of my research career, I have worked across four areas of particle technology: size reduction, size enlargement, powder flow and fluidisation, and electrical and environmental phenomena in particulate systems. A unifying theme throughout this work has been the relationship between bulk behaviour and single-particle characteristics, while accounting for the influence of the surrounding medium.

In reflecting on the historical development of particle technology, this talk will focus on my work on the attrition of particulate solids, the area to which I have devoted the greatest attention. Particulate solids exhibit an exceptional diversity of physical, chemical, and mechanical properties, and the study of attrition therefore requires careful consideration of both material properties and process dynamics. Particle breakage mechanisms, whether brittle or semi-brittle, depend not only on mechanical parameters such as elastic and plastic moduli and fracture toughness, but also on strain rate, particle structure, and interparticle interactions.

Under dense-phase flow conditions, particles experience multiple contacts with their neighbours, characterised by the coordination number. These conditions promote compressive stresses within particles, while interparticle force chains generate the shear and tensile stresses that lead to fracture. In contrast, under lean-phase flow conditions, particle stressing is dominated by collisions, which become the primary mechanism for breakage. Consequently, understanding attrition requires careful analysis of the flow regimes in which it occurs. To support such analysis, modelling tools including the Discrete Element Method (DEM), coupled with Computational Fluid Dynamics (CFD), have been employed to describe particle assemblies and their interactions with the fluid phase.

Experimentally, several techniques have been developed to characterise attrition under different regimes. For lean-phase conditions, we developed a single-particle impact tester together with two aerodynamic dispersion methods for generating controlled impact stresses. For dense-phase conditions, we employed the Bridgewater attrition shear cell. Analysis of particle breakage in dense flows is more complex, and predictive capabilities remain at an early stage of development. Furthermore, depending on particle structure and mechanical properties, a coupled effect may arise



in which impact stressing enhances the propensity for breakage under shear deformation. To investigate this behaviour, we developed the Particle Shear and Impact Tester. This instrument has been used extensively to evaluate enzyme dust release during attrition of detergent enzyme granules, an issue of practical importance in the detergent industry.

The presentation will provide a brief overview of selected analytical approaches and experimental tools developed for investigating the attrition of particulate solids.

Past, Present and Future Particle Technology - A Focused Personal Overview (Part 2)

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Like Mojtaba Ghadiri, I have had a wide-ranging research career which has, I hope, been unified to some extent by the same interesting tension between the bulk behaviour of particles in industrial processes and the underlying physics of the interactions between individual particles. As a new lecturer I was fascinated by the very wide range of behaviour exhibited by particles in different situations – particularly fluidisation and filtration in my case – but rather dissatisfied by the explanations, which acknowledged the dominant importance of particle size but seemed to gloss over the physics of particle contact. As Mojtaba and I both discovered, there is a large community of physicists and surface chemists working in this area from whom we, as engineers, can learn a great deal.

In fluidisation, the weight of the particles is balanced by the drag of the fluid so that quite small cohesive forces can be expected to have an effect on the macroscopic behaviour. I became quite fascinated by cohesion in fluidisation and in part of my talk I will summarise those studies.

One of the difficulties in investigating granular materials is that they are opaque, so that really knowing what is going on inside the flowing bulk or within a process is very difficult. In some ways, the major development in my research has been my adoption of positron imaging methods, particularly Positron Emission Particle Tracking (PEPT), and I shall talk a little about that very powerful technique.

If there is a tension between understanding bulk behaviour and single particle properties then there is also an interesting (and – in my view – productive) tension between curiosity-driven research and industrial applications. Engineers exist to build things and solve problems. We have to focus on finding solutions, but we also need to stay curious. Most of the projects I've been involved in during my career have had industrial involvement; some have arguably resulted in industrial impact while some have not, despite my high expectations! Among my attempts at industrial impact I think particularly of the commercialisation of ceramic filters, understanding of high shear mixer-granulators and the continuous twin screw granulators that have partially replaced them, processes for generation of micro-particles by precipitation from supercritical fluids, use of fluidised beds for direct solar power, improved control of

Advanced Modelling and Simulation for Granular and Multiphase Flows: Recent Advances and Future Opportunities

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Granular and multiphase flow systems are widely encountered in chemical, energy, pharmaceutical, and materials processing industries. Understanding particle–fluid interactions is crucial for optimizing industrial operations such as milling, mixing, and fluidization. In recent years, numerical simulations based on Eulerian–Lagrangian approaches have emerged as powerful tools for analyzing these complex systems. However, their application to industrial-scale processes remains challenging due to the extremely large number of particles, strong particle–fluid coupling, and the presence of complex moving boundaries. This presentation introduces recent advances in large-scale modeling and simulation for granular and multiphase flows using the Discrete Element Method (DEM) coupled with Computational Fluid Dynamics (CFD) and Volume of Fluid (VOF) approaches. First, a validated coarse-grained DEM–CFD framework for bead mill systems is presented. By combining coarse-graining techniques, an implicit drag-force algorithm, and a scalar-field-based wall boundary model, the proposed approach enables stable simulations of high-shear liquid–particle systems containing enormous numbers of beads while preserving macroscopic particle behavior. Second, recent developments in the simulation of gas–solid–liquid three-phase flows are discussed. A refined-grid model integrated with a coarse-grained DEM–VOF framework allows flexible grid selection independent of particle size while significantly reducing computational cost. Third, particle–fluid interactions in powder mixing are investigated using an advanced Eulerian–Lagrangian framework. Numerical results demonstrate that airflow can accelerate the mixing of fine particles through air entrainment and drag-induced particle motion. Finally, recent advances in heat transfer modeling within DEM-based simulations are introduced. Although the Discrete Element Method (DEM) coupled with Computational Fluid Dynamics (CFD) is widely used for solid–fluid systems, existing DEM heat transfer models have fundamental limitations. These arise from the soft-sphere contact model in DEM, where heat conduction depends on spring constants and requires complex modeling of particle contact states. In addition, conventional models show poor compatibility with scaling approaches such as the coarse-grained DEM. To address these challenges, a novel heat transfer model based on an Eulerian framework is developed. In this approach, particle motion is calculated by DEM, while heat transfer is solved using an Eulerian description, where solid-phase conduction is

represented through the void fraction without explicitly modeling particle contacts. Validation tests demonstrate that the predicted temperature field is independent of particle contact conditions and remains accurate when combined with the coarse-grained DEM. These results highlight the potential of the proposed model for efficient and reliable DEM–CFD simulations of industrial multiphase systems.

The author acknowledges financial support from the Japan Society for the Promotion of Science KAKENHI (JSPS Grant No. 24K22289), the Social Cooperation Program for Fundamental Technologies on Powder Process Digital Twin at The University of Tokyo, and the Social Cooperation Program for Digital Twin Fundamental Technology Course for Next Generation Resource Circulation Solutions at The University of Tokyo.

Bridging the Scales: Thermomechanical Modelling of Granular Materials

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In many granular material handling processes, friction and inelastic collisions cause heat generation and temperature rise, yet the self-heating phenomenon is not well understood. In this talk, we present a multiscale thermomechanical modelling framework to bridge microscopic and macroscopic behaviours. At the microscopic level, the thermal response of single particles during contacts is modelled using the finite element method (FEM), from which microscopic models for heat generation due to plastic deformation and frictional interactions were identified. At the macroscopic level, two complementary models were developed: a Discrete Element Method (DEM) model for granular flow and a FEM model for powder compaction.

First, a DEM model considering friction-induced heat generation and heat transfer is developed and validated. Experiments in a rotating drum under varying speeds and fill ratios show that denser particles generate more heat, higher rotation speeds promote temperature rise, and fill ratio has a minimal effect on thermal response. Key findings from the DEM model indicate that the coefficient of variation (CV) of particle temperature decreases and stabilises within five minutes of drum rotation, signifying uniform heat distribution. Simulated wall temperature distributions also match the annular patterns observed via infrared thermography, and increased drum speed expands the heated region on the wall and increases the heat absorbed by particles.

Second, an FEM analysis of the thermo-mechanical behaviour of powders during die compaction is performed. This model incorporates heat generated from both compression work and frictional interactions at particle-particle and die-wall interfaces. Results show that punch shape, compression speed, and die-wall friction significantly influence temperature and density distributions within the compact. Specifically, lower die-wall friction and reduced compression speed are found to decrease the tablet temperature upon ejection.

These multiscale models provide a comprehensive approach for predicting heat generation in granular materials across different regimes, from discrete flow to continuum-like deformation.

Powder Technology Opportunities and Challenges for Battery Electrode Manufacturing

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Lithium-ion batteries are now an essential part of everyday life. Increasing demand for these devices, driven by the urgent need to reduce carbon emissions, had led to increased scrutiny of the battery manufacturing process. In particular there is a drive to improve the efficiency of battery electrode production, reduce the requirement for hazardous solvents, and develop new methods which can provide better control over electrode microstructure.

In this presentation, recent advances spanning the breadth of the electrode manufacturing process are discussed. Current opportunities for particle technology to improve electrode manufacture are considered, alongside key outputs from the Faraday Institution funded research project Nextrode. An extensive physics based computational investigation of the electrode calendaring process and the effect of microstructural electrode properties on the electrode performance is presented, in conjunction with complementary machine-learning analysis (Figure 1).

Recently developed manufacturing techniques for solvent free electrode production are also discussed with a focus on key manufacturing constraints and opportunities for these techniques, such as reliance on fluorinated polymers, poor powder flow, and the potential to influence electrode microstructure and subsequent performance.

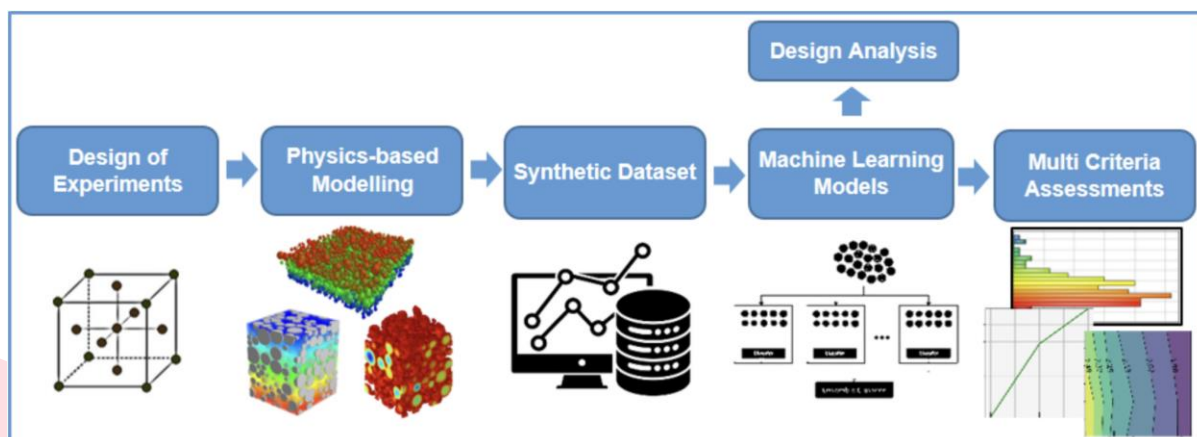


Figure 1: 3D physics modelling of battery electrode microstructures and machine learning framework (Ge et al, *Chemical Engineering Journal*, 2025, 526, 170784).

Engineering Powder Compaction: Past, Present and Future

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Where shall we begin? Bricks, ceramics, porcelain, terracotta incur packing and compacting powders in moulds. Powder metallurgy and sinter-forging dates back to the late bronze period. Pre-Columbian cultures in the Andes consolidated and sintered platinum and gold powders. Compressed tea bricks have been produced for 1500 years, not just for preservation but also for economic, logistical, fiscal, and cultural reasons, just like any modern complex formulated product in compact form. A papyrus dating back 3500 years lists hundreds of medicines formed into solid dosage forms, mostly hand rolled pills. Pill rolling has also been used in China, India, and the Middle East for 2000 years. Hypocrites and Galen worked 1500 years ago, and the European pharmacopoeia started appearing 500 years ago, likely helped by the invention of the print.

After the industrial revolution, in 1843 William Brockendon invented a “pill” making machine, a one tablet per cycle manual tool producing 5 tablets per minute. Operating on the same principles, about 100 year later, the motor driven Manesty “F press” produced 60 tablets/minute. The rotary tablet press was introduced 30 years later and its modern versions produce more than 8000 tablets per minute in normal operation. This accomplishment requires a fine-tuned formulation and a fine-tuned tablet press, e.g. engineering. Tablet compression consists of pressing a free flowing powder mixture into a solid compact using rigid dies and tooling. During compaction a range of densification mechanisms may be presents, including particle rearrangement, elastic and plastic deformation of particles as well as breakage or fragmentation, depending on the properties of the formulation constituents. The contact interactions between particles give rise to cohesion, determining the strength to tablets. Densification is a complex thermomechanical phenomenon, where the mechanical properties of the powder material change as the material densifies during densification.

We review the experimental characterization techniques developed for calibration of the Drucker-Praeger cap model used in finite element analysis of powder compaction [1]. We demonstrate that it is possible to produce identical looking tablets but with different internal density distributions and this affect tablet breakage and disintegration. We demonstrate finite element based digital tableting. Next, we return to formulation composition and introduce the concept of Successful Formulation

Window (SFW) which defines the operating space where prescribed tablet quality attributes can be met [2]. SFW is incorporated into the Virtual Formulation Laboratory, a software tool used to predict manufacturability of tablet using bulk powder properties, particle characteristics and molecular information.

Finally we introduce machine learning technologies to compaction, by linking molecular information directly to tablet manufacturability using the problem of sticking as demonstration case study. Sticking (undesired adhesion of powders to the surface of the compaction tooling), is a frequent and highly disruptive problem that occurs at the very end of the process chain when the tablet is formed. As alternatives to the mechanistic approaches to address sticking, we introduce machine learning strategies to predict sticking directly from the chemical formula of the drug substance, represented by molecular descriptors [3]. The methodology has potential to transform the development of medicines by providing manufacturability information at the drug screening stage and is potentially applicable to other manufacturing problems controlled by the chemistry of the drug substance.

We have got a glimpse in the possibilities offered by mechanistic and data driven models for compaction. But just because one thing seems logically connected with another thing, it doesn't mean that this connection actually exists. For example, we assembled a database with thousands of past and current medicines from public sources (e.g. the "Orange book"), together with the formulation composition from the actual leaflets for each dosage form. However, our proven machine learning methods were unable to extract compelling links between chemistry (molecular descriptors) and formulation composition. What does the future hold?

Acknowledgements: This work is based on the publications referenced below. The Co-authors are gratefully acknowledged.

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Powder Layer Formation and Its Characterisation for Powder Bed Fusion Additive Manufacturing

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In additive manufacturing techniques such as Powder Bed Fusion (PBF), spreading powders into thin layers is a key step. In PBF, the quality of the final artefact, particularly its definition, can be improved by using fine powders. However, cohesive interparticle forces in such powders can affect the quality of the spread layer by reducing the amount of powder delivered to the layer and by determining the occurrence of superficial defects. The effects of cohesion can be exacerbated by the use of high temperatures during the spreading process, which is typically used to reduce thermal stresses that can arise when the laser sintering/melting step is performed on a cold layer.

This note summarizes the most recent studies conducted at the University of Salerno to characterize the flowability and spreadability of commercial PBF polymeric powders at both ambient and high temperatures. The results of conventional methods for characterizing the flowability of powders, such as shear testing and rotating drum experiments, are critically compared with dedicated experiments on powder layer generation that were performed with an experimental setup that simulated the powder spreading process at operating temperatures. The quality of the powder spread was assessed by examining both the presence of defects and surface roughness using image analysis techniques. The occurrence of macroscopic defects is compared with changes in surface roughness and the flow properties of different materials at different temperatures. Powder flowability and spreadability show significant changes at different temperatures and are not strictly related to each other.

Towards a True Measurement of Powder Rheology

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Many powder processes operate under dynamic conditions, such as blending and mixing. To optimise these processes, it is beneficial to understand the prevailing shear stresses in the powder bed under these high strain rate conditions. Measurements of powder shear stress under quasi-static conditions is well established using shear cells. However, direct measurement of shear stress at elevated strain rates is limited to powder couette devices, which are difficult to operate particularly for fine cohesive powders. Couette devices also rely on an assumed shear stress profile, which has been shown to have inaccuracies due to poor powder gripping at the outer wall. Other commercial instruments for dynamic powder flow assessment are limited to dynamic angle of repose variation and torque or energy input in powder rheometers. As such, commercial rheometers cannot typically determine shear stress as a function of strain rate.

In this work we simulate the FT4 Powder Rheometer using the Discrete Element Method (DEM), calculating the prevailing shear stresses in the mobilised region in front of the blade. The shear stress is also determined from the impeller torque by taking account of the mobilised bed (non-zero velocity), which shows strong agreement between both approaches. This suggests that the shear stress can be determined from a rheometer torque measurement if the mobilised bed volume is known.

Rheometer measurements using several granular materials, coupled with high-speed camera measurements to establish the mobilised bed volume, enable the shear stress to be predicted from the above relationship. By measuring in the quasi-static regime and comparing to shear cell results, we show that the above relationship has promise. This approach enables the shear stress required for flow to be determined as a function of strain rate using a commercial rheometer, enabling true characterisation of powder rheology.

Explainable AI for Powder Characterisation

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The relationship between particle-level properties and bulk powder behaviour remains difficult to predict from first principles, presenting persistent challenges across pharmaceutical, food, chemical, and advanced manufacturing industries. Machine learning offers a pathway to establish quantitative structure-property relationships from experimental data, yet widespread industrial adoption requires models that are not only accurate but also interpretable.

This keynote begins with an introduction to AI methods applied to particle characterization, covering core concepts and practical applications across diverse powder systems. Case studies progress from conventional machine learning approaches for automated particle analysis and property prediction toward explainable AI methodologies that reveal which particle attributes most strongly influence bulk processing performance. This progression explores the future direction of the field, where transparency and interpretability become essential for regulatory compliance, industrial adoption, and scientific understanding.

Crystallogenesis – Challenges and Opportunities in Controlling Morphology Across Scales

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Crystallogenesis sits at the heart of manufacturing across pharmaceuticals, fine chemicals, food, and functional materials, where early molecular events determine form, shape, and downstream performance. Despite major advances in understanding nucleation, crystallisation processes remain challenging to control with the precision demanded, particularly as the systems of interest grow in complexity. Crystalline systems are inherently anisotropic, with directional variations in interfacial structure, surface chemistry, and molecular recognition shaping polymorphic outcome and habit; frameworks such as TiPOD and SinPOD show how interfacial and solvent-mediated interactions stabilise preferred orientations and early ordered clusters. These principles extend naturally—but not trivially—to larger and more complex modalities. Proteins and peptides introduce additional layers of complexity, including conformational flexibility, heterogeneous intermolecular interactions, and emerging secondary structure. Our recent work on the use of 3D nanotemplates for proteins and soft templates for systems such as insulin demonstrates how local environments can be modulated to enhance reproducibility, reduce induction times, and open new routes to controlling morphology and phase behaviour. For peptides, systematic studies using glycine homopeptides reveal how chain length, sequence, and protecting groups govern solubility and crystallisability, while more complex systems such as vancomycin and GnRH analogues highlight the growing importance of intermolecular interactions and secondary structure in determining crystallisation outcomes. Crystals subjected to processing conditions can undergo attrition, and their surprising ability to regenerate the fractured region and recover their original habit highlights the need for deeper insight into solid–liquid interfacial behaviour to achieve robust control of form, shape, and size. Together, these advances outline both the progress made and the emerging challenges as we seek to control morphology across increasingly complex systems, with crystallisation poised to play a central role in more efficient, sustainable, and resilient manufacturing pathways.

Tensor-Basis Neural Network Modelling of Solid Stresses in Granular Flows

Ali Ozel

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Accurate and reliable modelling of granular flows is crucial for understanding, designing and controlling large-scale particle technology processes such as silos, and drying tumblers. The hydrodynamics of these flows is driven by collisional dominated to frictional dominated (quasi-static) regimes as solid concentration increases in suspensions [1]. For industrial-scale applications, these flows can be modelled by continuum (Eulerian) approach which requires a constitutive relation for the solid phase stress. Considerable effort has been devoted in the literature on the development of stress modelling by adapting the kinetic theory of granular flows for rapid dense flows in the collisional regime [2], phenomenological rheology $\mu(I)$ -model in the frictional regime [3] and blending them in the transition regime. Recently, the computationally generated constitutive models for solid phase have been developed for dry and cohesive particles in unbounded gas-solid flows [4]. The data-driven modelling approach is advantageous because it learns constitutive behaviour directly from particle-resolved data, thereby capturing how microscopic contact mechanics and interparticle interactions develop the macroscopic stress. This makes it particularly suitable for granular flow with complex particle-particles interactions such as van der Waals, liquid bridge and electrostatics forces. In this study, we develop a Galilean-invariant Tensor Basis Neural Network (GiTBNN) model for the solid phase stress for dry granular flows using Discrete Element Model (DEM) simulation results.

We first performed DEM simulations of granular collapse of monodisperse, frictional, and slightly inelastic, spherical particles (Figure-1a & b). The Hertzian spring and dashpot model has been used for contact forces. Details of contact models can be found elsewhere [4]. We post-processed the DEM simulation results to compute the solid phase stress, σ_s . The solid stress tensor is then decomposed into isotropic and deviatoric parts as:

$$\sigma_s = p_s \mathbf{I} + \tau_s$$

where $p_s = 1/3 \text{tr}(\sigma_s)$ is the isotropic pressure and τ_s is the deviatoric stress tensor. Following [5], a GiTBNN is developed to model, τ_s . In this framework, the deviatoric stress is represented as a linear combination of scalar bases, λ_k , and tensor bases $\mathbf{T}^{(n)}$ as:

$$\tau_s = \sum_{n=1}^m g^{(n)}(\lambda_1, \dots, \lambda_k) T^{(n)},$$

where m is the order of the model and $g^{(n)}$ are scalar coefficient functions predicted by the neural network. For $m = 1$, the model gives the $\mu(I)$ -model with $\lambda_1 = p_s$, $\lambda_2 = |\mathbf{D}|$ (where $\mathbf{D}$ is the symmetric part of the velocity-gradient tensor) and $\mathbf{T}^{(1)} = \mathbf{D}$. For a high-order model $m = 3$, the scalar bases are $\lambda_1 = p_s$, $\lambda_2 = \text{tr}(\mathbf{D})$, $\lambda_3 = \text{tr}(\mathbf{D}^2)$, $\lambda_4 = |\mathbf{D}|$, $\lambda_5 = \alpha_s$ (solid volume fraction) and the tensor bases are $\mathbf{T}^{(1)} = \text{dev}(\mathbf{D})$, $\mathbf{T}^{(2)} = \text{dev}(\text{sym}(\mathbf{D}^2))$, and $\mathbf{T}^{(3)} = \text{dev}(1/2(\mathbf{D}\mathbf{T}^{(1)} + \mathbf{T}^{(1)}\mathbf{D}))$. Here, dev and sym refer to deviatoric and symmetric parts of given tensors.

The GiTBNN architecture embeds Galilean invariance directly into the constitutive model by construction, while retaining the flexibility of machine learning to represent nonlinear flow dependence. Both first-order and higher-order model predictions are assessed against the computed DEM solid stresses, which are taken as the ground truth. The comparison enables evaluation of the predictive capability of the GiTBNN framework for shear stress components over a broad range of local flow states.

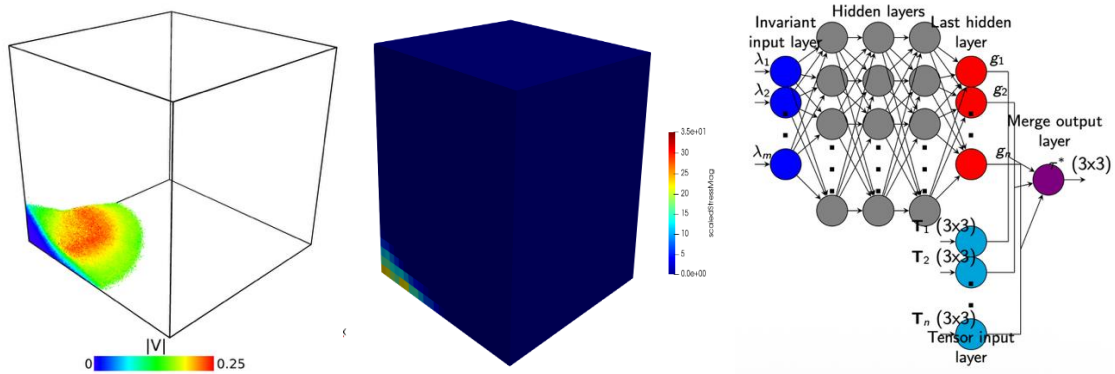


Figure 1: a) DEM particle velocities in a granular collapse, b) Computed solid stress magnitude using DEM dataset, c) Architecture of Galilean-invariant Tensor Basis Neural Network (GiTBNN) model : λ_k and $\mathbf{T}^{(n)}$ are scalar and tensor bases, τ_s^* is the predicted shear stress tensor.

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From Particle Calibration to Real-Time Optimisation: Virtual Prototyping with MercuryDPM

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Accurately predicting powder behaviour during handling and processing remains a critical challenge across sectors such as pharmaceuticals, food, and consumer goods. Creating reliable virtual prototypes of these complex granular processes requires overcoming significant hurdles, from handling complex industrial geometries to managing wide particle size distributions.

In this keynote, I will introduce MercuryDPM, an advanced, open-source particle simulation software, and discuss how its spin-off, MercuryLab, bridges the gap between high-fidelity physics and practical industrial application. I will walk through the complete end-to-end workflow of simulation-informed design, focusing on the journey from model calibration to real-time process optimisation.

First, we will address the critical step of model calibration—creating a true digital representation of an actual granular material. I will review practical methodologies combining direct experimental characterisation with indirect calibration using machine-learning techniques, including the open-source tool GrainLearning. Next, I will demonstrate how we can push beyond traditional computational limits. By applying Model Order Reduction (MOR) via pyMOR, we can transform these complex simulations into real-time models capable of on-the-fly optimisation.

Finally, I will ground these advancements in real-world industrial case studies—modelling processes such as hopper discharge, mixing, and packing. By linking simulation results directly to measurable physical parameters, this presentation will showcase how open-source particle simulations offers a powerful route to identifying inefficiencies, reducing segregation, and achieving profound performance gains in complex industrial systems.

Electrostatics on Particles

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When electrostatic phenomena in particulate systems are considered, the subject can be divided into two categories: application aspects and troubleshooting issues.

A wide range of applications of electrostatics has been developed, particularly for controlling particle motion using externally applied electric fields. A chronological overview of such applications is presented in Table 1. Notably, in most applications, the ion impact charging mechanism is employed to effectively charge individual particles, whilst tribocharging is used in electrophotography.

Conversely, in dry powder processes, it is widely recognized that tribocharging often results in unintended or undesirable particle behavior, including irregular motion due to electrostatic interaction, or even gas discharge due to charge accumulation.

However, the fundamental mechanism of triboelectric charge generation remains insufficiently understood. There is still ongoing debate regarding the primary charge carrier, whether electrons, ions, or material transfer. Table 2 presents historical data on the magnitude of charge generation in powders. Interestingly, these data lack detailed particle specifications, such as material type or particle size, with only the resistivity ($\rho \cong 10^{12} \Omega\text{m}$) being reported. Nevertheless, once electrostatic charge is measured, the observed order of magnitude tends to fall within a consistent range. Further systematic investigation is therefore strongly required.

A key challenge for the future lies in the *in-situ* measurement of particle charge in real systems, as well as in the advancement of measurement techniques and theoretical understanding. Ultimately, the ability to control particle behavior in practical processes through electrostatic interactions remains an important goal.

Table 1 chronology of applicational electrostatics¹⁾

1902	(one stage) electro precipitation	I
1932	electrostatic coating	I
1935	(two stage) electro precipitation	I
1938	electrophotography	T
1940	electrostatic coating (of sand paper)	I
1950	powder coating	I

Table 2 Charge generation on medium-resistivity powders²⁾

Operation	Charge-to-mass ratio ($\mu\text{C/kg}$)
Sieving	$10^{-5} - 10^{-3}$
Pouring	$10^{-3} - 10^{-1}$
Scroll feed transfer	$10^{-2} - 1$
Grinding	$10^{-1} - 1$
Micronizing	$10^{-1} - 10^2$

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- (2) J.A.Cross: Electrostatics, Principles, Problems and Applications, CRC Press (1987)

Segregation in Multi-Solid Fluidised Beds: Experimental Analysis and Model Predictions

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Multi-component fluidized bed technology is frequently employed in industrial applications requiring simultaneous processing of different materials or solids exerting separate functions. Binary- and ternary-fluidized beds are relatively common. As an example, conversion of solid biomass into syngas is operated in fluidized inert material, where severe operational issues like tar condensation and aerosol formation, corrosion, fouling, are mitigated by integrating specific tar-reducing catalysts (e.g. olivine). As uniform conditions are highly desirable to carry out the transformations, the efficiency of the resulting ternary bed (biomass, inert and catalyst) can suffer owing to solids' segregation. The present contribution discusses the fluidization and segregation behaviour of mixtures of a biomass (crushed olive pits), sand and olivine of given size, shape and density, at different compositions, by a thorough experimental characterization of the key fluidization and segregation properties.

To help interpretation of these experimental observations, a macroscopic model for mixing and segregation direction named Particle Segregation Model (PSM) is illustrated and discussed. Originally developed for segregation in two-component fluidized beds, the PSM has been recently conceptually extended to three-component systems. In a first part, the role of composition is investigated for a biomass-rich and a sand-rich mixture. Given the contrasting sizes and densities, the former system maintains its state of mixing at low olivine fractions. In the sand-rich mixture, the size-segregating behaviour leads to modest segregation of the biomass and olivine towards the bed surface and sand at the bottom. In a third examined mixture with extended olivine fraction, a similar behaviour to the sand-rich mixture is observed. Both tendencies are well captured by the PSM, whose analytical formulation allows drawing triangular plots that effectively compare experimental points and equilibrium lines. Overall, the study demonstrates the predictable possibility to exploit particle properties and mixture compositions as variables with which mixing can be promoted or segregation can be oriented towards the stratification of one or the other components.

Characterising Powder Triboelectric Charging in Shaking Systems: Experimental and Modelling Investigations

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The triboelectric charging of powders remains poorly understood due to the complexity of the governing mechanisms, limiting predictive numerical simulations and lack of established, reliable experimental characterisation methods [1]. An integrated experimental–numerical framework is employed to study the triboelectric dynamic behaviour of polypropylene powders in shaken cylindrical glass vials. Charges obtained from experiments performed at different sample masses and vial volumes are compared with corresponding DEM simulations (Figure 1), which account for tribocharging, polarization, and long-range electrostatic interactions [2]. Due to the difficulties in the calibration of tribocharging model parameters for both dielectric materials (polypropylene and glass), these are determined by matching the experimentally measured steady-state charges for one test case. Then, the results are exploited to analyse particle dynamics in the other cases and attempt to elucidate the role of particle–particle vs. particle–wall collision statistics. Charging dynamics and steady-state charge levels are discussed in the light of theoretical rate and saturation values. On the one hand, the influence of different modelling contributions is analysed. On the other hand, the joint simulated particle-scale results and experimentally observed total charge levels provide a useful dataset for a deeper understanding of how the contacts and collisions determine the collective behaviour.



Figure 2: Snapshots of the simulated 1.5-3 mm tri-disperse polypropylene particles in the shaken glass cylinder at different volumes (25cc, 40cc, 80cc, 200cc).

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AI-Assisted Prediction of Particle Impact Deformation Simulated by Material Point Method

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Study of particle impact, particularly that of elastic-perfectly plastic particles poses experimental and theoretical challenges due to the dynamic and non-linear nature of the phenomenon. Moreover, traditional numerical approaches such as the Finite Element Method (FEM) and the Discrete Element Method (DEM) encounter limitations in cases of large deformation impacts. To overcome these limitations, the current work employs the Material Point Method (MPM), a meshless computational technique that naturally accommodates large deformations. Subsequently, MPM is used to simulate the normal impact of an elastic-perfectly plastic spherical particle onto a rigid wall. To explore a wide range of parameters, five different values for the impact velocity (V_i), three for Young's modulus (E), four for density (ρ), and eight for the ratio of Young's modulus to yield strength (E/Y) are considered, leading to 480 simulations. This generates a large dataset covering a variety of deformation responses, from minor elastic deformation to extensive plastic flow. Considering the volume of the simulation data, a hybrid artificial intelligence (AI) framework is employed to find equations describing the relationship between the simulations' input (material properties and impact velocity) and output (expressions reflecting the deformation behaviour of the particle).

The first output parameter investigated is the equivalent plastic strain, ϵ_p , which is used as a measure of accumulated plastic deformation. The second output parameter is the deformation extent, defined as $1-(H_d/D)$, where H_d is the post-impact particle height and D is the original particle diameter. This metric quantifies the degree of flattening following impact. The AI framework derives dimensionless equations predicting ϵ_p and $1-(H_d/D)$ based on the material properties and impact velocity of the particle, showing a good agreement with the MPM results, as evidenced by a strong coefficient of determination (R^2) and small errors relative to the MPM data (refer to Figure 3). The identified equations reveal that both ϵ_p and $1-(H_d/D)$ depend on and can be determined from the yield strength of the material, Y , as well as the portion of the incident kinetic energy that is spent on inducing plastic deformation, $\rho(V_i^2 - V_y^2)$, with V_y being the yield velocity.

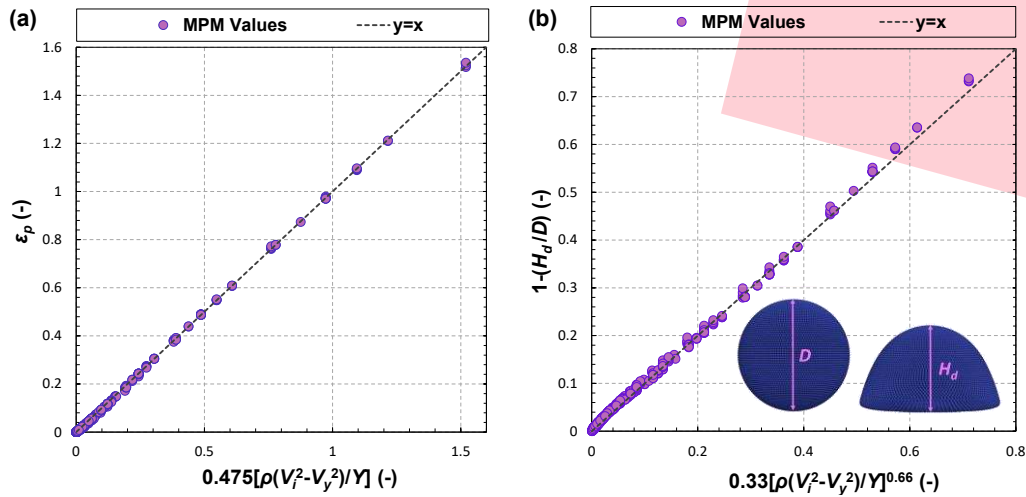


Figure 3. The simulations output parameters as a function of the equations identified by the framework for their prediction: (a) the equivalent plastic strain, ϵ_p , and (b) the deformation extent, $1-(H_d/D)$.

To verify the predictive capability of the framework beyond the training dataset, additional MPM simulations are performed for two cases with material properties and velocities outside the original parameter range. Consequently, the values predicted by the AI-derived equations demonstrate good agreement with these new simulations.

Furthermore, experimental validation is carried out using aluminium alloy, copper and solder particles impacted in an in-house device. In the device, particles are accelerated toward a rigid target by a vacuum-driven flow, collected after impact, and placed on a glass slide such that they rest on their deformed face. Scanning electron microscopy (SEM) imaging is then utilised to measure geometric parameters, from which H_d/D is estimated using a geometric assumption. As seen in Figure 4, the experimental values of the deformation extent closely follow the trajectory of the curve for the identified equation, indicating that the empirical equation provides a reasonable prediction of $1-(H_d/D)$.

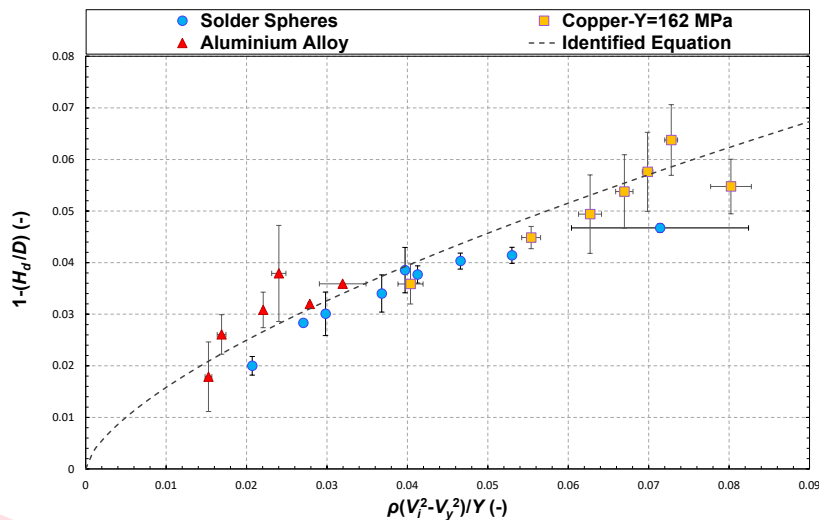


Figure 4. The deformation extent, $1-(H_d/D)$, as a function of $\rho(V_i^2 - V_y^2)$ for sample particles subjected to impact.

A Large-Scale DEM–CFD Simulation for Industrial Powder Die Filling with Particle Shape Effects

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Powder die filling is a fundamental unit operation in powder-based manufacturing, in which raw powder is introduced into a die as a preprocessing step prior to compaction. Achieving rapid and sufficiently uniform filling is directly linked to product quality and productivity, and die filling is widely employed across diverse industrial fields such as pharmaceutical manufacturing, powder metallurgy, ceramic processing, and food production. Owing to its industrial importance, the die-filling process has been extensively investigated in experimental and numerical studies. Despite extensive progress in powder simulations, achieving realistic simulations of industrial powder die-filling systems remains challenging. First, die filling is a gas–solid two-phase flow problem involving complex and moving wall boundaries. Second, industrial-scale systems contain hundreds of millions to billions of particles, making direct simulation with original particles computationally impractical. Third, real powders are composed of non-spherical particles, whose effects cannot be neglected in filling behaviour. Although all three aspects must be considered simultaneously for industrial die-filling simulations, no existing modelling framework can adequately address them at the same time. To overcome these limitations, this study develops a new DEM–CFD-based modelling framework specifically designed for industrial powder die filling.

To address these challenges, we develop a new DEM–CFD-based model by coupling three key methods with FELMI ^[1], our in-house DEM–CFD solver employing an implicit algorithm for the drag force term. Moving and arbitrarily shaped wall boundaries are modelled using the signed distance function–immersed boundary method (SDF–IBM) ^[2], which represents walls through a scalar field and wall volume fractions within CFD cells, enabling efficient treatment of moving and arbitrarily shaped geometries required for die-filling simulations. The issue of excessive particle numbers is addressed by a coarse-grained DEM ^[3], in which multiple original particles are represented by a single coarse-grained particle while ensuring energy consistency, allowing industrial-scale systems to be simulated at significantly reduced computational cost. Finally, the effects of particle non-sphericity are modelled using a rotational resistance model that introduces a rotational resistance moment acting on particles, enabling reproduction of non-spherical effects while using spherical computational particles and thus maintaining computational efficiency.

To validate the proposed model, two types of comparative simulations were performed for a linear shoe–die filling system, in which a shoe moves from left to right at a constant velocity of 0.1 m/s. First, the influence of rotational resistance was examined by systematically varying the parameter controlling the rotational resistance within the coupled DEM–

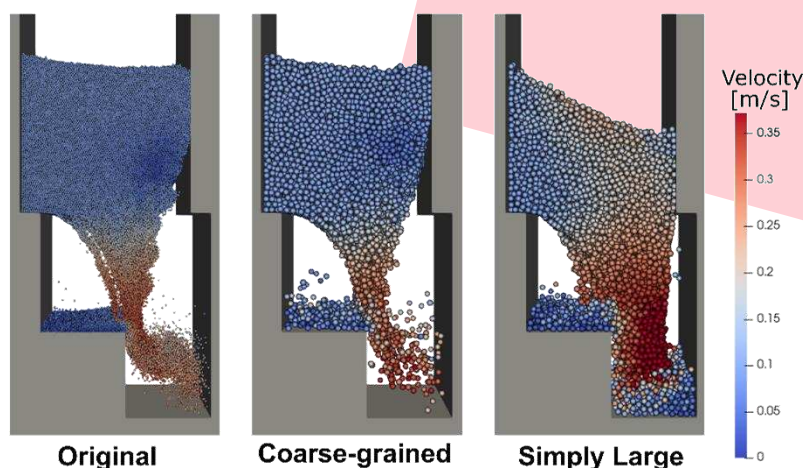


Figure 1. Comparison of filling behaviour

CFD model without the coarse-grained DEM. The simulations successfully reproduced physically reasonable filling behaviour. Furthermore, the results show a characteristic behaviour of non-spherical particles, in which larger rotational resistance leads to lower final filling rates. Second, the validity of the coarse-grained DEM with rotational resistance was evaluated by comparing simulations using original particles, coarse-grained particles with a coarse ratio of three, and simply enlarged particles with three times the original diameter. Figure 1 compares the filling behaviour among the three cases. The macroscopic filling behaviour of the original and coarse-grained particles showed excellent agreement. However, that of the simply enlarged particles was completely different, exhibiting faster filling due to reduced air drag effects. In addition, application of the coarse-grained DEM resulted in a substantial reduction in computational cost. These results demonstrate that the DEM–CFD model with rotational resistance appropriately captures the effects of particle non-sphericity in gas–solid die-filling systems and that the coarse-grained DEM with rotational resistance successfully reproduces the macroscopic behaviour of non-spherical particles at significantly reduced computational cost.

This study presents a novel coupled DEM–CFD model that enables realistic simulation of industrial powder die filling while accounting for moving complex boundaries, large particle numbers, and particle non-sphericity at low computational cost. Owing to its industrial relevance and general applicability, the proposed framework has strong potential for extension to a wide range of powder processes.

Acknowledgements

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Assessing the Feasibility of a Drag Force Flow Sensor for the Inline Monitoring of High Shear Wet Granulation Using the Discrete Element Method (DEM)

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High shear wet granulation (HSWG) is a widely used method in pharmaceutical tablet manufacturing to improve powder flowability, content uniformity, and processing efficiency. HSWG is a complex, multivariate process. Equipment, formulation and process parameters all impact granulation and the resultant granule properties which in turn influence downstream unit operations and properties of the resultant tablets. This presents challenges for process development and scale-up, which typically rely on traditional empirical approaches and trial-and-error methods.

In-line and at-line process analytical technology (PAT) provide real-time information of the granulation process, and offer opportunities for process development, control and scale-up.

One novel technology being explored is the Drag Force Flow (DFF) sensor as an in-line PAT tool to provide real-time monitoring of granulation dynamics. A DFF sensor is inserted into the granulation bowl. During granulation, particles collide with the probe, and the forces of these collisions are measured. [1]. Previous work has shown that force recordings from a DFF probe correlate with offline granule measurements taken from the FT4 powder rheometer [2], and that the force recordings can be used to predict tablet tensile strength [3].

However, current studies do not establish how DFF signals relate to particle properties. As the drag force exerted by a wet mass on an obstacle is governed by the flow's momentum, which is intrinsically linked to the density of the wet mass, force recordings can theoretically provide insights into the density of the particles. It was further hypothesised that as particle size will impact the rate of particles colliding with the probe and the contact area of collisions, it may be possible to understand particle size distribution from DFF recordings.

This work uses Discrete Element Method (DEM) simulations to develop machine learning models of particle size and density using forces recorded by the DFF probe. DEM allows for the exploration of a wide parameter space, which would be time-consuming and challenging to achieve experimentally. In this work DEM was used to create a computational model of a DFF probe in particulate flow. This allows

assessment of how particle properties such as size, density and friction affect the forces experienced by the probe, and support development of models predicting particle properties.

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Statistically Robust and Efficient Method for Calibration of DEM Parameters in Particulate and Fluid-Particle Processes

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In the last three decades, Discrete Element Method (DEM) and CFD-DEM simulations have proved their huge potential in helping to understand and predict the particulate solids behaviour in diverse industrial applications. However, the success of simulated trends and values strongly rely on the knowledge and availability of particle-scale material parameters that, in turn, can be complex to determine from experimental, bulk-scale tests. Simply simulating the bulk behaviour in characterisation devices (e.g. shear/compression tests, dispersion) as a function of different combinations of parameters (e.g. Young's modulus, friction coefficient, surface energy) can be costly in terms of time, inaccurate, insensitive to some parameters and yield little statistical significance of the fitted values. In the present contribution, we describe a computational methodology combining Bayesian statistics with DEM simulations, where the iterations of the former efficiently and effectively drive the parameter sets to be used in the latter until convergence. The method proves robust and in terms of statistical information on the final parameter values and efficient in terms of moves in the space of parameters. The following open-source tools are used: GrainLearning [1] for Bayesian statistics calibration and MFIX for the DEM simulations.

The computational framework is demonstratively employed to calibrate mechanical parameters against experimental measurements for two cases: (i) glass beads in a shear cell test and (ii) an air-driven impactor of particles against walls at different inclination angles for electrostatic charging of particles.

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Dynamic Adhesion Measurement of Powders using the Drop Testing Method: Defining a Standard Operating Procedure

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Powder adhesion often presents major challenges within the pharmaceutical industry as it significantly affects powder flowability. While measuring adhesion alone cannot resolve powder flow problems, understanding its relationship with powder flow, especially through modelling, presents a major advancement. Traditional methods such as atomic force microscopy (AFM) and centrifuge method were previously utilised to measure the adhesive force of particles; however, these methods are both time and cost intensive necessitating the need for a more practical solution. This work endeavoured to develop a novel standard operating procedure for measuring the effective work of adhesion of both regular (aluminium-alloy) and irregularly (ibuprofen) shaped powders using the drop test method. For optimisation and accuracy in obtaining the critical diameter of adhesion, the drop test rig was further developed so as to ensure reliable and repeatable measurements of the impact velocity and contact time, which previously posed major challenges. A total of 30 iterations was undertaken to ensure the repeatability of the impact time, by releasing the dropping platform at a height of 15 cm (for ibuprofen powders), resulting into an average time of 12.99 ± 0.30 ms. This generated an impact velocity of 1.54 ± 0.036 m/s. The corresponding, contact time was simultaneously measured to be 80.96 ± 1.17 μ s. The choice of height at 15 cm for the ibuprofen powders, enabled a thorough detection of particle detachment by mitigating the wobbling effect so as to ensure the tensile forces act evenly on the adhered particles upon impact of the dropping platform carrying the aluminium substrate. Additionally, a drop height of 10 cm was implemented for the spherical aluminium-alloy metal powders as any height above this resulted to no particles adhering on the substrate after the drop test. The 10 cm drop height resulted into an impact velocity of 1.23 ± 0.002 m/s and a contact time of 83.03 ± 0.65 μ s.

The effective work of adhesion, Γ of ibuprofen powders across four different sample volumes: 7 mm³, 21 mm³, 42 mm³, and 49 mm³ was measured. Establishing a minimum number of analysed particles is imperative, as falling below this threshold significantly compromises the accuracy of the measured critical diameter. A minimum of 640 particles was required resulting into an effective work of adhesion of 19.6 ± 2.9 mJ/m². Moreover, the effective work of adhesion, Γ of spherical Aluminium-alloy powders (7.7 ± 1.8 mJ/m²) was also assessed. It is important to note that the minimal

threshold established for a sample is dependant to the particle size distribution. Hence, for any given sample, a threshold for the number of particles initially dispersed on the substrate needs to be established to ensure the accuracy of results. Additionally, the choice for the drop height is also material dependant so as to ensure that there are particles still adhered on the substrate after the drop test to enable analysis. Furthermore, artificial intelligence is incorporated in parallel to effectively determine the critical diameter and compare it to the manually calculated values allowing for an efficient image analysis.

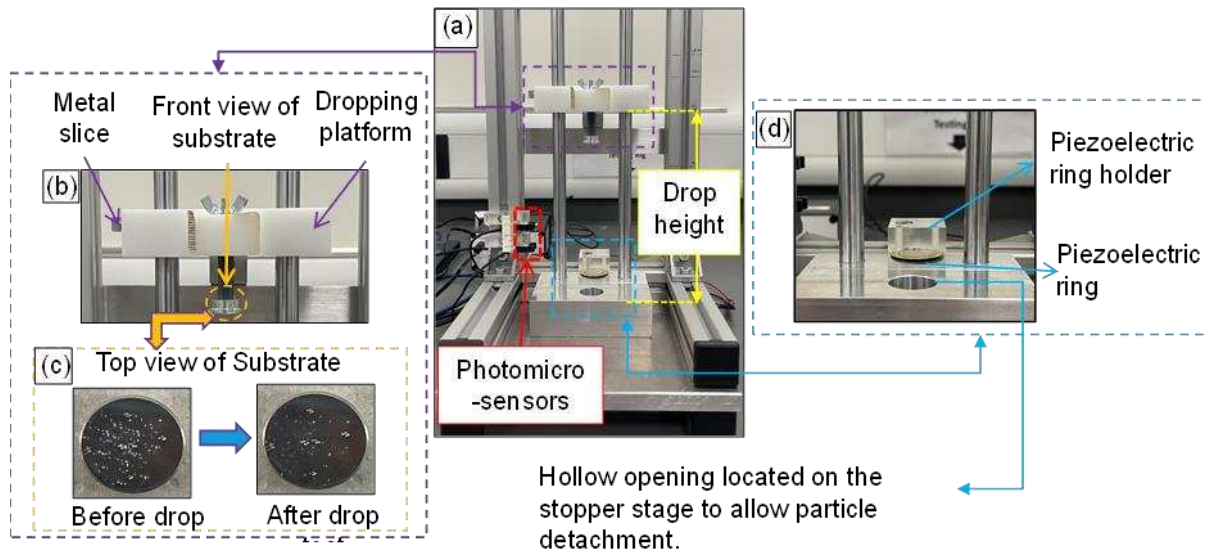


Figure 1: (a) The overview of the in-house drop test rig consisting of (b) the dropping platform carrying the (c) aluminium substrate and (d) stopper stage holding the piezoelectric ring.

Data Quality in Powder Characterisation: Challenges for AI-Assisted Properties Prediction

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Particle technology has progressed from reliance on single measurements toward more integrated and data-driven approaches that better capture the complex behaviour of powders and particulate systems. This study presents a broad experimental investigation of more than sixty powders covering a wide range of pharmaceutical powder systems. The aim is to systematically evaluate the strengths and limitations of commonly used techniques for particle size, shape, and flow characterisation, while building a structured experimental dataset to support the development of AI-assisted predictive models.

A combination of established and advanced methods was selected to provide a comprehensive assessment of particle size, morphology, and bulk powder performance. These include laser diffraction, dynamic and static image analysis, angle of repose, shear cell testing, FT4 powder rheometry, and Granupack measurements, alongside in-house methods such as a Drop Test approach for assessing particle adhesion. Together, these techniques provide insight into both fundamental particle properties and process-relevant bulk behaviour.

The study evaluates the suitability and limitations of each method across diverse powder systems, with particular attention to how measurement principles, data quality, and experimental variability influence reported results. Such differences can affect material classification and process understanding and may introduce bias or noise into datasets used for modelling. By comparing outputs across multiple techniques, the work identifies areas of agreement as well as gaps and uncertainties in current characterisation practices.

Understanding these limitations is critical for AI-based modelling, where inconsistent or technique-dependent data can directly impact predictive reliability. This work supports the development of more robust, reliable AI-assisted workflows for powder characterisation across pharmaceutical and wider particulate material applications.

Discrete Element Modelling of a Mechanochemical Encapsulation Process

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Mechanochemistry is a green chemistry process that allows the syntheses and transformations of powders with little or no solvent. The process is based on the supply of mechanical energy, generally using high-energy ball mills or extruders. Despite the potential of this process, there are still scientific locks at the molecular, particle and process scales. The link between mechanical energy and the chemistry modifications needs to be understood. In literature, the former has been assessed by the Discrete Element Method (DEM) for some mechanochemical reactions. This study provides the first investigation of an API encapsulation by mechanochemistry using a DEM model at the particle scale. The nature of the powder and of the process requires the consideration of normal and tangential elastic forces, rolling friction and cohesion. Unlike most works in literature, our study explicitly considers the powder particles in addition to the milling ball, which will allow in the future to analyse the mixing and collision heterogeneities. Simulations were conducted for different quantities of powders and vibration amplitudes of the mill. The total collision energy per mass for each case is computed. Our recent experimental measurements of the apparent reaction rate constant allow the preliminary investigation of its possible correlation with the collision energy estimated by DEM.

Finite Element Method Modelling of Dissolution of Sustained Release Tablets

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The pharmaceutical industry constantly faces challenges presented by the ever-increasing time and cost of developing new products. Moreover, the lack of comprehensive process understanding often results in quality issues with already registered products, leading to financial losses. In order to retain their competitiveness, manufacturers need to develop drug products that are robust to changes in raw material attributes and process parameters.

The purpose of our research is to create a modelling framework for the design of sustained release pharmaceutical tablets. In order to develop a technique that is agnostic to the size and shape of the tablets, we used the Finite Element Method as the modelling tool. Our method aims to combine the Drucker-Prager Cap (DPC) model-based simulation of powder compaction with a description of the dissolution process that relies on the modelling of diffusion.

The tablets used for the study consist of caffeine as drug, hydroxypropyl-methylcellulose (HPMC) as matrix polymer and CaHPO_4 as filler. Tablets were prepared with HPMC concentrations of 5-10-15-20-25-30-35 w/w% and their in vitro dissolution profiles were recorded.

The constructed diffusion model is based on the assumption that initially water is transported inside the tablet via the available pore space. This pore space is defined by the distribution of relative density resulting from the simulation of compression by the DPC model. This way, the model is capable of accounting for inhomogeneous density distributions, and we can study how the settings of tablet compression influence the dissolution profile. Owing to its excellent solubility, the dissolution of caffeine is considered to be instantaneous when water penetrates into a part of the tablet. This is followed by the diffusion-based transport of the drug outside the tablet. In order to describe the behaviour of these tablets, the effect of swelling and gel formation must also be accounted for. The swelling strain in turn effects the porosity of the tablet, and when the criteria for gel formation are satisfied, the diffusion coefficients are significantly decreased, leading to slow drug release that takes hours.

Packing and Cohesive Properties of Aggregates of Non-Spherical Particles

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Granular materials often consist of particles whose shape strongly governs their packing behaviour and mechanical response. We investigate the microstructure and cohesive strength of aggregates composed of two different particle shapes (hexapods and pentagon-platelets) using an in-house DEM platform. Both shapes are defined by an aspect ratio describing the transition from near-spherical forms to elongated or branched nonconvex geometries. Spherical agglomerates are generated by radial compaction for a range of aspect ratios and friction coefficients to analyse their densest jammed configurations (Figure 1).

Hexapods exhibit strong mechanical interlocking and form porous yet robust aggregates, while platelets favour layered, anisotropic structures with enhanced face-face contacts. We quantify packing fraction, connectivity, and bulk modulus to characterise how shape and friction control aggregate organisation. The packing fraction shows a non-monotonic dependence on aspect ratio due to steric constraints, rotational hindrance, and emerging local order.

Cohesive strength is assessed by introducing friction and adhesion forces and performing diametral compression on the spherical agglomerates. Peak stress increases with particle aspect ratio for both shapes, reflecting interlocking in hexapods and concentrated force-chain transmission in platelets due to chains of face-face contacts. Overall, particle aspect ratio significantly enhances agglomerate stability through combined interlocking and adhesive interactions, providing insights for designing advanced granular materials in geomechanics, materials engineering, and additive manufacturing.

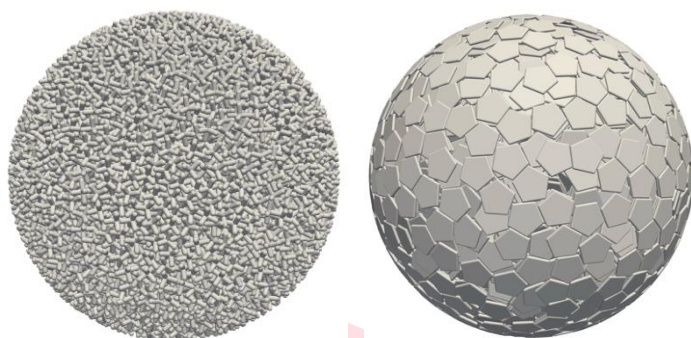


Figure 1: *Final jammed configurations of hexapod and pentagon-platelet particles obtained via radial compaction for aspect ratios of 5 and 11, respectively.*

Towards an Unified Model of Dense Powder Flow in Agitated Devices

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Powder handling often involves convective agitation operations, such as homogenisation or mixing, which must be controlled for ensuring product quality, low energy consumption, low product waste and process safety. Powder is known to be a state of matter that is difficult to model on a large scale, specifically in industrial equipment. In fact, the sizing of powder agitation devices and the choice of operating parameters are often carried out empirically or according to default rheological models. Dimensional analysis can help rationalising these operations. Based on small-scale experiments, it requires establishing an extrapolation basis composed of geometric similarities and the choice of an invariant. Using this method therefore requires precise knowledge of the phenomena involved. Numerous articles have relied on physical approaches to study the action of different blade systems on the powder flow, focusing mainly on the recirculation zone near free surfaces. While this mechanism is essential for powder mixing, it overlooks an important aspect which is the flow of powders in the dense submerged region where friction forces predominate.

Recently, Boussoffara et al. [1] modelled dense-phase flow in a horizontal powder mixer agitated by a simple blade-equipped device, which can be described by an effective friction coefficient correlated with an Inertial number [2]. Although this work represents a fundamental advance in understanding the mechanisms at play in agitated devices, it still needs to be consolidated and supplemented in order to become a robust design tool. In this communication, we will present how this model applies to various more complex equipment geometries featuring several rows of horizontal or inclined paddles held on one or two horizontal shafts, and a vertical one. Its ability to take into account filling ratio and particles sizes effects is discussed. Being used as an invariant basis for scaling-up processes, this model could pave the way for rational design of blenders.

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[2] GDR MiDi, 'On dense granular flows', Eur.Phys.J.E., vol. 14, pp. 341-365, Aug. 2004

CCC-ParaSolS: A UK Collaborative Computational Community in Particulate Solids Simulation

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Particulate solids encompass natural soil deposits, pharmaceutical powders, food ingredients (e.g., powdered milk, flour), aggregates and cement used in construction, etc. They are often inputs to manufacturing processes or are produced as intermediate/final products and as such, they have significant economic and societal importance. For example, they are fundamental to the UK chemical and pharmaceutical industry which annually generates over £60bn of exports and directly employs more than 130,000 people across over 4,000 businesses. However, particulate systems are complex and contain material behaviours that are difficult to understand and predict. The Discrete Element Method (DEM) is a computational method that simulates granular materials at a particle level, allowing insight into the complex behaviours that are difficult to observe experimentally or with other computational tools. However, DEM can come with high costs, both in terms of computational requirements and licences for commercial codes. Both of these costs can be overcome by running open-source codes on GPUs and high-performance computing (HPC) systems, but making this switch can be prohibitive for users.

CCC-ParaSolS is an STFC-funded project (UKRI/ST/B000493/1) to create a multi-disciplinary Collaborative Computational Community in particulate solids simulations, with a particular emphasis on DEM and open-source software: <https://www.ccc-parasols.ed.ac.uk>. The multi-disciplinarity of this community aims to overcome the issue of developments happening in discipline silos, inhibiting full exploitation of methodological advancements. Since the beginning of 2025, CCC-ParaSolS has held hybrid network events at various UK locations: Edinburgh, Abingdon, Manchester and Belfast. These events have included the delivery of training to lower the barriers to adopting open-source DEM codes and accessing HPC. Following a community consultation, we are undertaking a code development project to add GPU capabilities to the established MercuryDPM code. Being able to efficiently run on GPUs will be essential to exploit the next generation of UK HPC systems. Code benchmarking cases are also being developed as a technical focus. The CCC-ParaSolS project is working towards establishing a long-term Collaborative Computational Project supported by CoSeC: the Computational Science Centre for Research Communities.

Combined Surface- and Density-based Approach for Spreadability Study of Metal and Polymeric Powders in PBF processes

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Powder Bed Fusion (PBF) is an Additive Manufacturing process; a powdered material is transformed in a 3D item by selective fusion following a layer-by-layer approach. Defects and poorly spread layers result in defected or imperfect final products. Despite the efforts in producing many indices and methods to express powders' spreadability, every index fails in univocally describing powder spreading behaviour. In this work three different analysis methods were employed to better understand the aspects that mainly affect spreadability and the relationship between different spread layer properties. Two polymeric powders and two metal powders were tested in spreading experiments. Every powder was purposely designed for additive manufacturing processes. Tests consisted in spreading the powders in a pocket bed of 100 μm depth, at different spreading speeds: 50, 75, and 100 mm/s. The obtained layer was firstly analysed in place by means of shadowgraphy and laser profilometry; subsequently, the powder was removed from the layer and weighed to calculate layer's density. Profilometer's results were used to calculate statistical parameters of the layer's surface. Additionally, both profilometer and shadowgraphy data were processed applying wavelet transform and obtaining a power spectrum and a characteristic wavelength. Three indices were defined and calculated from the data of the three different methods. It was not possible to define a direct relationship between the indices, suggesting that the methods highlighted different aspects of the same layer. However, all the indices and the calculated parameters, showed a consistent variation, in the order of 8-13%, with increasing spreading speed.

Analysing the Effects of Powder Flow on Battery Powder Spreading for Dry Manufacturing Using DEM

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As customer demand and policies are driving industry away from internal combustion engines, battery manufacturing for electric vehicles is establishing its presence in the motor industry. Conventionally, lithium-ion batteries are produced using wet slurry casting which involves using toxic NMP solvent and energy intensive drying and solvent recovery. This emphasizes the need to develop dry manufacturing methods for battery production.

Powder spreading additive manufacturing (PSAM), conventionally used in powder bed fusion for metal 3D printing, can prove to be a good dry alternative for battery manufacturing. Similar to wet coating, PSAM of dry battery powders can simply be done using a blade to spread powder onto the current collector. Challenges arise when using battery powders mainly due to 1) high cohesion between particles and 2) a smooth current collector surface to spread the powder on. Engineering the particle properties may prove to be the solution that would make this manufacturing method work.

In this work, the effect of particle properties such as static and rolling friction coefficients and surface energy are studied using Discrete Element Method for NMC622 particles. By varying these properties, the effect on powder spreading is studied. Coupled with this, a measurement of flowability is taken by simulating a modified, miniturised FT4 rheometer model. This study aimed to draw a correlation between powder flowability and spreadability while trying to understand the effect of each of the coefficients on these measured properties. It was concluded that the surface energy has the highest effect on the spreadability and flowability of the battery powder as it amplifies the effect of friction. It creates arcs/bridges restricting powder flow, and causes the powder to act more like a solid than a fluid. Generally, a low flowability correlates to poor spreadability, and vice versa. However, in a counter intuitive case, a low flowability run was achieved with very high friction coefficients and zero surface energy but produced a reasonably good average layer height. This leads us to say that the powder flowability measured from an FT4 should be treated with caution when trying to predict its spreadability. Coupling it with experimental surface energy measurements and/or shear cell measurements may be the way forward to predicting spreadability.

Heat Transfer Analysis of Immersed Probe in a Fluidised Bed for Particle Based Energy Storage

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Fluidised bed reactors are widely utilised in industry, especially in particle based thermal energy storage systems, as they provide high heat transfer rates, excellent temperature uniformity and effective solid–gas contact. To achieve optimal design and performance improvement, precise prediction of the heat transfer mechanism within the fluidised bed is essential, which requires quantifying the individual contributions of particle- and gas-dominated heat transfer mechanisms. Numerical models of the existing research often rely on simplified assumptions such as constant wall temperature throughout the probe circumferential or constant heat flux, which cannot accurately capture the discrete particle–wall and gas–wall heat transfer contributions.

In this study, an immersed probe in a fluidised bed is simulated by combining a Computational Fluid Dynamics (CFD) and Discrete Element method (DEM) framework implemented in MFIX software. The model includes a sphere probe initially at 25°C is placed in a bed containing fine particles at 200°C. The study explicitly incorporates particle–wall conduction, particle–fluid–wall conduction, and gas–wall convection at different circumferential sections through user-defined heat transfer formulations.

The results showed that heat transfer from the fluidised bed to the immersed sphere reached steady-state conditions within 3 seconds, yielding temperature distributions in good agreement with Di Maio et al. The heat transfer coefficient was found to be 258 W/m²·K at minimum fluidisation velocity ($U_{mf} = 0.5$ m/s) conditions, which is consistent with existing literature.

Furthermore, a parametric investigation across different superficial velocities reveals that heat transfer increases up to 297 W/m²·K at 1.5 U_{mf} before decreasing to 150 W/m²·K at 3 U_{mf} . Particle–wall and particle–fluid–wall conduction dominate at low velocities (between U_{mf} and 1.5 U_{mf}), whereas gas convection becomes increasingly dominant at 3 U_{mf} when particle–wall contact frequency diminishes. To resolve circumferential effects, the probe surface was divided into several angular sectors. While temperature distributions remain marginally uniform at U_{mf} , significant angular non-uniformities emerge at 3 U_{mf} , invalidating the uniform temperature assumption. These findings provide mechanistic understanding into the transition from particle-dominated to gas-dominated regimes, demonstrating that excessive superficial velocity significantly reduce overall heat transfer efficiency.

Powder Flow Behaviour and Performance Prediction in Handling and Powder-Bed Fusion Processes

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Powder flow behaviour and powder-air interactions play a critical role across bulk solids handling and powder-bed fusion processes. A series of studies was undertaken to characterise these behaviours, develop predictive dimensional models, and establish links between powder properties, process performance, and final product quality.

Powder behaviour was examined in industrially relevant handling systems, including bin discharge, and linear shoe-die filling. Flow initiation from an arching state was explored under imposed differential air pressures, leading to a dimensional model predicting the critical pressure required to break arches as a function of orifice size. Mass flow rates were measured under varying pressure gradients, enabling development of a complementary model relating discharge rate to differential pressure and outlet geometry. In linear shoe-die systems, gravity-driven and suction-assisted filling mechanisms were analysed using internal differential pressure measurements to capture air movement during powder transfer. Dimensional models were subsequently derived to relate delivered mass to pressure gradients, shoe velocity, and die-punch motion. These studies identified the key dimensionless groups governing the behaviour of fine and cohesive powders under differential pressure, strengthening predictive capability for industrial process design.

The same principles were applied to Selective Laser Sintering (SLS). Relationships between the flow properties of virgin and reused PA12 powders and the resulting part density and mechanical strength were established, with strong correlations demonstrating that powder flow characteristics can be used to predict final part quality before printing. Further evaluation of powder reuse in SLS revealed substantial changes in powder behaviour across reuse cycles and corresponding variations in manufactured parts, supporting improved recycling strategies and reduced material waste.

Overall, this work provides an integrated understanding of powder-air interactions and their influence on both industrial handling systems and additive manufacturing, contributing to more consistent, efficient, and sustainable powder-based processes.

Past, Present and Future of Seeded Granulation

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As a result of a completed research programme (2005–2011) funded by the Engineering and EPSRC in collaboration with P&G, Hosokawa Micron, Pfizer, and Borax Europe Ltd, a novel method for the scale-up of batch high-shear granulation was developed. This method enables the production of granules containing a large particle core, hereafter referred to as seeded granules.

Scanning electron microscopy (SEM) images of over 100 seeded granules were featured on the front cover of KONA Powder and Particle Journal (2011), as illustrated in Fig. 1, while Fig. 2 presents a representative SEM image of an individual seeded granule. These granules demonstrate significant advantages over conventional granules, particularly in terms of uniformity in shape, well-defined internal structure, controlled dissolution rates, and consistent physical properties.

Subsequent research efforts have focused on advancing the understanding of seeded granulation through both computational modelling and experimental investigations, encompassing a range of batch and continuous granulation systems. More recently, this approach has been adopted by several large industrial organisations across sectors including food processing, pharmaceuticals, powder metallurgy, and detergent manufacture. The present work provides a comprehensive overview of more than two decades of research in this field, encompassing prior developments, current investigations, and future research directions aimed at elucidating the underlying mechanisms governing seeded granulation.



Fig 1 Front cover of KONA shows SEM over 100 seeded granules.

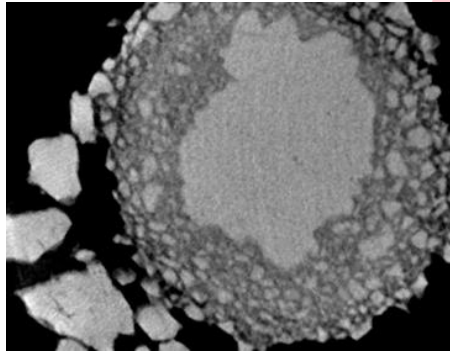


Fig 2 X-ray CT scan of a seeded granule.

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Microstructural Tuning Of NMC₆₂₂ Dry Electrodes Properties through Fluorine-Free Binder and Carbon Particle Interactions for A Reduced Reliance on Fluoropolymers in Dry Electrode Processing

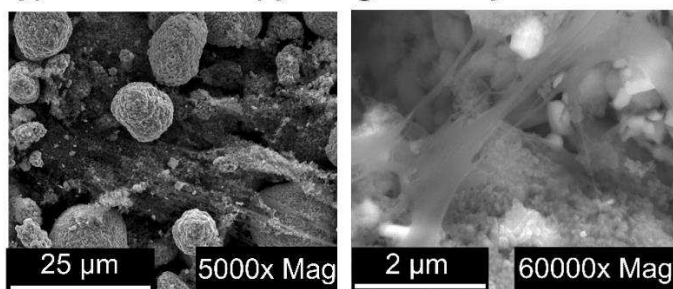
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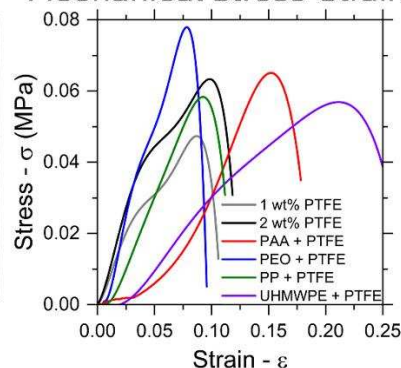


Battery electrode manufacturing has relied on slurry-cast, wet electrode processing as the dominant production process since the introduction of the lithium-ion battery. As our understanding of the environmental impacts (energy use in drying, toxic organic solvents) and electrode constraints on overall achievable thickness and energy density has matured, the limitations of wet processing have become barriers to achieving low-cost, high energy density batteries. In recent years, dry electrode processing has experienced a surge of interest in both research and manufacturing with promises of directly addressing these limitations through elimination of the solvent altogether. Dry processing is governed by particle interactions, as applied heat and mixing act to shear polymer particles for electrode cohesion. Unfortunately, a ubiquitous polymer used in this process is PTFE, a fluoropolymer with associated environmental concerns, owing to its near-unique ability to easily fibrillate.

Typical Microscopy Images of Dry Electrodes



Mechanical Stress-Strain



Here we investigate alternative electrode components, using both fluorine-free binders and different conductive additives, in combination with reduced quantities of PTFE. We show that it is possible to reduce the overall PTFE content while maintaining the mechanical processability of the electrode, to ensure compatibility with electrode processing techniques and optimal performance. We demonstrate how the different microstructures of the electrodes, generated from the particle interactions during mixing, contribute to the bulk properties of the electrode with the ability to tune the mechanical properties of electrodes arising through choice of electrode components.

Conceptual Design of Tribo-Plasma Fluidised Beds for Ammonia Production

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Over the past century the Haber-Bosch process has been the dominant process worldwide for producing ammonia, which is highly energy intensive. A promising energy efficient alternative is dielectric barrier discharge (DBD) reactors using non-thermal plasma. The main issue regarding these reactors is their industrial scalability, as they are limited by the plasma volume. Thus, in this study we address this limitation by proposing a conceptual design of a tribo-plasma fluidised bed reactor. The electrical discharges arising from contact electrification (tribocharging) due to particle-particle and particle-wall collisions will drive plasma generation and hence chemical reactions.

We design the spatially homogenous tribo-plasma fluidised beds via Eulerian-Eulerian modelling where the transport equations for mass, momentum, total energy for gas and solid phases, and an additional transport equation for charge evolution in the solid phase are solved. The solid phase properties closures such as viscosity, diffusivity, charge conductivity and diffusion have been developed by Kinetic Theory of Granular Flows with charged particles [1,2]. The charge discharges are evaluated using the Paschen law. Occurring at ambient conditions, non-thermal plasma arises from these electrical discharges. We also track neutral plasma species, including electrons, ions, and excited molecules in electron-impact reactions, ionisation, excitation and recombination processes for ammonia production. Additionally, the role of charge in governing the particle hydrodynamics of the system has also been assessed, with emphasis on pressure-dependent charge accumulation. A simulation campaign has been performed by varying particle diameter, particle material properties, bed packing fraction, and particle mixtures to evaluate the feasibility of tribo-plasma fluidized beds. The whole modelling framework will provide insight into the conditions under which triboelectrically generated discharges can sustain plasma reactions in gas–solid reactors. In a future study, this framework will be extended to 3D fluidized-bed simulations to investigate reactor-scale behaviour and scale-up potential. These results will also inform further benchtop studies.

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A Multiscale DEM-Machine Learning Framework for Efficient Prediction of Particle Fracture during Lithium-Ion Battery Electrode Calendering

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Calendering plays a decisive role in shaping the microstructure and the resultant performance of lithium-ion battery (LIB) electrodes, yet fracture-resolved Discrete Element Method (DEM) simulations remain computationally expensive when brittle particle breakage and repeated-stress weakening must be captured in detail. This study presents an efficient multiscale framework that combines DEM and machine-learning surrogate modelling to predict particle fracture and mechanical evolution during electrode calendering.

At the particle scale, a DEM framework incorporating the Tavares UFRJ Breakage model is employed to represent fracture initiation, repeated-stress weakening, and fragment generation in brittle active material particles under compression. Based on a validated parameter set, a systematic design-of-experiments (DOE) study is performed to quantify the sensitivity of key breakage-model parameters and to generate a high-quality simulation dataset spanning the relevant process space. Using this dataset, a machine-learning surrogate model is developed to rapidly predict both calendering pressure-compression behaviour and particle breakage responses, providing an efficient alternative to repeated high-cost DEM simulations. The surrogate captures the nonlinear dependence of the mechanical response on model parameters while preserving the essential fracture-induced transitions observed in the full DEM results.

A Macroscopic Comminution Model for Wet Granular Media : from Mineral to Lignocellulosic Feedstock

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Milling is one of the most widely used processes in the industrial sector. While dry and wet milling have been extensively studied and are well understood in literature for diverse application (pharmaceutics, food industry...[1]), unsaturated milling remains poorly understood. Nevertheless, because drying operations are energy- and cost-intensive, this specific grinding condition is attracting growing interest in various industrial sectors, such as the biofuel industry [2]. The presence of water induces changes in the rheological behavior and densification properties of the feedstock. These modifications in mechanical properties strongly affect energy transmission and particle size reduction. This presentation introduces an experimental methodology to characterize powder densification and to relate it to grinding efficiency using a laboratory-scale vibratory ball mill [3]. The objective is to propose a generic macroscopic comminution model that accounts for the presence of water. The study starts with a mineral granular medium (quartz sand), which neither absorbs water nor swells, and is then extended to more complex biological feedstocks, such as lignocellulosic biomass, which are subject to such phenomena.

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Micro-scale Investigation of Shear-induced Fabric Evolution and Crushing in Carbonate Sands

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Over 35% of the ocean floor is covered by carbonate sediments having more than 30% carbonate minerals (Rogers, 1957). Carbonate sands are porous in nature due to their biogenic origin. Despite having a higher peak friction angle of 45-50° when compared to silica sands (30-35°), carbonate sands crush under normal stress (Semple, 1988). This innate nature of carbonate sands is a challenge in process of geotechnical foundation and retaining structure designs. In the UK, the presence of carbonate sands is majorly found in the NW Scottish coastal systems of Orkney and Shetland.

The early studies on granular soil started in the early 1970s, when the concept of granular 'fabric' - the statistical arrangement of particles, contacts, and voids - was introduced by Oda (1972), who used 2D thin sections and optical microscopy to manually quantify particle orientation. He observed that depositional fabric significantly influences mechanical properties such as strength and dilatancy. This was later formalized as a second-order tensor (Oda, 1982) and the later extended to fourth-order representations (Imseeh et al., 2018) to capture full micro-structural anisotropy.

Parallely, the macro-scale behaviour of granular sand has been studied extensively through experiments (Oda, 1975, Airey and Wood, 1987, Li et al., 2017). And the introduction of Discrete Element Methods (DEM) by Cundall and Strack in 1979 allowed for the idea of simulating particles to understand the micro-scale behaviour (Katagiri et al., 2010, Shi et al., 2015, Nguyen et al., 2021). Researchers focused on understanding the force chains and contact networks (Thornton, 2000; Fonseca, 2012). This eventually led to the extension of the critical state theory, in which granular fabric evolves toward a steady state under sustained shear. The fabric anisotropy was introduced as the third parameter to the critical state of the granular soil. Li and Dafalias (2012) observed that upon shearing, all the specimens become anisotropic and have a fabric tending to be coincident with the loading direction and hence the Anisotropic Critical State Theory (ACST) was established. However, the ACST has been developed and validated considering non-crushable spherical silica sand particles, where particle geometry remains constant during shearing.

Coop and Lee (1993) demonstrated that the particle crushing behaviour of carbonate sands shifts the critical state line (CSL) downward in the e - $\log(p')$ space. Cho et al (2006) have demonstrated that the irregularity in the shape of the particle affects the coordination number, compressibility and stiffness of the material. Other researchers (Zhao & Zhou, 2017; Shi et al., 2020) also support this observation showing the particle shape (defined by sphericity, roundness, and angularity) directly influences fabric anisotropy development. Furthermore, angular particles interlock more strongly, developing higher fabric anisotropy under shear (Kawamoto et al., 2018). And carbonate crushing progressively rounds particles and reduces angularity (Coop, 1990; Wu and Wang, 2024). Therefore, it is a limitation in the present literatures that the effect of shape characteristics and the particle crushing behaviour have not been considered in the study of fabric evolution and framing of the ACST.

Many researchers studying the fabric characteristics and its evolution have preferred to investigate the soil under one-dimensional compression under tri-axial conditions (Oda et al., 1985, Oda et al., 2004, Majmudar and Behringer, 2005, Yang et al., 2008, Fonseca et al., 2013a, Druckrey et al., 2016, Alam et al., 2018, Sun et al., 2019). While DEM has proven effective in simulating granular behaviour, most studies have focused on idealized spherical or non-crushable particles, limiting their applicability to crushable carbonate sands with complex particle morphologies.

Furthermore, the application of DEM to study fabric evolution under simple shear conditions—which better represent in-situ stress paths—has not been extensively investigated. Under simple shear conditions, the soil samples are naturally consolidated as it would be present at any site, whereas in triaxial conditions, the soil typically consolidates isotropically, which may not represent in-situ conditions.

Therefore, in my research, I plan to perform an extensive DEM-based investigation using YADE software to simulate the behaviour of carbonate sands while considering its shape characteristics and particle crushing behaviour under both triaxial and simple shear conditions. The DEM model shall be developed and duly validated by performing physical simple shear experiments and observing single-particle crushing behaviour. The parametric study will consider variable relative density, normal stress, and strain rate to capture the coupled effects of particle shape characteristics and crushing behaviour on fabric evolution. Based on the insights from triaxial simulations, we aim to extend the ACST by introducing particle breakage as a fourth parameter alongside void ratio, mean stress, and fabric anisotropy. Subsequently, the simple shear DEM simulations will be utilized to propose modifications to strength parameters for improved estimation of foundation capacity in soil-structure interaction problems involving crushable carbonate sediments.

Understanding Particle-Droplet Collisions

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Collisions between unsupported particles and droplets occur in many natural and industrial systems, ranging from rain droplet interactions with atmospheric particles to the dynamics of droplets, semi-dried droplets and particles in spray drying process equipment. This work uses binary particle-droplet collisions to build understanding of these collisions, significantly extending the very experimental space that has been investigated previously. It explores smaller droplets (400 μm) and focuses on droplet-particle size ratios >1 . It also systematically explores the impact of particle density and wettability, by looking at the behaviour of hydrophobically coated particles and uncoated, hydrophilic particles, as well as particles of different materials. A customised experimental set-up and high-speed camera is used to image collisions and build a regime maps of collision outcome based on Weber number and collision offset, and get insights into the physics driving the behaviour of these systems. The results show that the importance of wettability and the density on the collision outcome. The poorer wetting of the hydrophobic particles impeding the transition from separation to coalescence as collision offset is reduced. The influence of Weber number definition is also explored and discussed and a definition with wider applicability proposed.

Transient Inhalation Effects and Triboelectric Interactions in Swirl-Based Dry Powder Inhalers

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Flow-independent aerosolization is a key requirement for swirl-based Dry Powder Inhalers (DPI) delivering carrier-API formulations [1]. This work evaluates the impact of transient inspiratory flow conditions on deaggregation and emission through high-fidelity CFD-DEM simulations.

Four inhalation profiles are analysed: a step input, a clinically representative asthmatic trace, and two linear ramps with identical peak inspiratory flow rate (60 L/min) but different accelerations (8.0 and 3.9 L/s²). The Eulerian-Lagrangian framework couples airflow dynamics with particle-scale mechanics, resolving carrier-API agglomerates, hydrodynamic forces, adhesive collisions, and particle-wall interactions.

Triboelectric charging is modelled according to the “condenser model” proposed by Matsusaka [2], including charge exchange during contacts, electrostatic forces and polarization effects via the “effective dipole model” [3], developed in-house and integrated into the DEM formulation.

Results show a strong sensitivity to flow acceleration: ramped profiles delay API detachment and emission, while the lowest acceleration significantly reduces fine particle fraction despite identical peak flow. The model clarifies how inspiratory transients govern deaggregation kinetics, charge build-up, and delivered dose, providing insight for the design of flow-robust DPI.

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Investigating the Role of Temperature on the Calculated Work Function of Polymer Surfaces

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Triboelectric charging presents a persistent challenge in industries that handle powders during manufacturing processes. Repeated particle–particle and particle–wall collisions can generate significant electrostatic charge on both particles and vessel surfaces, leading to adhesion to equipment walls, agglomeration, electrostatic discharge, and associated problems such as blockages, destabilised formulations, and fire hazards. Despite its industrial importance, the fundamental mechanisms underlying triboelectric charging remain poorly understood, and numerous rigorous yet inconclusive studies have only deepened this uncertainty.

Recent studies have shown that even nominally identical materials can develop systematic charging tendencies and may arrange themselves into so-called identical-material triboelectric series [1]. These observations suggest that nanoscale variations between surfaces that are chemically identical may produce asymmetric charge transfer during contact.

At the macroscale, it is known that stress and strain gradients can influence triboelectric charge transfer through the flexoelectric effect [2]. In this work, we propose that thermally induced atomic vibrations at finite temperatures generate natural fluctuations in the surface work function, which may provide a mechanistic explanation for tribocharging between identical materials.

To investigate this hypothesis, we employ first-principles density functional theory (DFT) calculations to examine how temperature influences the work function of amorphous polymer surfaces, specifically polyethylene, nylon-6, and polytetrafluoroethylene. Amorphous surface structures with realistic densities were first generated, after which molecular dynamics simulations were performed to sample thermally accessible configurations. Representative structures extracted from these simulations were subsequently analysed using DFT to determine the distribution of surface work functions as a function of temperature.

Our results reveal a clear statistical variation in the calculated work functions of these materials at finite temperatures. This finding has important implications for modelling triboelectric charging using work functions obtained from zero-Kelvin DFT calculations. More broadly, it suggests that materials at non-zero temperature exhibit a distribution

of electronic states at their surfaces, which could plausibly enable charge transfer between otherwise identical materials during contact.

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Design and Modelling of Triboelectric Charge Measurement Rig using CFD-DEM Approach

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Particle charge characterisation as a function of size is an important aspect in industries involving particle handling and manufacturing, as it can provide insights into important processing attributes such as flowability and mixing. Existing instruments, such as the Faraday cup electrometer measures only the net charge of particles, while the electrostatic classifier is designed for large particles. A new device has been developed to measure the charge distribution of particles in the range of 30 μm to 200 μm . The particles are first dispersed via a pulse of pressurised jet and enter a cyclone where they exhibit frequent collisions with the wall, acquiring charge. When the air flow is stopped, the particles leave the bottom of the cyclone and enter a charge classification chamber where a high DC voltage is applied across the electrodes, which segregate the particles based on charge and size. The lateral position of particles collected at the bottom plate allows the calculation of the charge on individual particles as a function of size for a certain potential difference applied at the electrodes.

A coupled CFD-DEM approach is used to optimise the design of this device. Turbulence in the air flow is modelled using the RST model, while the particle-particle and particle-wall contacts are modelled using the Hertz-Mindlin contact model. Spherical glass beads of sizes ranging from 50 μm to 110 μm are used as the test case for the geometry optimisation. Charging of particles is considered due to impact on the wall as well as due to rolling. It is found that all particle sizes reach the equilibrium charge level before exiting the cyclone chamber. The smaller particles exhibit greater lateral displacement compared to the larger particles due to lower axial velocity in the chamber. The particle charge is then back calculated from the lateral displacement at the bottom plate of the chamber using a 2D numerical model and compared with the CFD-DEM predicted charge on each particle. A good agreement is obtained between the particle charge predicted using the CFD-DEM model and the back-calculated charge based on particle location and size.

Development of a New Particle Charge Classifying Chamber

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Characterising particle charge is a critical requirement in many industries that rely on powder handling, processing, and manufacturing. Understanding how particles acquire and retain charge provides valuable insight into key behaviours such as flowability, segregation, and blend uniformity. Conventional instruments, however, have notable limitations. For example, a Faraday cup electrometer measures only the overall or net charge of a sample, while electrostatic classifiers are generally intended for much larger particle sizes and are not optimised for the intermediate range relevant to many industrial powders.

To address this gap, a new experimental device has been developed that enables measurement of the charge distribution of individual particles. In this system, particles are initially dispersed by a short pulse of pressurised air, allowing them to enter a cyclone chamber. Within the cyclone, the particles undergo repeated collisions with the chamber walls, which leads to triboelectric charging. Once the flow is halted, the particles settle and exit through the cyclone's base, entering a charge classification chamber.

In this chamber, a high DC voltage is applied across parallel electrodes, creating an electric field that deflects the particles based on the magnitude and polarity of their charge as well as their aerodynamic size. The particles are collected on a bottom plate, and their lateral landing positions are recorded. These positions form the basis for calculating the charge carried by each particle, enabling the construction of a complete charge–size distribution for a given applied potential difference.

The presentation will describe the design and development of this new measurement rig, followed by an overview of experimental trials conducted using glass beads as model particles. The results demonstrate that the device can successfully resolve the charge on individual particles and reveal the statistical distribution of particle charging within a sample. Notably, the measurements show clear evidence of bipolar charging, where particles within the same population acquire both positive and negative charges.

Improving Single Droplet Drying Models for Spray Dryer CFD Simulations Using Physics-Informed Neural Networks

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In the food and pharmaceutical industries, spray drying is a key technology for producing powders, and computational fluid dynamics (CFD) simulations are used to analyse and optimise this process. Central to such simulations is the single droplet drying (SDD) model, which provides the drying rate of a droplet as it transforms into a particle. This drying rate is strongly influenced by changes in the internal resistance to mass transfer, which is governed by the particle structure that develops during droplet drying.

Many simulations currently rely on semi-empirical SDD models such as the Characteristic Drying Curve (CDC) and Reaction Engineering Approach (REA), which are obtained by fitting model parameters to experimental data. These approaches are useful for reproducing overall drying curves but suffer from drawbacks: they are unable to predict behaviour under conditions outside their fitted range and cannot represent internal moisture gradients. As a result, they provide limited insight into the moisture content near the droplet surface, which is crucial for estimating the drying rates and particle stickiness.

Internal diffusion-based models, which numerically solve Fick's Second Law, offer a more detailed description by capturing internal moisture gradients and surface moisture content, even though they still typically require some fitting to experimental data. However, their computational expense makes them unsuitable for use in full-scale spray drying CFD simulations that track thousands of droplets simultaneously.

This work explores the potential of Physics-Informed Neural Networks (PINNs), which have been reported to achieve good accuracy when predicting the solutions of partial differential equations (PDEs), as surrogates for internal diffusion-based SDD models. The ultimate aim is to develop a *parameterised* PINN-based SDD surrogate that predicts the solution of Fick's Second Law across varying conditions – including droplet diameter, droplet temperature and initial moisture distribution – while explicitly representing internal moisture gradients, being more computationally efficient than numerical internal diffusion-based models, and more robust and accurate than CDC and REA models. The presentation will describe progress towards this goal.

Developing A Process Workflow to Predict Particle Size Changes in Agitated Filter Drying

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Active pharmaceutical ingredients are typically produced by crystallisation from solution, following which they are filtered, washed and dried. These steps are typically carried out in an agitated filter dryer (AFD), which heats the liquid through the vessel walls whilst the bed is agitated to improve heat and mass transfer. This agitation causes undesirable particle size changes due to breakage and agglomeration. The rates are dependent on process parameters (e.g., impeller speed and operation) and material properties (e.g., hardness and flowability).

In this research we aim to understand how process parameters and initial particle size distribution affect size distribution changes in AFDs, by developing and carrying out drying experiments in a small-scale jacketed vessel, which mimics the AFD process. A population balance model is coupled with differential equations for moisture evaporation and temperature rise throughout the bed, to predict particle size distribution from a given drying operation. By comparison to pilot scale results and iterating the model, we aim to develop a process workflow by which new APIs can be characterised to determine the viability of drying in an AFD and the optimum operational conditions.

Xerode: Dry Battery Electrode Printing

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Traditional battery electrode manufacturing is energy-intensive, relying heavily on solvent-based processes that not only increase costs but also slow down production. The growing demand for energy-efficient, sustainable, and custom-designed batteries in sectors such as consumer electronics and electric vehicles requires a shift in manufacturing methods.

At Xerode, we have developed a game-changing solution for battery manufacturing. By eliminating the need for solvents in the electrode printing process, we reduce energy consumption, cut production times, and enable highly customised battery designs for various applications including wearables, consumer electronics and specialised electronics.

Xerode's proprietary dry electrode manufacturing process transforms battery materials into toner-like substances, allowing them to be printed directly onto substrates using a dry, modular approach. Our technology offers rapid prototyping, full freedom of form factor, advanced microstructure control and compatibility with a wide range of chemistries. This makes it a versatile solution for both small-scale and large-scale battery manufacturers.

Since completing the Faraday Institution Industry Sprint programme, Xerode has made substantial progress in both technological development and market outreach, successfully demonstrating our distinctive capabilities and generating strong interest across multiple market segments. This poster presents the core capabilities, key performance indicators, and commercial opportunities associated with Xerode's dry electrode printing technology, alongside the current IP status and potential avenues for strategic industry collaboration.

Hybrid Mechanistic–Machine Learning Platform: From Formulation and Process Parameters to Performance and Inverse Design

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Manufacturing of solid oral dosage forms involves a sequence of unit operations that transform complex powder blends into structured tablets with defined performance. While process models for these unit operations are relatively well developed, broadly applicable product performance models remain scarce. Existing models are often either highly empirical—tied to narrow formulation and process windows—or fully mechanistic but too computationally intensive for routine use. There is therefore a clear need for mechanistic product models that capture the key rate processes governing performance, and for hybridization with machine learning to make these models practically usable in design and optimization.

This work presents a hybrid mechanistic–machine learning framework that links routine formulation and process descriptors to time-dependent product performance, such as swelling, disintegration. A mechanistic core describes the evolution of internal structure and mass release using coupled single-particle and population-balance models. This provides a physics-based forward mapping from internal material parameters to performance profiles, representing a product performance model.

On the other side, a supervised artificial neural network (ANN) “mapper” is trained to infer the key mechanistic parameters from standard formulation and process inputs (e.g. excipient type, binder and disintegrant levels, liquid-to-solid ratio, porosity, skeletal density). Sensitivity analyses are used to identify the most influential parameters and inputs, thereby clarifying dominant levers for critical quality attributes (CQAs).

On the current dataset, the hybrid framework can generate swelling and disintegration curves for new formulations without manual parameter fitting, acting as a fast surrogate to the full mechanistic workflow. Ongoing work aims to embed this forward model within inverse optimization schemes so that target performance (e.g. desired disintegration or swelling profiles) can be systematically mapped back to feasible combinations of formulation and process parameters, moving towards a practical digital design tool for tablet performance.

Deep Learning for Analysis of Powder Triboelectrification

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Triboelectric charging has been recognised for millennia, yet its underlying mechanisms remain poorly understood. In powder-handling industries, tribocharging causes flow instabilities, segregation, and safety risks [1]. Identifying the particle properties that govern charge accumulation would enable improved material and process design, however progress has been limited by the large number of interacting factors influencing charging behaviour. Significant disagreement persists regarding the dominant charging mechanism, with recent reviews suggesting that conflicting experimental findings arise from multiple competing processes acting simultaneously [2]. Consequently, the fundamental properties controlling tribocharging, and their combined effects, remain unclear. Machine learning methods offer a promising approach for analysing high-dimensional datasets and capturing complex interdependencies, while enabling the incorporation of previously underutilised data types such as imaging and structural descriptors [3].

This study applies deep learning to investigate relationships between physical, chemical, and electrical properties of particles and their triboelectric behaviour. 35 different powders are characterised using multiple experimental techniques, combining measurements of surface morphology, size distribution, and hygroscopicity with imaging data. Molecular and electronic descriptors obtained from established databases are incorporated to capture mechanisms relevant to charge transfer. The experimentally measured saturation charge, obtained via aerodynamic dispersion, is predicted by the model. Interpretability analyses, including feature importance and sensitivity mapping, identify the properties most strongly associated with charge accumulation, providing insight to guide the design of powder systems that minimise triboelectric effects.

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Digital Twin Development for Solid Waste Packaging in Nuclear Decommissioning

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Nuclear decommissioning requires the safe sorting and packing of radioactive components such as vessels and glove boxes. Current manual and remote-handling approaches expose workers to radiation, limit operational time, and incur high costs. Autonomous robotic systems offer a promising alternative, but recent UK NDA demonstration projects have highlighted a key challenge: packing solutions generated by optimisation software must be mechanically feasible and executable by real robotic manipulators.

A PhD project within the SATURN CDT is developing a digital-twin (DT) framework to address this issue. The system integrates: (i) a robotic arm with a gripper for object placement; (ii) RGB-D cameras to detect deviations between predicted and actual packing states; and (iii) a DT engine based on DigiDEM, a discrete-element-method implementation using a digital approach that makes handling of arbitrary (irregular) geometries relatively easily. The DT performs packing optimisation, communicates desired position and poses to the robot, and continuously updates itself using machine-vision feedback to remain aligned with physical reality.

Once validated, this framework will allow practical assessment of packing algorithms before deployment, overcoming limitations of existing methods that prioritise space utilisation while neglecting stability and robotic packability. Because the DT is continuously updated and remotely accessible, it supports virtual testing, improved planning, and integration with multi-robot systems. This work represents a significant step toward safer, more efficient, and cost-effective nuclear waste packaging, contributing to the broader digital transformation of nuclear decommissioning.

Data-Driven Modelling of Diffusion Coefficients in Simple Fluids and Porous Media

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Characterisation of reactive-diffusive transport in porous systems is crucial for the design of processes for solute uptake, release, and conversion. Conventional parameter estimation of diffusion coefficients, reaction rates, and reaction orders necessitates advanced, extensive calibration experimental techniques. We present a data-driven computational framework using physics-informed neural networks (PINNs) to directly extract transport parameters from spatiotemporal concentration fields obtained via fluorescence imaging. Governing PDEs describing transport and reaction kinetics are incorporated directly into PINN training alongside boundary conditions and interior observations within a multi-objective loss function. Minimising this loss function converges on best-fit transport parameters and reconstructs concentration fields for comparison with observed propagation. As an illustrative example, Rhodamine B diffusion in aqueous solution has been studied. The developed PINN predicted a diffusion coefficient of $D = 3 \times 10^{-10} \text{ m}^2/\text{s}$, consistent with literature values, while reconstructing the concentration field with low error (see Figure 1). The framework will be extended to coupled reaction-diffusion systems for simultaneous multi-parameter estimation and validated using particle-laden hydrogel systems with varying particle sizes and hydrogel loadings. This approach provides an easy-to-set-up, cheap, imaging-based characterisation methodology for particulate transport in complex media.

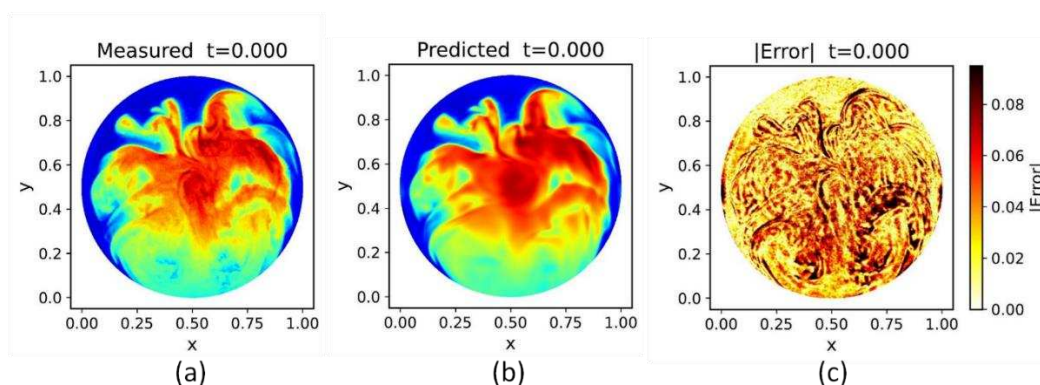


Figure-1: a) Image of Rhodamine B concentration (ground truth), which is the input for the data-driven computational framework, b) Concentration predictions by the developed model, and c) the relative error between ground truth and predictions.

An Opensource CFD Model of Gas-Solid Vortex Chambers: Single Phase and Multiphase Operation

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Fluidization is widely employed in industrial gas-solid operations, from non-reactive to reactive processes. Enhanced solid mixing and the higher velocities experience in a fluidized bed lead to better heat and mass transport, but transfer coefficients remain limited by the achievable gas-solid slip velocity, which is necessarily lower than the particle terminal under earth's gravity. Fluidizing solids against a centrifugal field instead allows overcoming this limit and maximise transport. Rotational (high-g) fluidized beds can operate at much higher slip velocities and accelerate heat and mass transfer by orders of magnitude [1], facilitate the fluidization of cohesive powders, allows for more compact reactors with a lower contact time and better selectivity [2].

Traditional mechanically rotating fluidized beds (RFBs) have been used to process fine materials but large moving parts are an important scale up challenge [3]. Similar rotating fluidized beds can be obtained in a static geometry, solid vortex reactors (GSVRs), using a set of tangential inlets to impart the swirling motion to the solids (Fig 1a). The resulting centrifugal force pushes the solid phase outwards while the radial drag pushes them inwards towards a central chimney. Depending on this force balance, the system may develop into a stable rotating (aerated) fixed bed or a rotational (expanded) fluidized bed. GSVRs have shown potential in particle processing (drying, coating) and reactive processes (e.g. pyrolysis, CH₄ coupling) as a form of ultra-short contact time device [4–7]. Stator–Rotor Vortex Chambers (STARVOCs) have been recently proposed as much more flexible RBF that can be operated with or without a motor using a tangential gas injection to impart momentum to a rotor-chamber and the solid phase. While sharing some scalability issues with RFBs, STARVOCs can achieve rotating speeds up to 4 times higher than GSVRs at lower gas throughput [8].

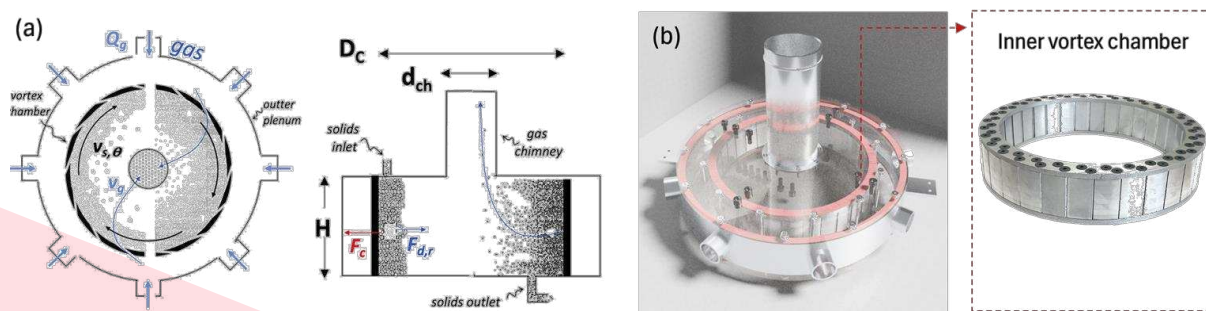


Figure 1. (a) Top and side schematic of a radial GSVR. (b) Prototype and inner chamber at Heriot-Watt University

The design and control of high-g gas-solid devices is a substantial technical challenge. While RBFs can deliver an independent control of the swirl and the gas throughput, the external energy input and moving parts complicate scale up and applicability. GSVRs involve no moving parts, but suffer from high frictional losses, and a more complex design where the geometry and inlet configuration determines the efficiency in the transport of angular momentum to the solids. In both GSVRs and certain STARVOC configurations, one cannot control independently the radial and azimuthal drag force, and consequently, bed stability, uniformity and expansion, are directly linked to the unit geometry, inlet design and solid properties [9]. High-g units are conceived for specific feedstock and loading and cannot easily adapt to wide changes in particle properties, handle a large solid throughput or target its residence time.

Control, adaptability and scalability are important challenges in high-g GSVRs. It is hard to capture their complex hydrodynamics in 0D models [10], so design ultimately relies on computational fluid dynamics (CFD) models calibrated with measurements of solids velocity and void fraction. In this contribution we introduce a new, fully opensource (OpenFOAM) computational platform to simulate single radial GSVRs. Single-phase and multiphase operations are described with transient RANS (Reynolds Stress Model RSM) and Two-Fluid Model (TFM) and validated with experimental data at small scale, including measurements of pressure, pressure drop and solid velocity fields [10,11]. This computational framework allows us to study the transient response of a wider radial unit under construction at Heriot-Watt University (Fig 1b) and to investigate the response of high-g rotational beds to varying solid loading (Fig 2) and inlet configurations. Understanding this dynamic is fundamental step to address control and scale up issues with the design of multimodular devices that could enable independent control of swirl, expansion, throughput and solid phase residence time.

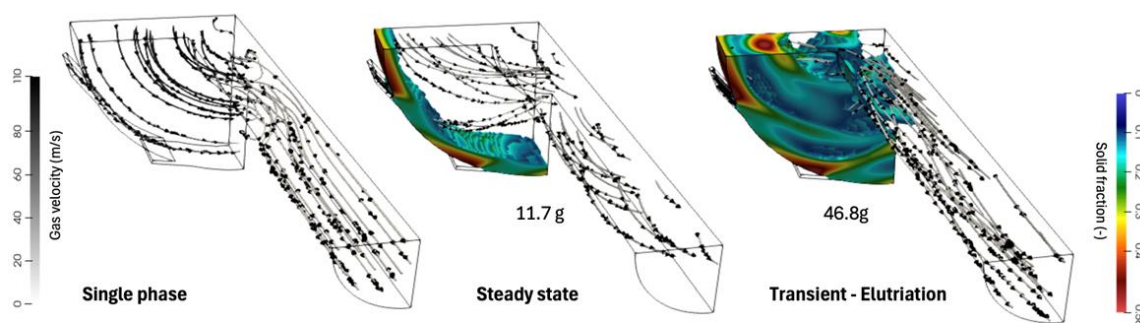


Figure 2. Bed development under increasing solid injection load. Gas velocity and solids volume fraction. GSVR refers to [12]

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Cost-Optimal Cutting and Packing for Nuclear Decommissioning

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During nuclear decommissioning, large structures must be cut into smaller parts before packing, and the cost of these two processes is tightly linked. Cutting parts into smaller pieces improves packability and can reduce the number of containers needed but increases cutting effort. Cutting minimally saves effort but produces large, inefficiently shaped parts that require more containers. Because packing performance depends directly on how a structure is cut, the two processes should be optimised together rather than independently. However, this is not what has usually happened in practice!

A voxel-based optimisation method is introduced to minimise the combined cutting and packing cost. The structure is voxelised, and total cost is defined as the weighted sum of cutting volume and the number of containers required. A genetic algorithm (GA) generates candidate cutting patterns, evaluates them by cutting and then packing the resulting parts, and iteratively evolves towards lower-cost solutions. Packing uses a container-by-container strategy that fills each container with a selected subset of parts, repairing failures by replacing only items that cannot be placed.

A glove-box case study compares two container types (i.e., box and drum) with different sizes and packing costs. In both cases, the algorithm steadily reduces total cost over GA generations. The box container achieves a lower final cost despite requiring more cutting, because the resulting smaller pieces pack more efficiently. Additionally, a high cutting-cost scenario shows that when cutting is heavily discouraged, the algorithm produces fewer cuts but much poorer packing, demonstrating the limitations of minimal-cutting strategies that ignore packing effects.

This integrated method captures the essential trade-off between cutting effort and packing efficiency, works for arbitrary structures and container types, and outperforms approaches that treat cutting and packing as separate problems.

A Gaussian Process assisted Multi-objective Optimisation Framework for Precision Probiotic Tablet Manufacturing

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Tablet is a widely used dosage form for probiotic delivery due to its stability, ease of administration, and scalability for industrial production. However, probiotics are highly sensitive to mechanical and thermal stresses during powder compaction, often resulting in significant viability loss and suboptimal tablet structure. In this work, a finite element (FE) model integrating the Drucker–Prager Cap (DPC) framework with probiotic thermal tolerance was developed to predict both probiotic survival and tablet porosity during powder compaction and was validated against experimental data. Based on the FE-generated dataset, Gaussian Process Regression (GPR) coupled with active learning (AL) was employed to construct data-efficient surrogate models for viability and porosity, providing reliable predictions with quantified predictive uncertainty. Finally, multi-objective optimisation (MOO) using Non-dominated Sorting Genetic Algorithm II (NSGA-II) was performed with an ϵ -dominance strategy that explicitly accounts for surrogate prediction uncertainty in the optimisation process, enabling robust identification of processing conditions that simultaneously maximise probiotic survival and achieve desirable tablet porosity. This integrated modelling and optimisation framework provides practical guidance for the rational and Quality-by-Design (QbD)-oriented development of robust probiotic tablet formulations.

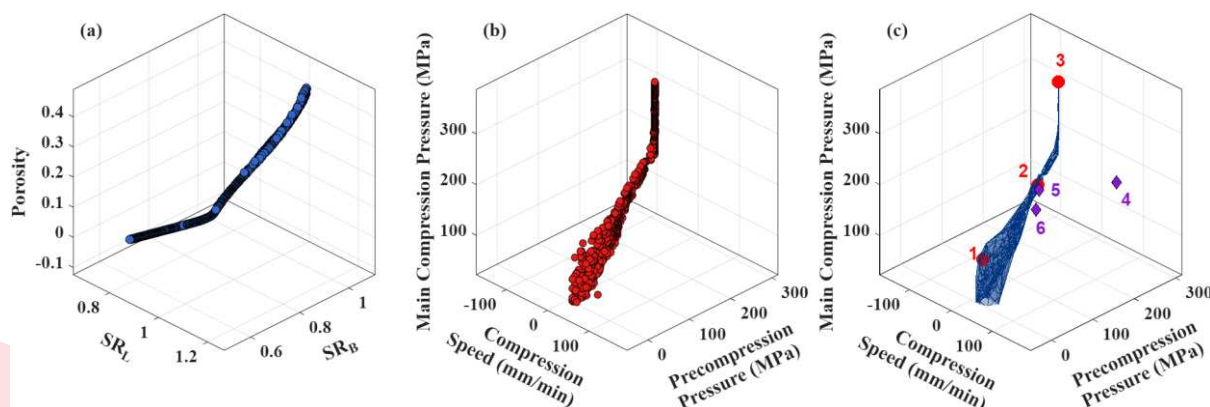


Figure 1 Pareto front obtained using NSGA-II (a); corresponding optimal process conditions (b); feasible design space (c).

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