BEAR

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BEAR Conf '24

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Acknowledgements

We would like to thank all the people who contributed to this publication.

Front Cover
Separated Vortex Ring behind a Porous Disc
Chandan Bose (University of Birmingham) & Ignazio Maria Viola (University of Edinburgh),
OpenFOAM Journal Cover 2022.

Cite

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FOREWORD

DR DIETMAR HEINKE

CHAIR OF THE BEAR USER GROUP

The BEAR PGR Conference served as a gathering for BEAR users to convene and learn about the captivating research conducted by Postgraduate Researchers (PGRs) and academic staff utilizing the University's supercomputer, BlueBEAR. The BEAR PGR Conference takes place annually and offers PGRs a valuable opportunity to gain conference management experience, enhancing their curriculum vitae.

This year's conference spanned two days and featured poster presentations and talks encompassing a wide range of disciplines including fluid dynamics, design optimisation, psychiatry, neuroscience, genetics and neuropsychology. We were privileged to host three distinguished keynote speakers, namely Dr Neil Ashton (Worldwide Tech Leader, Amazon Web Services), Jack Style (EvoPhase, COO) and Dr Kit Windows-Yule (Assistant Professor, Chemical Engineering)

We trust that these abstracts will prove highly stimulating and motivate you to delve deeper into the presenters' research and explore how BlueBEAR can contribute to your own research endeavours.

The conference culminated in the announcement of the best poster and talk winners. Given the outstanding quality of presentations, selecting the winners was no easy task. However, we are delighted to acknowledge Aaron Wiggin as the recipient of the best poster award, commending his engaging and clear presentation. Additionally, Katherine Jeynes-Cupper earned the best talk award for his visually impactful delivery. We extend our gratitude to Lenovo for generously providing tablets as prizes for the winners.

These proceedings and the conference as a whole would not have been possible without the remarkable efforts of numerous dedicated individuals working tirelessly behind the scenes. We extend a heartfelt thank you to the Organizing Committee, comprised of Leonard Nicusan, Will Peace, Khirzra Wadood, Ioanna Giannakou and Benjamin Jenkins and Kirsty McCready as well as the advisory Committee members: Aslam Ghumra, Dr Stephanie Thompson, and Debbie Carter.

Dietmar Heinke

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Worldwide Tech Leader for CAE at Amazon Web Services

JACK SYKE

EvoPhase - COO

DR KIT WINDOWS-YULE

Assistant Professor in Chemical Engineering

CONTRIBUTORS TALKS

Winner for best talk:
Katherine Jeynes-Cupper

CONTRIBUTORS POSTERS

Winner best poster
Aaron Wiggin

DAY 1

Time	Speaker	Title
09:3	Coffees, Networking and Posters (Atrium)	
10:00	**Welcome by Dr Dietmar Heinke**	
10:10	Carol Sandys Head of ARC	BEAR State of the Union
10:30	Keynote: Neil Ashton	How HPC, ML and Cloud Computing are helping to move towards a digital design process for the automotive and aerospace industries
11:10	Coffee Break (Atrium)	
Session 1: CFD Session (G35)		
11:30	Chandan Bose	CFD / OpenFOAM User Group
11:50	Roberto Hart-Villamil	On the AI driven geometry optimisation of a stirred tank CFD model in laminar flow
12:10	Xue Lian	Coupled SPH-DEM method for simulating coarse food particles in a non-Newtonian conveying fluid
12:30	Lunch (Atrium)	
13:00	Poster Session (Atrium)	
Session 2: Short Presentations (G35)		
14:00	Kamilla Kopec-Harding	R User Group
14:10	Kamilla Kopec-Harding	Research Data Science Group
14:20	Lu Hai	FEM / Abaqus User Group
14:30	Josephine Bates	Using data analytics to break down outcome measures in liaison psychiatry
14:40	William Peace	Investigation of high gas flow rates on hydrodynamics in two phase gas-liquid stirred tanks using Positron Emission Particle Tracking (PEPT)
	END	

DAY 2

Time	Speaker	Title
09:30	Coffees, Networking and Posters (Atrium)	
10:00	**Day 2 - Welcome**	
	Session 3: DEM Session (G35)	
10:10	Keynote: Jack Sykes	EvoPhase - A University of Birmingham Spin-Out
10:50	Dominik Werner	Optimising Mixing Processes with DEM: From Problem Identification to Solution
11:40	Daniel Rhymer	A world of pure imagination? Understanding the dynamics of Vertical Stirred Mills within chocolate processing.
12:00	Lunch Time + Posters (Atrium)	
13:00	Keynote : Dr Kit Windows-Yule	AI-based optimisation of industrial processes and process equipment
	Session 4: Biological Presentations (G35)	
13:40	Andrew Quinn	CHBH-on-BEAR: cluster computing for neuroimaging analysis
14:00	Kirsty McCready	Deconstructing the Ceratopteris genome
14:20	Margarita Sarant	In search of the big data benefit when predicting language outcome after stroke using machine learning
14:40	Coffee Break (Atrium)	
15:00	Katherine Jeynes-Cupper	mobileRNA: A new tool for efficient analysis of RNA expression in multiple genomes
15:20	Christopher Mahony	Runx1 Is A Key Transcription Factor That Drives Synovial Fibroblast Pathogenicity In Rheumatoid Arthritis
16:00	Awards and Wrap-Up	
	END	

CFD USER GROUP

Chandan Bose
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The OpenFOAM and Fluid Dynamics special interest user groups, operating under the aegis of the Birmingham Environment for Academic Research (BEAR), serve as pivotal platforms for advancing computational fluid dynamics (CFD) research at the University of Birmingham. Established to address the growing demand for sophisticated Computational tools and methodologies in fluid dynamics, these groups harness the collective expertise of researchers, fostering an environment of innovation and collaboration. Recent initiatives includes the plan for a series of workshops, seminars, and hands-on training sessions focused on OpenFOAM, a leading open-source software for CFD analysis.

These activities will not only bolster the technical proficiency of our members but also stimulated collaborative research endeavors within and beyond the University. Looking ahead, these two special-interest groups are committed to expanding their impact through the creation of a robust network of fluid dynamics researchers. Plans include the establishment of an annual Fluid dynamics symposium, and the development of an online portal for resource sharing and discussion.

These initiatives aim to catalyze the exchange of knowledge, facilitate interdisciplinary projects, and ultimately, contribute to cutting-edge advancements in fluid dynamics research. As we move forward, the OpenFOAM and Fluid Dynamics user groups will continue to play a critical role in shaping a dynamic and collaborative research landscape at the University of Birmingham. Through these concerted efforts, we anticipate not only the advancement of CFD technologies but also the nurturing of the next generation of researchers equipped to tackle the complex fluid dynamics challenges of the future.

ON THE AI DRIVEN GEOMETRY OPTIMISATION OF A STIRRED TANK CFD MODEL IN LAMINAR FLOW

Roberto Hart-Villamil
email: rxh659@student.bham.ac.uk
Roberto Hart-Villamil(1) , Andy Ingram(1) , Christopher Windows-Yule(2) , Andrei L. Nicuşan(1) , Santoshkumar Gupta(3) , Waldo Rosales(4) , Adam Kowalski(4)

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Viscous mixing in stirred tanks is a process employed in a wide range of industries and requires a thorough understanding of the material properties and the hydrodynamics within the system. Using Computational Fluid Dynamics (CFD), mixing environments can be fully simulated to highlight regions of poor mixing and predict the influence of parameters such as impeller shape or material properties. This study applies a novel AI-driven technique to improve axial mixing in a poorly performing lab-scale ploughshare mixer. In laminar flow, the rate of mixing is a function of the rotation rate and the mixer geometry [1]. Therefore, mixing can be improved by either increasing the rate of impeller rotation or by instead modifying the impeller geometry such that the mechanism responsible for axial mixing is promoted.

Using HARPPP, the AI-driven tool from EvoPhase, the components of the ploughshare shape were generalised and an optimisation strategy using evolutionary algorithms was applied to morph the geometry shape for maximum axial mixing. In each epoch, 48 simulations are run in parallel, each running for approximately 20 hours. Illustrated in Figure 1, each simulation possesses three passive scalars initially occupying a third of the available volume along the shaft axis (left, middle, right of tank). After 10 seconds of rotation, the uniformity of each passive scalar is evaluated, and a measure of mixing error is input to HARPPP which then applies multi-objective optimisation to minimise each mixing error.

ON THE AI DRIVEN GEOMETRY OPTIMISATION OF A STIRRED TANK CFD MODEL IN LAMINAR FLOW

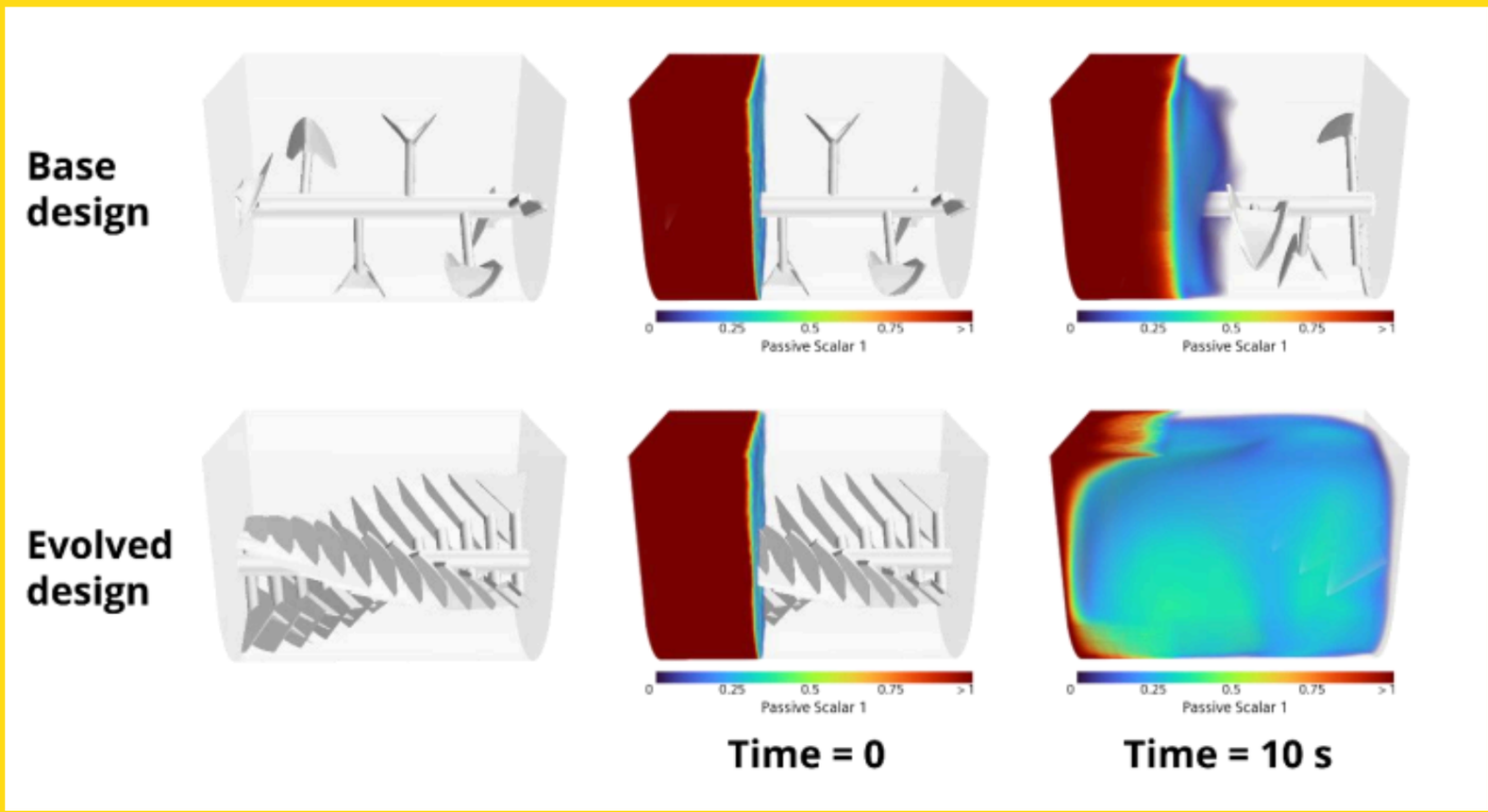

Figure 1. A comparison between the performance of the base design (Top) and an evolved design (Bottom). In the second column, a single scalar tracer is depicted initially occupying the left-most third of the tank. The third column reveals the concentration of the tracer after 10 seconds of simulation.

Upon exploring a wide range of impeller shapes, the algorithm discovered that a double-helix design was able to promote axial mixing far more efficiently than any other design. Illustrated in Figure 2, the evolved designs achieved a 1000x mixing improvement over the base design for the same power requirement. The generality of this technique allows for future application on a wide variety of unit processes unrelated to mixing.

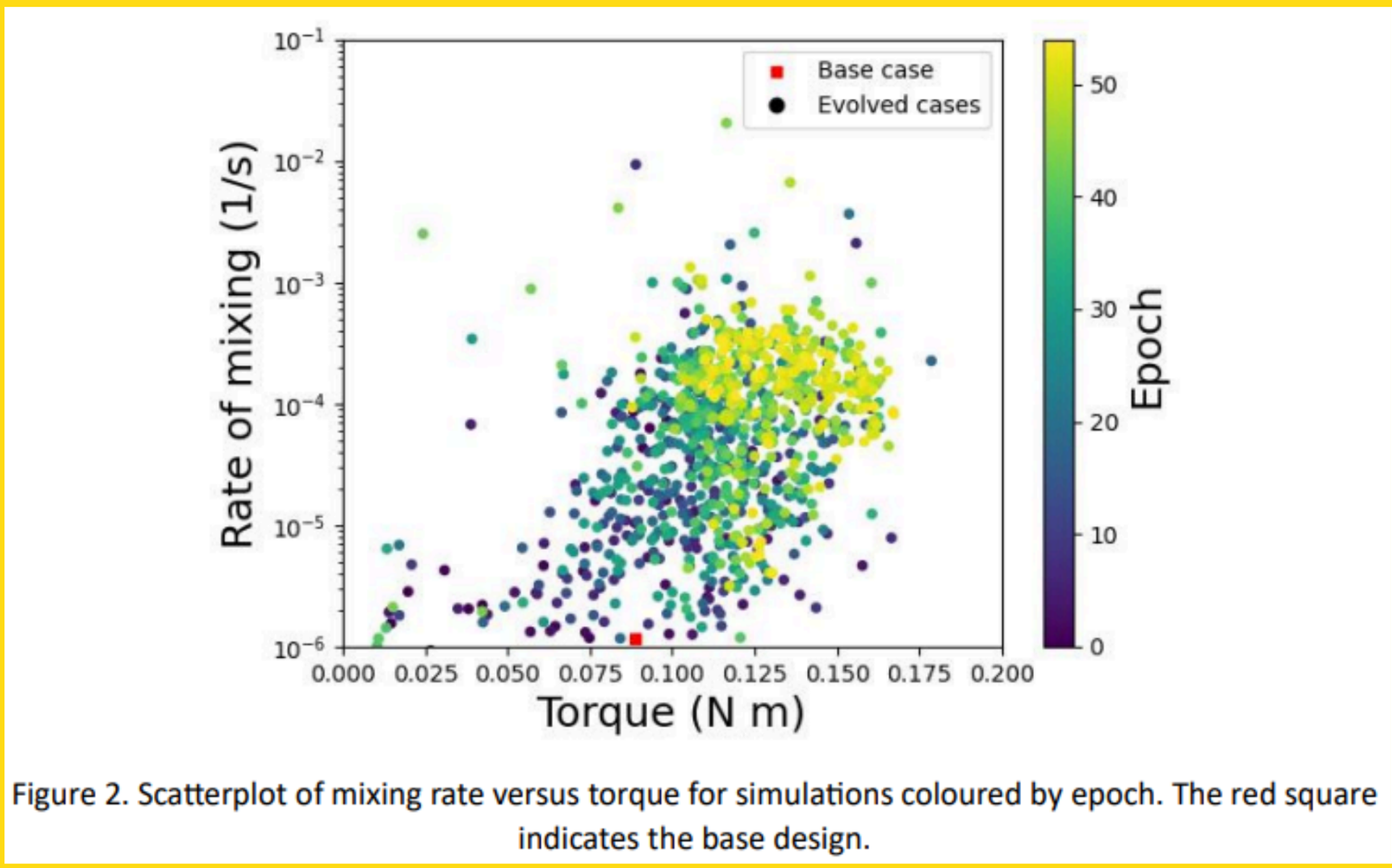

Figure 2. Scatterplot of mixing rate versus torque for simulations coloured by epoch. The red square indicates the base design.

References [1] G.B. Tatterson, Fluid Mixing and Gas Dispersion in Agitated Tanks, McGraw-Hill, USA, 1991

COUPLED SPH-DEM METHOD FOR SIMLATING COARSE FOOD PARTICLES IN A NON-NEWTONIAN CONVEYING FLUID

Xue Lian
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Xue Lian(1) , Mostafa Barigou(1)
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A Lagrangian particle-based numerical framework, utilizing smoothed particle hydrodynamics (SPH) coupled with a discrete element method (DEM), was employed to simulate the flow characteristics of coarse food particles in a non-Newtonian conveying fluid within a horizontal pipe. Nearly neutrally buoyant nearly spherical calcium-alginate particles were used as model food particles. The capability of the SPH-DEM methodology was successfully validated in non-Newtonian single-phase as well as in two-phase particle-liquid flows by comparing the local phase velocity flow field, radial particle distribution, and particle passage times with experimental Lagrangian measurements obtained by a technique of positron emission particle tracking (PEPT). The simulations also yielded accurate predictions of flow pressure drop. In addition, detailed information was afforded on local particle spin, fluid pressure, and carrier fluid vorticity. The results demonstrate the high capability of the proposed numerical framework to predict the complex features of complex particle-liquid flows in pipes.

R USER GROUP

Dr Kamilla Kopec-Harding
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In this talk we introduce the University of Birmingham R User Group, a special interest group for R practitioners at the University. We'll cover the purpose of the group, how we fit in with other R groups locally and nationally, highlight upcoming events and our plan for the coming year. We'll look at our Organising Team and how it is structured to ensure that the group is sustainable and continues to grow.Finally, we'll talk about how you can get involved!

RESEARCH DATA SCIENCE GROUP

Dr Kamilla Kopec-Harding
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In this talk, we introduce the Research Data Science Service, a new addition to the Research Software Group. We are a team of “Research Data Scientists” available for hire across the university who provide support to researchers through both free and funded engagements. As part of Advanced Research Computing (the people who bring you BlueBEAR), the Research Data Science Service exists to facilitate data intensive research, increase the competitiveness of funding applications and support open science by sharing best practices around sharing data and or code. In this presentation, we’ll introduce the team, tell you about the services we offer and how to get in touch!

FEM / ABAQUS USER GROUP

Lu Hai
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Abaqus is an efficient software application to provide advanced solutions in several fields. However, it is quite hard for the beginners to start their research with the software while some specialists also would get stuck in with their modelling because of the intricate functions and multiple parameters. UoB Abaqus special interest group (SIG) intends to provide an integration platform for the beginners and specialists to learn and communicate, then generate more outcomes. Resource library and community are provided for people to ask for solutions and share ideas. More engagement of researchers and advancements are expected to be generated in all fields through Abaqus SIG.

USING DATA ANALYTICS TO BREAK DOWN OUTCOME MEASURES IN LIAISON PSYCHIATRY

Josephine Bates
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Supervisor: Dr Adam Hickson (Consultant psychiatrist, Devon Partnership Trust)

Introduction
Performance measures are used to record both the emergency department and inpatient referrals to the liaison psychiatry team, and the responses to those referrals. At Devon Partnership Trust (DPT), this captures (on CHIT sheets) the date and time, location and driving reasons for both the patients' admission and for referrals to liaison psychiatry. Subsequently, the main aim of the liaison psychiatry team when making contact with referred patients is noted, and whether this aim was achieved. The mental state of the patient is assessed to record a clinical judgment of whether their condition had improved as a result of contact with the team both after a single session (global outcome 1, GO1) or multiple sessions (global outcome 2).

Aim: To audit the performance measures after assessments of liaison psychiatry inpatient referrals.

Methods
All CHIT sheets for referrals in May 2023 were collated. Data about the referrals were extracted, including their temporal characteristics, main aims and outcomes. Bootstrapping was applied to the data to allow for high granularity in visualising the distribution of referrals across the month. Kendall's tau correlational analysis was performed to assess whether referral time, patient age or the main aim of referrals were associated with GO1. R version 4.3.0 was used to complete this analysis.

Results
78 referrals were collected and analysed. Patient ages ranged from 18-85, and were non-normally distributed. There was a non-uniform distribution of referrals across the month. The Kendall's tau correlation coefficients for associations between referral time, patient age and the main aim of referral to GO1 were 0.080 ($p = 0.470$), 0.108 ($p = 0.274$) and -0.067 ($p = 0.561$), respectively.

USING DATA ANALYTICS TO BREAK DOWN OUTCOME MEASURES IN LIAISON PSYCHIATRY

Discussion

It was predicted that referrals would have a uniform distribution across the different dates within the month of data collection. Because of the naturally limited number of actual referrals, bootstrapping to apply the identical data distribution across 7,800 referrals was a useful method of testing this prediction with advanced descriptive statistics. BEAR facilitated this through the provision of a coding platform for higher-performance data analysis. No meaningful correlations were found between referral time, patient age or referral aims, with GO1. This audit sparked regional discussion regarding the use of performance measures for referrals in liaison psychiatry. DPT considered the accuracy of performance measure recording, the internal validity of the options for referral reasons and aims of contact, and the threshold for deciding when aims of contact are achieved. This allowed a contrast of what DPT wants the liaison psychiatry performance measures to indicate, versus what they do indicate.

USING DATA ANALYTICS TO BREAK DOWN OUTCOME MEASURES IN LIAISON PSYCHATRY

William Peace

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Two-phase gas-liquid stirred tanks are used in a variety of industrial sectors. However, despite their ubiquity, the understanding of these systems is significantly limited when compared to single-phase equivalents. Most quantitative investigations have been limited to systems at very low gassing rates (<1 VVM), which are unrealistic when compared to typical pilot scale production facilities.

In this investigation, Positron Emission Particle Tracking (PEPT), a non-invasive measurement technique has been used to study the fluid dynamics of a 200mm diameter gas-liquid stirred vessel at industrially relevant gas hold-ups and superficial gas velocities. Flow dynamics have been studied in both the flooded and dispersed aerated regimes for a viscous Newtonian aqueous glycerol solution. Gas flow rates have been varied between 1.6, 3.0 and 5.0 VVM for both cases, corresponding to industrially relevant superficial gas velocities of 0.0053, 0.01 and 0.0167 m/s . For all cases, a single-phase measurement has been performed as a control experiment.

From the PEPT measurements, velocity scalar and velocity vector fields have been derived, alongside a calculation of the degree of dispersion in the system, providing an alternative quantitative measure of mixing time and performance. The three-dimensional nature of PEPT has been exploited by examining the particle trajectories as well as three-dimensional maps of poorly dispersed regions in order to identify areas in the vessel which experience poor localised mixing. The flooded experiments identified a high-velocity bubble plume along the vessel axis dominating the flow, matching previous qualitative observations. The dispersed experiments highlighted a strong impact of the gas flow rate on the hydrodynamics, with the direction of the high velocity out jet becoming more vertical as the gas flow rate increases.

ABSTRACT SUBMISSION FOR CONFERENCE WORKSHOP: ENHANCING PARTICLE MIXING EFFICIENCY IN ROTATING DRUMS USING DISCRETE ELEMENT METHOD (DEM)

Dominik Werner

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This workshop offers an insightful exploration into the application of the Discrete Element Method (DEM) for optimising industrial processes, particularly focusing on particle mixing in rotating drums. Despite the widespread utilisation of rotating drums in various industries, achieving uniform mixing remains a challenge due to segregation. This practical session will demonstrate how DEM can be employed to diagnose and resolve non-ideal mixing by implementing design modifications such as drum inserts.

Participants will engage in a hands-on exercise using a JupyterLab notebook that includes data from more than 20 DEM simulations. These simulations represent a range of scenarios depicting different degrees of mixing efficiency in rotating drums. Through guided analysis, attendees will learn how to use advanced post-processing software to evaluate each simulation and determine the most effective configuration.

The workshop is designed to be accessible for engineers and researchers, regardless of their prior experience with DEM. By the end of this session, participants will have a solid understanding of how to apply DEM to enhance equipment performance and prevent costly operational issues.

Attendees will leave equipped with the skills to apply these techniques to their own work, driving forward the efficiency and reliability of their processes.

A WORLD OF PURE IMAGINATION? UNDERSTANDING THE DYNAMICS OF VERTICAL STIRRED MILLS WITHIN CHOCOLATE PROCESSING

Daniel Rhymer

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While it would be nice to imagine a Willy Wonka world where perfectly smooth chocolate is produced by waterfall, the reality is very different. Cocoa liquor is a particle-laden slurry, and these particles need to be reduced in size to create the smooth texture and desired mouthfeel needed for tasty chocolate. A vertical stirred mill is often used to achieve this, as they have greater specific energy transfer and a smaller physical footprint than other grinding techniques [1], but there is still little understanding about its exact dynamics on an industrial scale. This is a problem not just within chocolate, but industry as a whole, as grinding is the most commonly used step in manufacturing. Up to 4% of global electricity consumption goes into reducing the size of materials [2]

Simulation has opened a new world of possibility to explore the detail of vertical mills and the talk presents a validated simulation using the Discrete Element Method (DEM) technique and experimental data from particle tracking data. The model is trained and optimised using machine learning and while there are limitations in trying to align complex multiphase systems, a good level of agreement with the experimental results can be reached. The model can also reproduce the dynamics of unseen trials to the same level of accuracy as the initial training set, further validating the optimal conditions and means the model can be used with confidence beyond the experimental trials. This truly unlocks a world of pure imagination in better understanding and optimising the process, improving efficiency and tackling the climate crisis

CHBH-ON-BEAR: CLUSTER COMPUTING FOR NEUROIMAGING ANALYSIS

Andrew Quinn
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I will outline how science and teaching at the Centre for Human Brain Health have been adopting cluster computing solutions with BlueBEAR. Central to this is a collaborative website which we use to collate neuroimaging-specific documentation and tutorials as a supplement to the BEAR technical docs. https://chbh-opensource.github.io/chbh-on-bear/

DECONSTRUCTING THE *CERATOPTERIS* GENOME

Kirsty McCready
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Supervisor: J.C. COATES, A.R.G PLACKETT

Seeds are a recent evolutionary innovation that arose once from an ancestral spore-based reproductive mechanism that is still present in living seedless plant groups (e.g. mosses, liverworts and ferns). How this dramatic transition to seed-based reproduction occurred is currently unknown. Here we carry out RNA sequencing to unravel the genetic mechanisms controlling reproduction in the model seedless plant Ceratopteris richardii. However, the recently published C. richardii genome is large, and its completeness and accuracy remain largely untested.

Alignment of reads to a reference genome or transcriptome is a common first step in the analysis of RNA sequencing data. We investigate the efficiency and accuracy of mapping RNA sequencing reads to the published C. richardii transcriptome and genome using the pseudoalignment algorithm Salmon. We show that only 50% of reads mapped confidently to the transcriptome, with 25% mapping better to non-coding regions of the genome, and 25% not mapping at all. We further extract and de novo assemble the 291 million reads into 211,000 genes, 822 of which are not present in the current published genome annotation. This work demonstrates the need to carefully analyse the way we process new genomes to avoid losing important biological information.

IN SEARCH OF THE BIG DATA BENEFIT WHEN PREDICTING LANGUAGE OUTCOME AFTER STROKE USING MACHINE LEARNING

Margarita Sarant
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In our study, we investigated the learning curves of two models, ResNet18 (a deep Convolutional Neural Network) and logistic regression, to assess their performance in predicting post-stroke language recovery for different sample sizes. Utilising machine learning in this field is particularly relevant for aiding the rehabilitation process of stroke patients. This, however, faces some challenges such as dealing with high-dimensional neuroimaging data and the scarcity of large training datasets.

Our dataset consists of 758 stroke patient MRI scans and corresponding tabular data from the PLORAS project. We employed a 2D representation of 3D MRI data for the ResNet and three tabular measures for the logistic regression model. The task was to classify patients into aphasic or non-aphasic categories based on their performance on tasks from the Comprehensive Aphasia Test.

We divided patients into five groups, ensuring balance on relevant clinical information, and trained both models using cross-validation. To explore the dimensionality of our imaging data, we performed Principal Component Analysis (PCA) on the 2D brain scans, identifying components explaining 95% of variability.

Surprisingly, logistic regression consistently outperformed ResNet in our classification tasks, achieving a maximum accuracy of 81.4% compared to ResNet's 80.7%. Both learning curves exhibited a plateau, suggesting a saturation point in accuracy improvement with increased sample size. Notably, ResNet's performance using reconstructed images from only 20 out of 632 identified PCA components was comparable to its original image performance.

This hints at ResNet potentially missing subtle patterns crucial for enhanced performance, possibly due to the limited sample size. A larger dataset might enable the true potential of deep learning in predicting language recovery post-stroke, emphasizing the significance of big data in this context.

MOBILERNA: A NEW TOOL FOR EFFICIENCY ANALYSIS OF RNA EXPRESSION IN GENOMES

Katherine Jeynes-Cupper
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A growing number of studies have employed genomic analysis with next-generation sequencing technologies to differentiate genome-wide variations between treatment and control samples. However, instances in which biological samples contain genetic sequences from multiple organisms, such as those from plant grafting experiments or pathogen infection experiments, pose challenges related to correct mapping across multiple reference genomes. Mapping algorithms are designed to find the most suitable alignment in the provided reference. Therefore, when multiple references are involved, the independent mapping approaches of the same sample on separated genomes is not an efficient solution to correctly map RNA reads to the genome of origin. Here, we introduce a pipeline integrated into an R package, mobileRNA, which perform simultaneous alignment of transcripts and small RNA sequencing samples using two independent reference genomes.

Using real and simulated datasets, we show that mobileRNA can place reads to their genomic origin more accurately than previous approaches. The results demonstrated that the mobileRNA method retrieved results with less data noise; however, the similarity of the two genomes used as references plays the main role in the expected confidence in the discrimination of the placed reads across the two genomes.

RUNX1 IS A KEY TRANSCRIPTION FACTOR THAT DRIVES FIBROBLAST PATHOGENICITY IN RHEUMATOID ARTHRITIS

Christopher Mahony

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Mahony C(1), Kemble S(1), Chin P(1), Prada C(2), Hackland J(1),Nisa P(1), Marsh LJ(1), Keane P(3), Bonifer C(3), Buckley CD(2), Sansom S(2), Mark Coles(2) and Croft AP(1)#

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corresponding author

Background: Fibroblasts are key effector cells in rheumatoid arthritis (RA) underpinning joint inflammation and damage. Synovial tissue fibroblasts are heterogenous and acquire pathogenic cell states that either drive inflammation or tissue damage. However, the molecular mechanisms underpinning fibroblast heterogeneity and pathogenicity are poorly understood.

Methods: To identify key regulators of fibroblast behaviour, we performed combined scRNAseq and scATACseq analysis of synovial fibroblasts from the serum transfer induced arthritis model in mice and compared these data to additional scRNAseq data from collagen induced arthritis and antigen induces arthritis models. We have also performed lentiviral mediated overexpression of RUNX1 and bulk RNAseq. Ongoing validation is being performed using multiplex imaging, spatial transcriptomics (10x Visium platform), conditionally inactivating Runx1 in murine fibroblasts, pharmacological inhibition and ChIP-Seq.

Results: We identified Runt-related transcription factor 1 (Runx1) expression (scRNAseq) and motif activity (scATACseq) to be highly specific to sub-lining synovial fibroblasts which have been implicated in driving synovial inflammation. Runx1 motif activity and gene expression were also found to be upregulated during joint inflammation in mice and in patients with RA. RUNX1 overexpression showed that activated genes are upregulated in patients with RA and active joint inflammation, compared to those patients in clinical remission. Further analysis of publicly available data from RA synovium showed robust RUNX1 expression in synovial fibroblasts. Multiplex imaging showed RUNX1 to be enriched in perivascular fibroblasts compared to interstitial fibroblasts.

RUNX1 IS A KEY TRANSCRIPTION FACTOR THAT DRIVES FIBROBLAST PATHOGENICITY IN RHEUMATOID ARTHRITIS

Christopher Mahony
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Furthermore, RUNX1 expression was increased in perivascular fibroblasts in active RA compared to early RA. We next confirmed that RUNX1 expression in synovial fibroblasts is controlled by inflammatory stimuli using confocal imaging and analysis of publicly available Hi-C data. Examining publicly available ATAC-Seq data as well as coexpression analysis using spatial transcriptomics and scRNAseq data from murine models of arthritis highlighted several direct RUNX1 target genes. We are now performing functional experiments to validate RUNX1 targets to explore how RUNX1 regulates fibroblast pathogenicity.

Conclusion: Our analysis identifies RUNX1 as a novel regulator of disease associated, synovial fibroblast behaviour in inflammatory arthritis and a potential novel therapeutic target to modulate fibroblast-driven pathology in RA.

Optimisation of a vibro-packing process through simulation and experiment*

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Characterising and Modelling Low Dose Formulations in a Continuous Tabletting Line Using Process Analytical Technology*

Eleonora de Giorgi
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* We are unable to reproduce the above posters due to sponsors request

GRANUTOOLS™ POWDER FLOW CHARACTERIZATION

Data Driven Method Using Powder Characterisation Tools to Calibrate DEM Simulation

B. D. Jenkins[1,2], A. L. Nicusan[1], A. Neveu[2], G. Lumay[2,3], F. Francqui[2], J. Seville[1], C.R.K. Windows-Yule[1]

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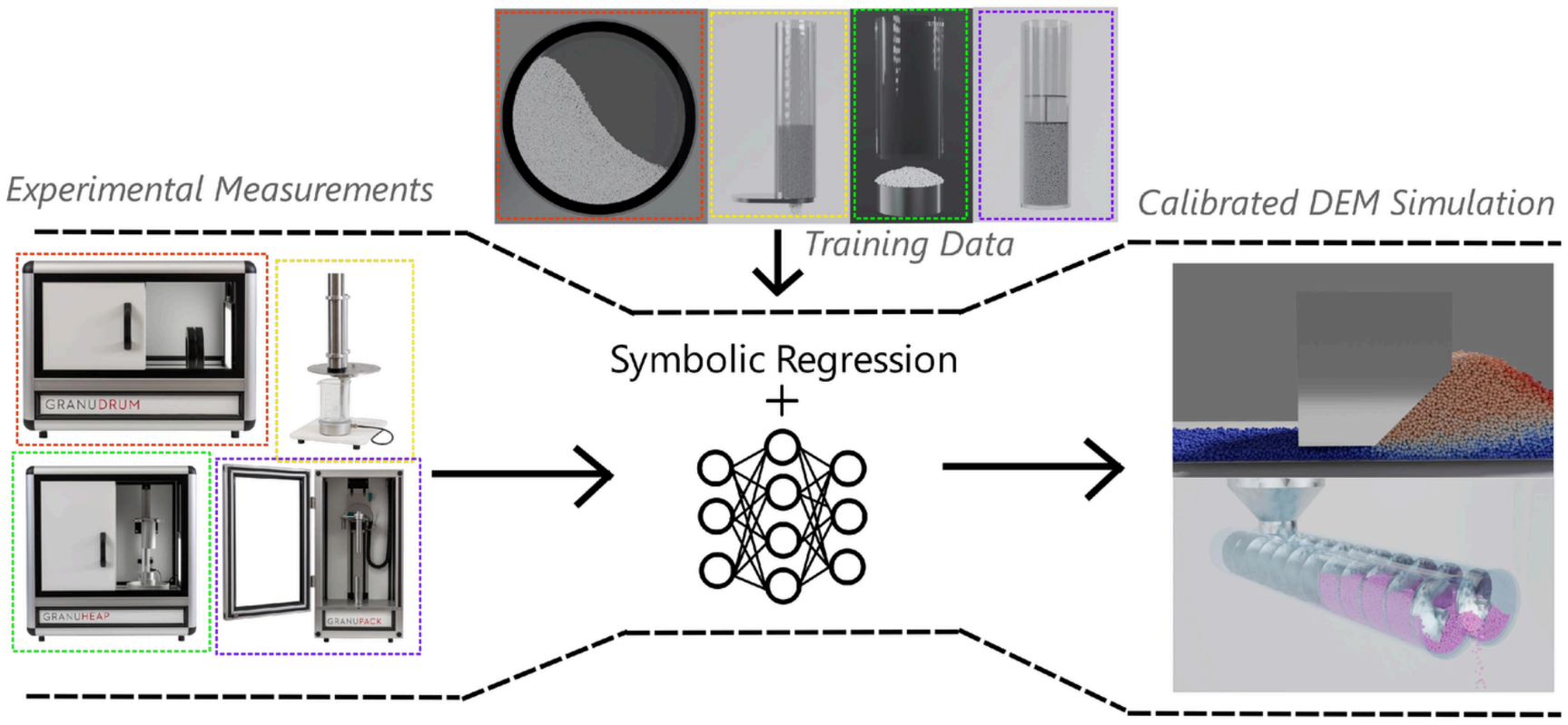
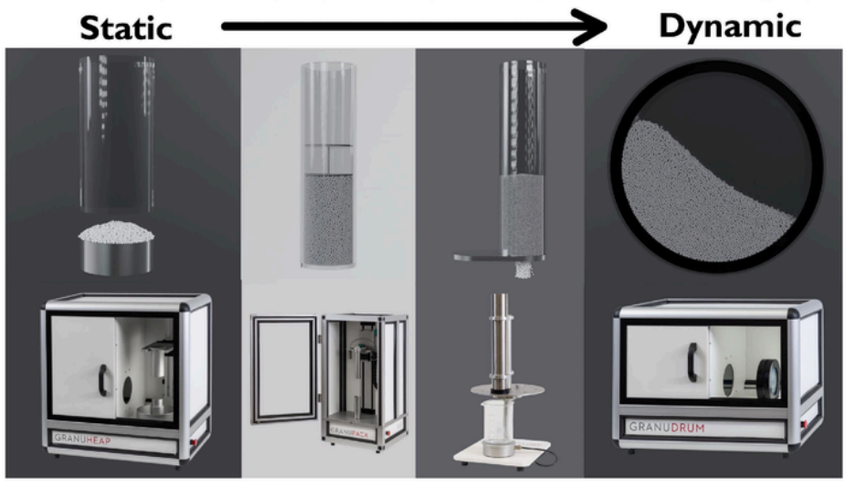


INTRODUCTION

- Calibrating Discrete Element Method (DEM) simulations is time consuming and non-standardised. Often, calibration is done poorly leading to inaccurate simulations [1].
- A computational inexpensive but accurate approach to DEM simulation calibration is required that all DEM users can use.

MATERIALS AND METHODS

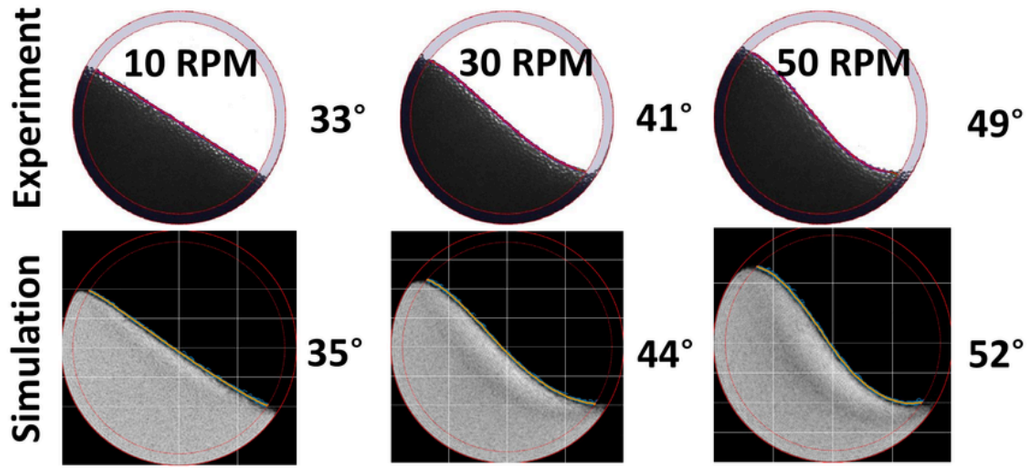
- A series of digital twins of powder characterisation experiments were developed to generate data of measured values of powder bulk measurements (angle of repose, cohesive index) at over 3000 unique combinations of particle properties (friction, cohesion strength).



- This dataset was used to develop both a set of mathematical equations using symbolic regression in the open-source package MED as well as train a neural network.
- Measurements from the powder characterisation powder experiments can be substituted into the mathematical equations or put into the neural network input to get out a set of calibrated particle properties that can be used to accurately recreate the powder in a DEM simulation.

RESULTS

- A set of symbolic equations were tested to calibrate the sliding and rolling friction of one of the simplest materials; 1mm glass beads.
- Experimental measurements of 3 bulk measurements of the glass beads were used including the angle of repose and dynamic angle of repose.
- The calibrated sliding friction and rolling friction values from the symbolic equations were, 0.78 and 0.094 respectively.
- These values were then validated again in the rotating drum to ensure the dynamic angle of repose in the calibrated simulation matched the experimental results which they did closely over several rotational speeds.
- In the future this validation needs to be done in different experiments.



CONCLUSIONS

- Data driven calibration techniques can be used to accurately calibrate real materials but lots of further testing is required.
- Further work needs to be done to calibrate cohesive strength of materials and more bulk measurements need to be included.

REFERENCES

1. Windows-Yule, C. R. K., & Neveu, A. (2022). Calibration of DEM simulations for dynamic particulate systems. *Papers in Physics*, *14*, 140010. https://doi.org/10.4279/pip.140010

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UKRI Engineering and Physical Sciences Research Council

EP/L015153/1

DEVELOPMENT OF A DIGITAL PLATFORM FOR THE OPTIMIZED PRODUCTION OF IN-HOUSE OF POLYMER PRODUCTS.

Lucia Blanco Loarte - Aquapak Polymers Ltd
Christopher Windows-Yule – University of Birmingham
Joseph Wood – University of Birmingham

Oluwatobiloba Henry – University of Birmingham/ Aquapak Polymers Ltd

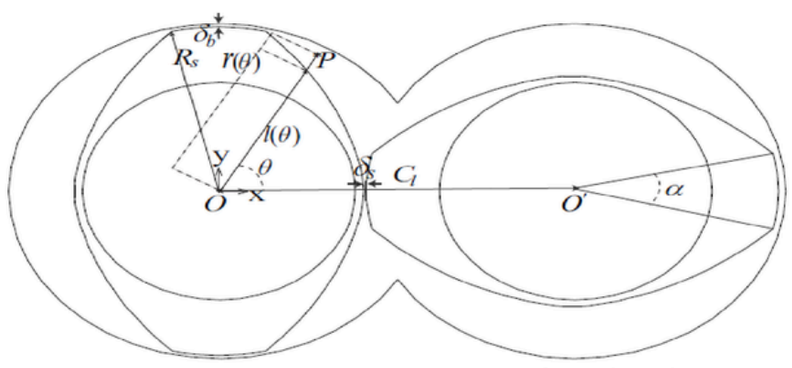
INTRODUCTION

The waste plastic crisis is one of the great challenges facing society today, polluting our soils and waterways, and contributing to the wider climate crisis.

Amongst all technology currently available to counter plastic pollution, **twin screw (TS) polymer extrusion** presents itself as a highly efficient and scalable technology [1]. This enables Aquapak polymers Ltd to process polymers into functional and sustainable products across a variety of industries such as food packaging, automotive manufacturing, etc [2].

TWIN SCREW EXTRUDER MODEL DESIGN

MATHEMATICAL DESIGN OF TWIN SCREW EXTRUDER GEOMETRY



$$\rho_c = \frac{C_l - \delta_s}{R_s},$$
$$\beta = \arccos\left(\frac{\rho_c}{2}\right)$$
$$\alpha = \frac{\pi}{e} - 2\beta.$$

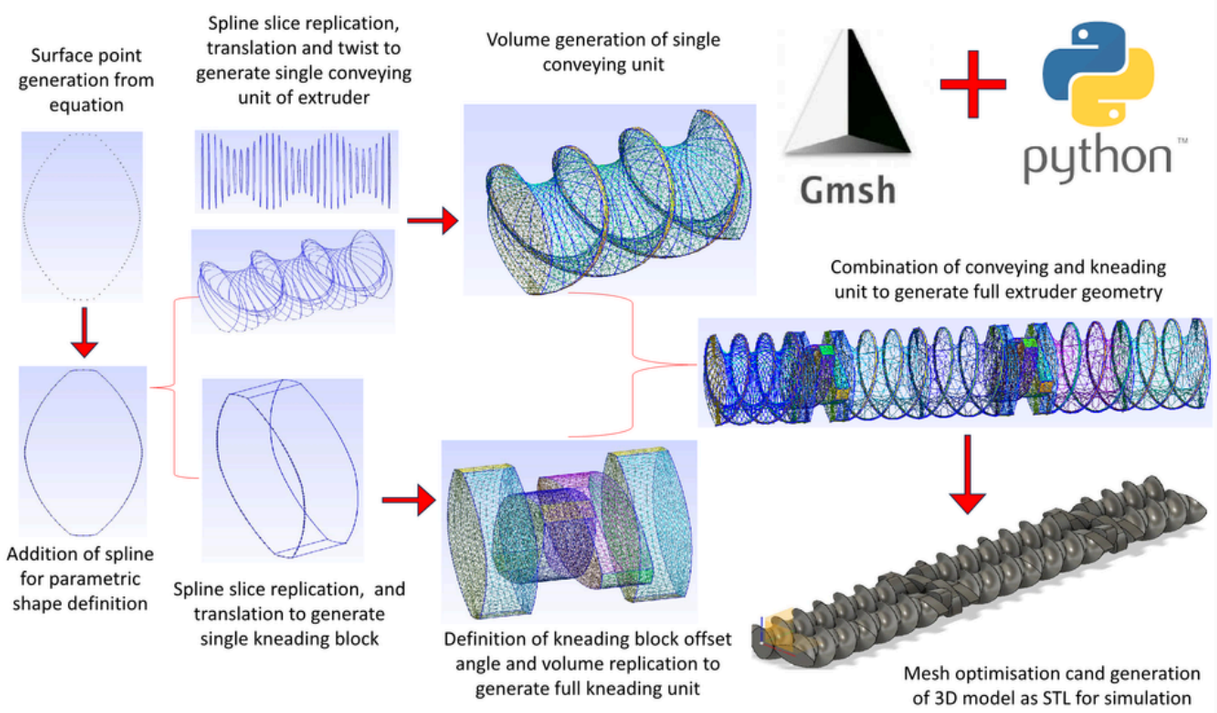
Valid for $0 \le \theta \le \frac{\pi}{e}$

Number of flights (e)
Screw radius (R_s)
Center distance of screws (C_l)
Clearance between screws (δ_s)
Clearance screw-barrel (δ_b)

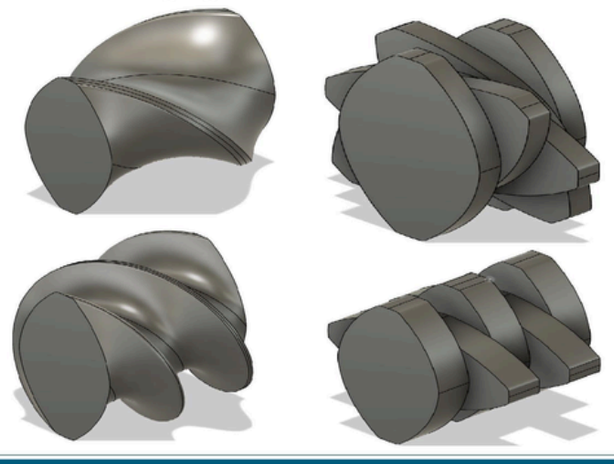
$$l(\theta) = \begin{cases} R_s(\rho_c - 1) & 0 \le \theta \le \frac{1}{2}\alpha \\ R_s\left[\sqrt{\rho_c^2 - \sin^2(\theta - \frac{\alpha}{2})} - \cos(\theta - \frac{\alpha}{2})\right] & \frac{1}{2}\alpha \le \theta \le \frac{1}{2}\alpha + 2\beta \\ R_s & \frac{1}{2}\alpha + 2\beta \le \theta \le \frac{1}{e}\pi, \end{cases}$$

- Extruder surface geometry definition via **Booy's equation for intermeshing self-wiping twin screw extruders** (TSE) [3].

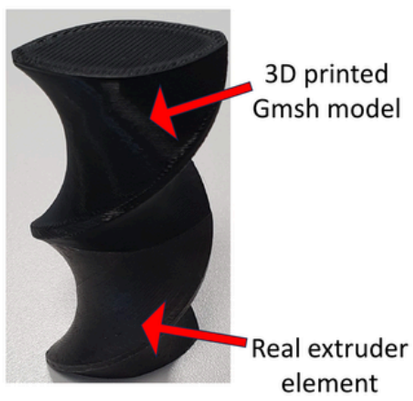
- Computational model of TSE via **Gmsh**, using **Python API** for simulations.



- Limitless possibility in extruder geometry and design generation via Gmsh.



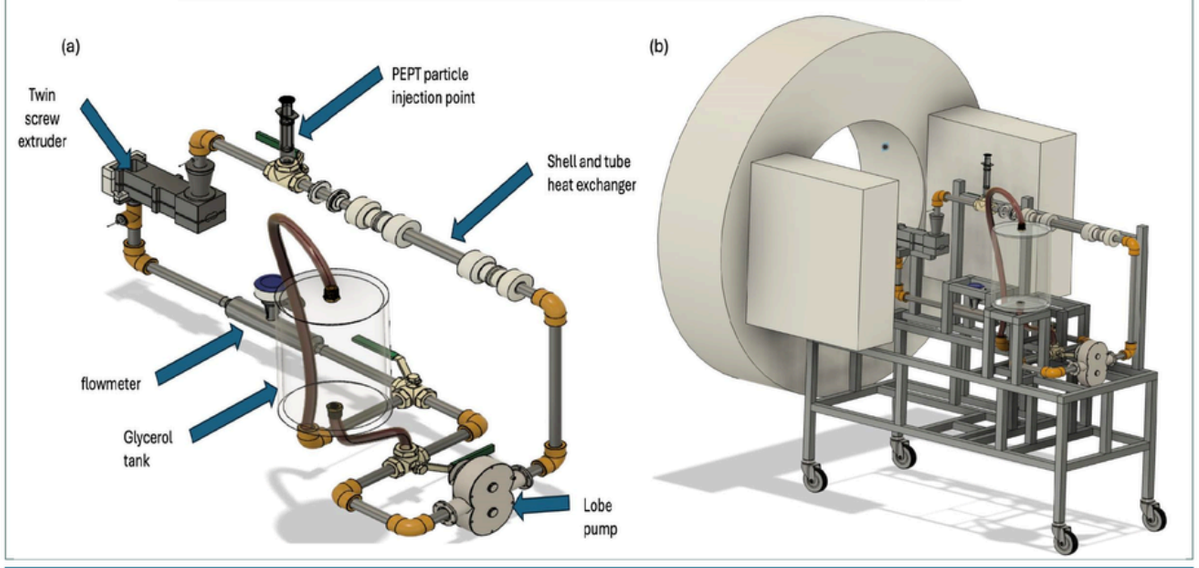
- Geometry verification through fit check



PRELIMINARY TESTING

HIGH VISCOSITY NON-NEWTONIAN & NEWTONIAN MIXING

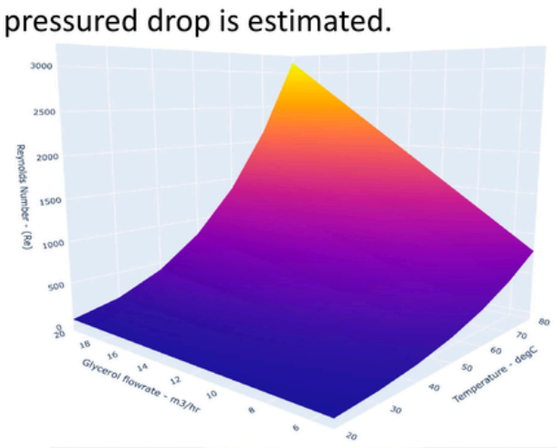
PEPT ANALYSIS: a non-destructive, invasive radioactive experimental technique to map flow trajectory, 3D velocity vector field and shear stress field and validate CFD simulation of high viscosity laminar TSE mixing in an 18 mm diameter TSE, with L/D=10, using Fluorine-18 doped ion exchange resin [4].



RESULTS

TSE PEPT RIG OPERATING CONDITIONS

Deduction of Reynolds number response surface in laminar flow regime, based on flow and temperature range of glycerol for high viscous flow. From which total rig pressured drop is estimated.



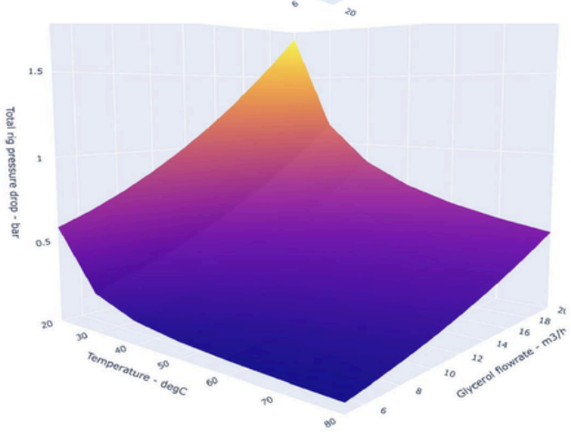
$$Re = \frac{\rho u d}{\mu}$$

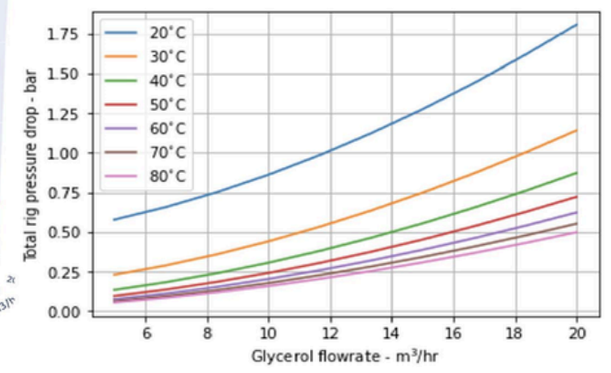
$$\Delta P_{rig} = 1.25\left(\sum \Delta P_{pipe} + \sum \Delta P_{fitting}\right)$$

$$\Delta P_{pipe} = f\frac{L}{D}\frac{\rho u^2}{2}$$

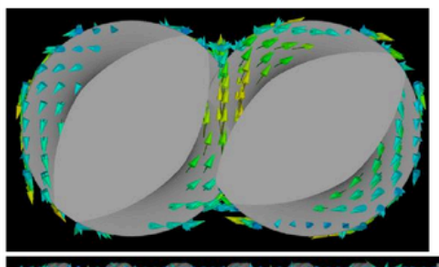
$$\Delta P_{fitting} = \rho K\frac{u^2}{2}, \quad K = \frac{K_1}{Re} + K_\infty\left(1 + \frac{25.4}{d}\right)$$

$$f = 0.316Re^{-0.25}$$



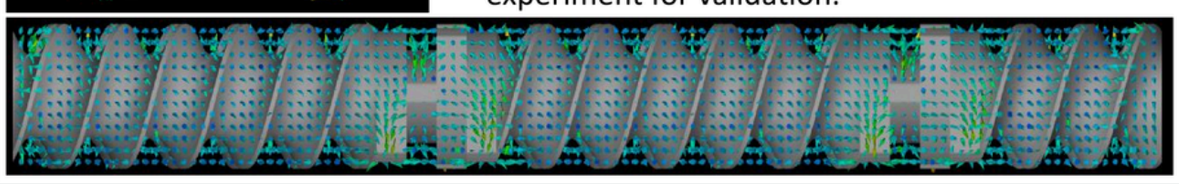


CFD SIMULATION OF TSE MIXING



- TSE Newtonian flow CFD model development. A simple case of 3D velocity flow field extraction from simulation, using Flow3D.

- Velocity field to be superimposed with PEPT experiment for validation.



FUTURE WORK

- Further development of CFD model to TSE mixing in high viscosity flow.
- Assembly of TSE PEPT rig and experimental campaign.
- Validation of CFD model of TSE high viscosity flow using PEPT.
- Increasing complexity of CFD model of TSE through inclusion of polymer multiphase reactions, heat transfer and venting.

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[1] Chen B, Zhu L, Zhang F, Qiu Y. Process development and scale-up: twin-screw extrusion. In: Developing solid oral dosage forms. Elsevier; 2017. p. 821-68 .
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Bootstrapping, in a liaison psychiatry clinical audit

Dr Josephine Bates, Dr Adam Hickson; Devon Partnership NHS Trust

NHS
Devon Partnership
NHS Trust

INTRODUCTION

> Liaison psychiatry - the sub-specialty that handles mental health on medical and surgical wards/ in the emergency department.
> Referrals are made by parent teams to liaison psychiatry, categorising a 'main aim of referral' - there are 10 possible options on DPT's referral sheets:

Assessment and diagnosis; providing guidance; signposting; assessment and risk management; mental capacity assessment; Mental Health Act assessment; medication management; disturbed behaviour management; brief psychological interventions; other treatment

AIM: Audit of outcomes following referrals to liaison psychiatry

METHODS AND ANALYSIS

> 78 referrals made in May 2023 - comprehensive sample
> Bootstrapping used during data exploration
> Correlational analysis (Kendall's tau)

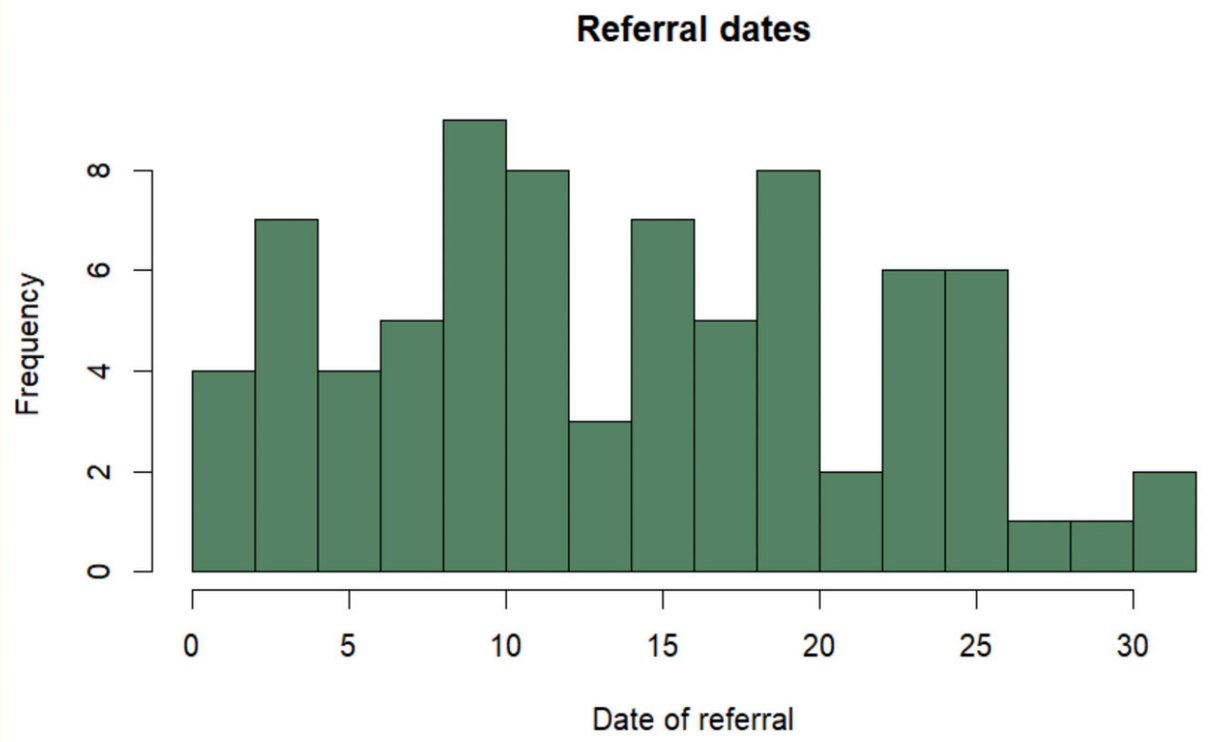
RESULTS

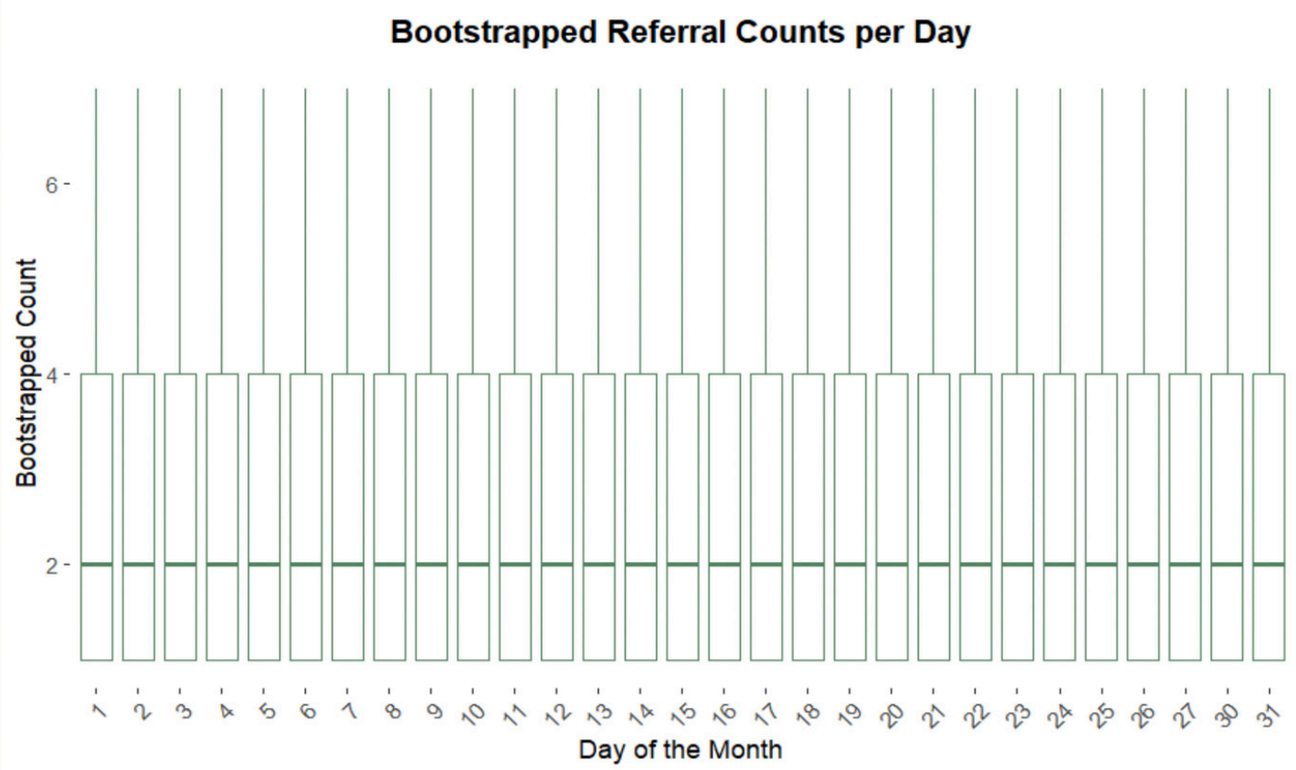
> Age range was 18-85, mostly 30-45; > 30 men, 48 women
> Referrals were mostly made between 08:00-12:00, then 22:00-00:00

Aims of referral:
> 66.7% for 'Assesment and management of risk'
> 23.1% for 'Assessment and diagnosis'
> 11.5% for the other 8 categories.

Outcomes (GO1):
> 35.9% minimally improved after assessment
> 33.3% had no change after assessment

Correlational analysis:
> Referral time ~ Outcome: T=0.080, p=0.470
> Age ~ Outcome: T=0.108, p=0.274





DISCUSSION

> 7,500 bootstrapped datasets - counts on each day represented in the box plots.
> Central limit theorem: all days will converge to a normal distribution in terms of the number of referrals.
> Value in this audit - demonstrated uniform distribution across each day when the dataset is large enough.

Discussed this at a medical writing workshop in an international clinical conference - lack of awareness about bootstrapping. Impression of this equating to incorporating falsified data.

Take home point: bootstrapping is not falsifying data. It was used in this audit as a technique for data exploration.

> How to better educate about statistical methods among clinicians?

Other points about clinical audit:
> Who records the data?
> Who decides the categories?
> What does 'achieved' mean??
> What are the outcomes really measuring? Performance measures are estimates, cannot assess uncertainty.
> Removing redundant parts of measured outcomes, e.g. GO2 (used 11.5% of the time)

References
Cevenini, G. and Barbini, P. (2010) 'A bootstrap approach for assessing the uncertainty of outcome probabilities when using a scoring system', BMC Medical Informatics and Decision Making. 10: 45.
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mobileRNA: A new tool for efficient analysis of RNA expression in multiple genomes.

Katie Jeynes-Cupper, Dr Estrella Luna-Diaz, Dr Marco Catoni

1 Introduction

- In genomic analysis, it is challenging to distinguish genetic sequences from multiple organisms within samples, such as plant grafting or pathogen-infection experiments.
- Here we address the lacks of a standardised approach.

2 Previous methods

Typically, reads are aligned to each genome separately, followed by post-alignment screening of genetic variants. These approaches can introduce high rates of false positives - incorrectly assigning RNAs to a genome.

But why?

- Alignment algorithms are designed to place reads in the best location in a genome reference.
- If a read is better suited to another location within a genome that was not provided, it cannot be considered.

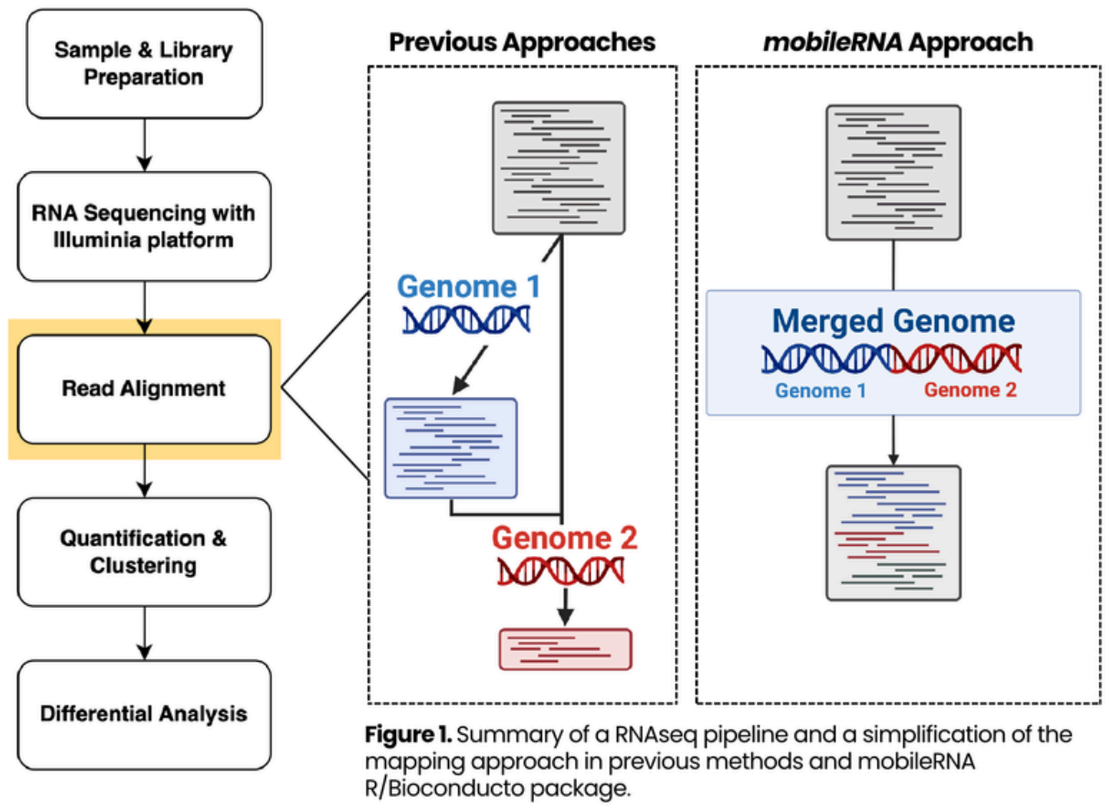


Figure 1. Summary of a RNAseq pipeline and a simplification of the mapping approach in previous methods and mobileRNA R/Bioconducto package.

3 *mobileRNA, an* R/Bioconductor package

Bioconductor
OPEN SOURCE SOFTWARE FOR BIOINFORMATICS

A Preprocessing uses alignment & clustering algorithms to place reads to multiple genomes in unison with a merged genome reference.

B Analysis isolates differential RNA expression & visualises results with PCAs, heatmaps, tables.

Testing The Method

- Created simulated mRNAseq & sRNAseq data to replicate 3 different grafting experiments.
- Data analysis against *mobileRNA* and recent methods from plant grafting studies.

5 Results

We show that this approach more accurately places reads to their genomic origin and reduces background data noise. Genetic similarity plays the main role in the expected confidence.

Comparing *mobileRNA* to other methods

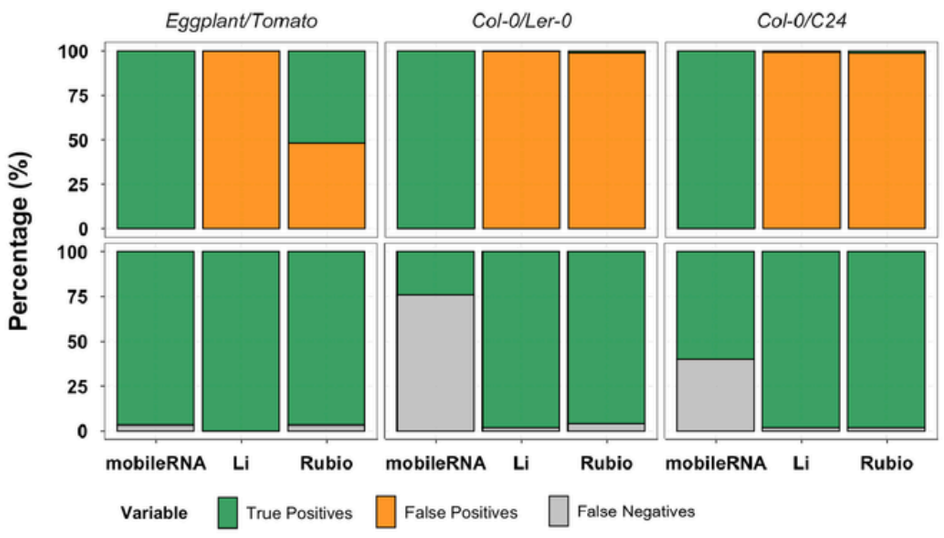


Figure 2. Results from the simulated sRNAseq analysis, replicating plant grafting in three different experiments. Where the name represents a scion/rootstock combination with the aim to locate the root-to-shoot mobile small RNAs. Eggplant/Tomato represents grafting of Solanum lycopersicum and S. melongena. Col-0/Ler-0 and Col-0/C24 refer to grafting of Arabidopsis thaliana accession. Col-0 refers to Columbia accession, Ler-0 refers to Landsburg accession and C24 accession.

Using genetic similarlity as in indicator to predict the output

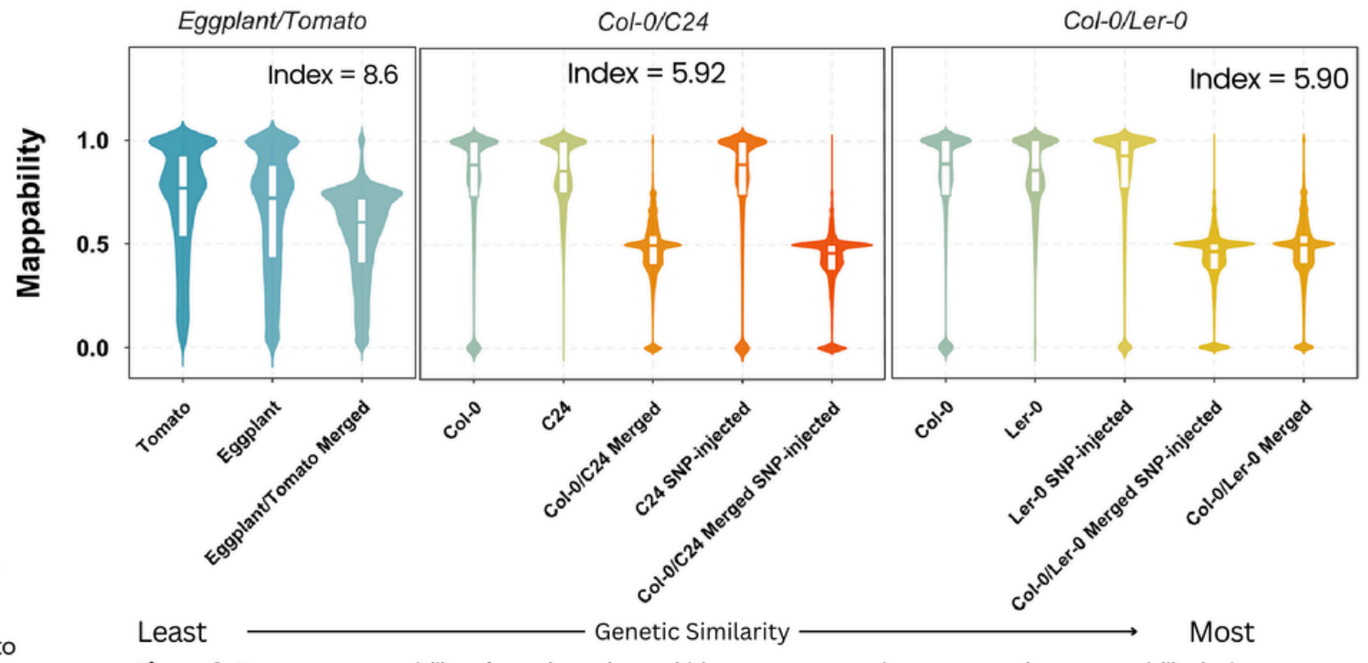
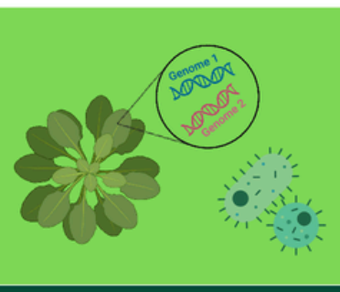


Figure 3. Genome mappability of exonic regions within a genome and accompanying mappability index. Mappability is between 0-1 where 1 refers to regions which are highly unique and 0 refers to regions which are highly repetitive within the genome

6 Conclusions & Applications

For both mRNA & sRNA reads, the ***mobileRNA*** method was more accurate at discriminating the genomic origin. Although primarily designed for plant grafting experiments, it could have the potential to apply to ecological samples, pathogen-infection samples, or microbiome samples.



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SIMULATING THE SOLUTION:

Exploring computational techniques for dispersion and dissolution of pharmaceutical powders

Presented by: Khizra Abdul Wadood [1,2]
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Project Supervisors:
Dr Andrew Ingram[1], Dr Christopher Windows-Yule Kit[1] and Dr Matthew Molloy[2]
Affiliations:
1. School of Chemical Engineering, University of Birmingham, UK
2. Oral Product Development, Pharmaceutical Technology and Development, Operations, AstraZeneca, Macclesfield, UK

1. Motivation

Formulating an effective pharmaceutical composition, while achieving precision using powders and solvents is quite a challenge in the industry. The conventional trial-and-error methods for rare or expensive substances are often impractical and cost prohibitive. Instead, adopting a modelling methodology emerges as an evidently more feasible substitute.

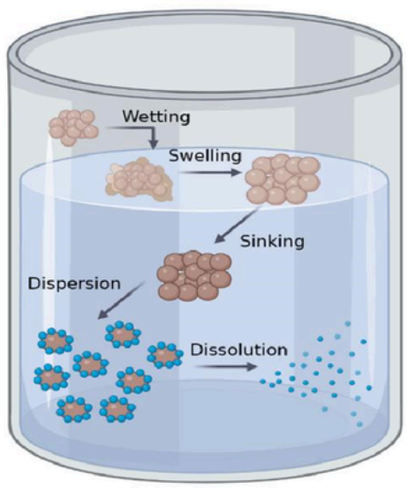

Fig 1: Powder Dissolution Profile

2. Objectives

- Proposing a modelling approach for several stages of mixing powders at a range of scales
- Identification of the key measurable particle properties for calibration of models
- Scaling up the model for reliable prediction of mixing strategies

3. Modelling Techniques

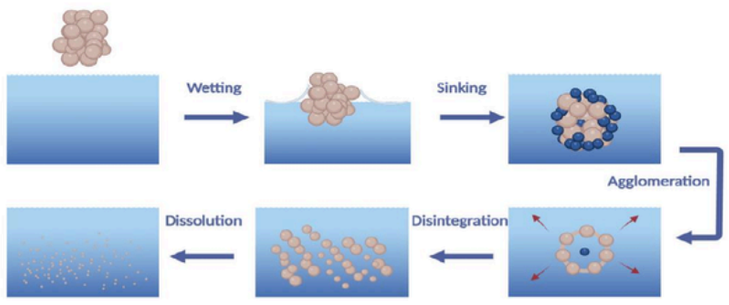

Fig 2: Stages of powder dissolution process

When considering the entire process, computational challenges emerge. So, a sensible approach is to focus on individual stage and governing forces in the respective phase of the dispersion. Simulating powder and multiphase flow, accounting for wicking and capillarity, requires critical steps.

An appropriate CFDEM solver is essential that accounts for two-way coupling and consider incorporating hydrodynamic forces, surface tension, and gravity to get refined simulation. Then, the simulation provides the key understanding and insights via dimensionless numbers like the Bond and Capillary numbers.

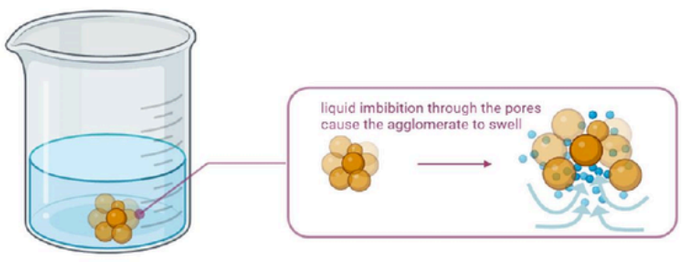

Fig 3: Swelling of the agglomerate immersed in the solvent

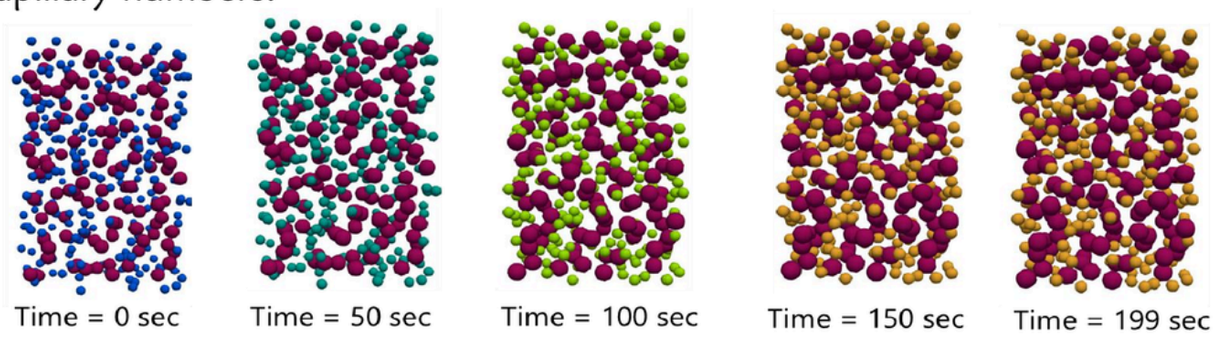

Fig 4: DEM Simulation of Swelling of particles

4. Way forward

In conclusion, the project aims to create process simulations based on DNS or CFD-DEM. The models will be studied on micro-and-meso scales initially to investigate the dominating parameters in the dissolution process. The project seeks to provide predictive and scalable models for pharmaceutical powder mixing using computational tools such as Lethe, LIGGGHTS, and OpenFOAM. Given their broad industry utilisation, these models are poised to be widely implemented and adaptable.

5. References

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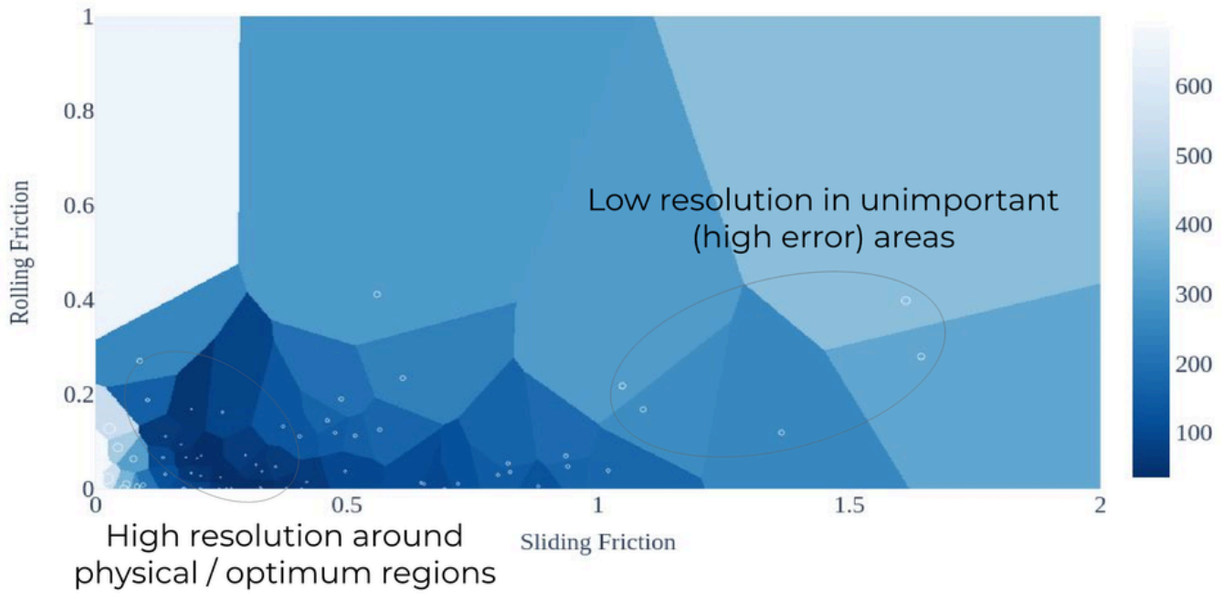
Andrei Leonard Nicusan
Dominik Werner
Jack Sykes
Dr. Kit Windows-Yule
Prof. Jonathan Seville

Data-Driven Engineering Open-Source Ecosystem

Learning Simulation Parameters from Experiments

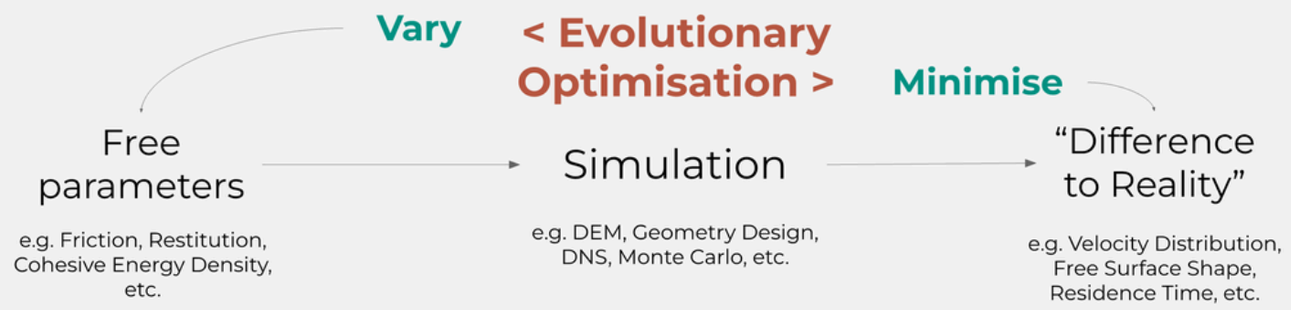
Problem: what microscopic parameters do I need to match a macroscopic measurement?

Manual calibration is tedious and error-prone
Grid-based calibration is expensive and limited

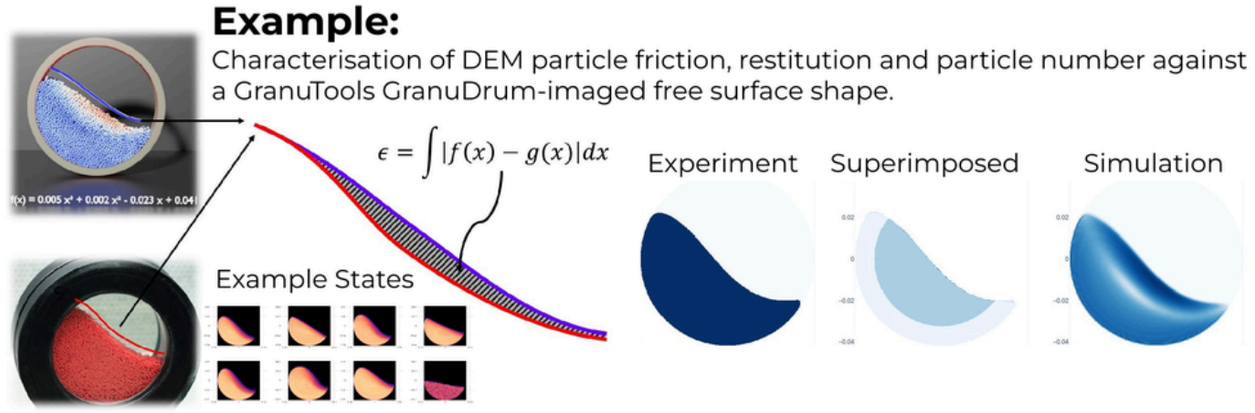


ACCES

Autonomous Calibration and Characterisation using Evolutionary Software



Example:
Characterisation of DEM particle friction, restitution and particle number against a GranuTools GranuDrum-imaged free surface shape.



Discovering Equations / Laws from Data

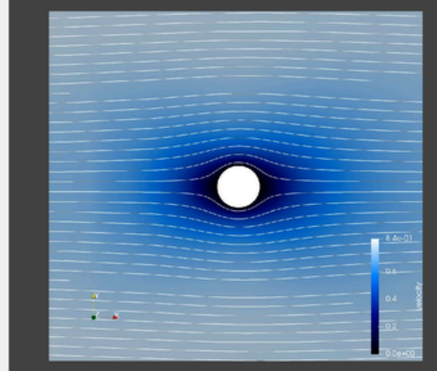
M²E³D: Multiphase Materials Exploration via Evolutionary Equation Discovery

Classical approach: find a predetermined model's / equation's coefficients that fit experimental data.
ML / AI: find a blackbox, uninterpretable surrogate model.

M²E³D: **find the equation itself!**

- Autonomously discover the equations required to accurately reproduce a system's full, three-dimensional dynamics.

1. Re-"discovering" Stokes' Law



- Used direct numerical simulations (DNS) of flow around a static 3D sphere
- Ran 32 combinations of the particle radius, fluid dynamic viscosity and velocity (0.02 < Re < 0.7)
- With **no a priori information**, we let M²E³D discover the equation fitting the resulting drag force

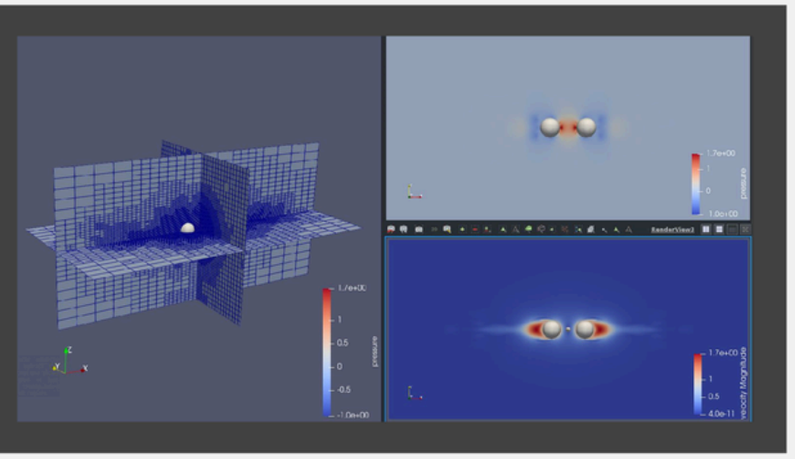
M²E³D found the equation on the left!

$$\frac{(-0.249 - 1.039)uR}{\frac{-0.069}{\mu}} = 18.67\mu Ru \approx 6\pi\mu Ru$$

So we can automatically derive what the finest human minds did 170 years ago - What about applying the SymbolicRegression.jl engine to XXI century problems?

2. Fluid drag on a DEM particle - without simulating the fluid!

$$\Delta C_D(Re, s^*) = \frac{2Re + 21.45}{1.82Re\ s^* + 0.1Re + 0.037}$$



Interactive Example

Example ACCES Workflow:
Learn Physical Parameters

"Find particle-particle friction and restitution"

Take Macroscopic Measurement

Choose Response Parameters & Goals

ACCES Calibrates Parameters

Characterised Material

Example M²E³D Workflow:
Learn Multiphase Coupling

Run Microscopic Experiments

Find Drag Relation

Derive Correlations

Combined:
Optimise Entire System Design

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Machine learning accelerated structure searching of heavy metal imidazole metal-organic frameworks

UNIVERSITY OF BIRMINGHAM

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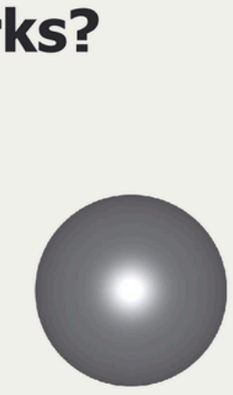
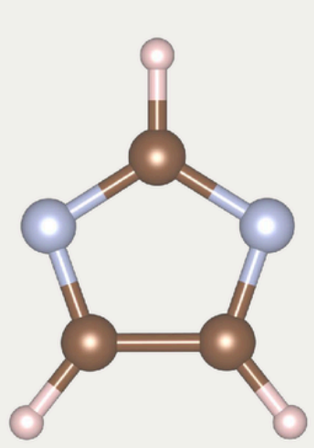
Why heavy metal metal-organic frameworks?

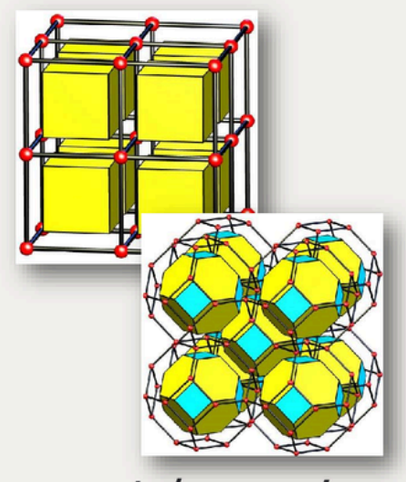
Concern around the use of heavy metal elements (e.g. Cd, Hg, Pb) in modern applications comes from their toxicity. Transforming these metals into functional materials allows us to maximise our available resources. We look towards metal-organic frameworks, whose stability and porosity promise constraining toxicity while further capturing additional heavy metal toxins.



heavy metals (e.g. Cd, Hg, Pb)



organic linkers (e.g. imidazole)



metal-organic frameworks[1]

How do we predict stable framework structures?

Generate sensible starting structures

Quantum mechanical approach

Structural relaxations using coarse density functional theory

Density functional theory is a quantum mechanical modelling method used to calculate energy and other properties of atomistic systems.

~1 hour/100 atoms
128 CPUs

Filter for candidate structures

Machine learning accelerated approach

Structural relaxations using machine learned potentials

~100 s
1 CPU

Filter for candidate structures

Criteria:
- ❑ *Low energy*
- ❑ *Multiple instances*
- ❑ *Physical sense*

Structural relaxations using fine density functional theory

~1 day
128 CPUs

Identify stable structures

Characterise using density functional theory

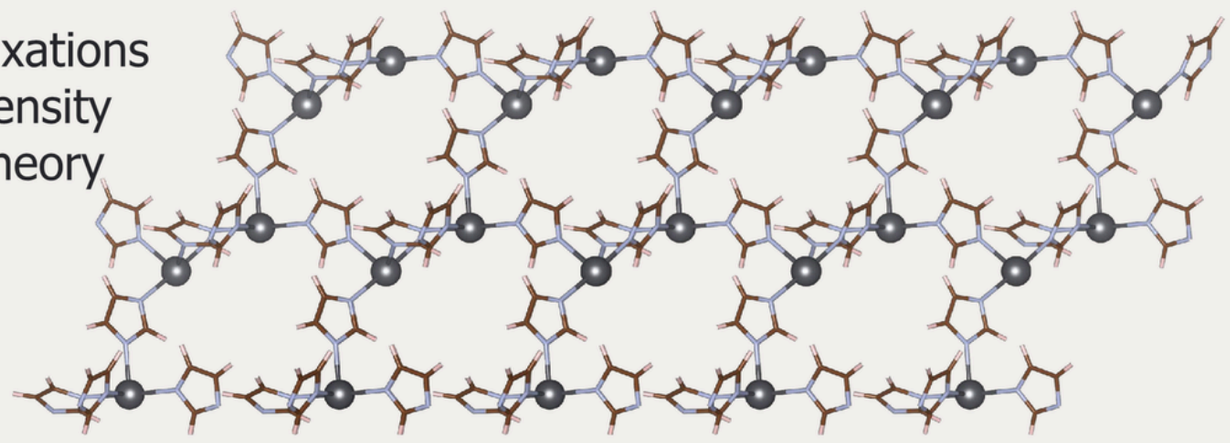
Repeat 1,000,000+ times to cover search space

What makes a "sensible" structure?

We use chemical information (e.g. symmetry, stoichiometry) to guide our initial guesses.

What are machine learned potentials (MLPs)?

MLPs replicate the potential energy surface described by quantum mechanics. Developments in message passing neural networks have increased the accuracy of MLPs for atomistic systems, with claims of foundational MLPs recently developed for use with most (if not all) material systems[2].



What comes next?

We simulate material properties and identify key experimental signatures that our collaborators can observe.

Acknowledgements & References

We would like to give thanks to funding organisations, UKRI and EPSRC, as well as thank the computing facilities that made this research possible, namely University of Birmingham's BlueBEAR and Sulis Tier 2 HPC.

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Ab initio statistical mechanics study on the compounds and disorderd phases in hcp Ti-O and Ti-Nb system

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Introduction

Oxygen (O) and niobium (Nb) are two representative alloying elements of hexagonal close-packed (hcp or α) titanium (Ti), the addition of O can improve the mechanical properties of α Ti to form high-temperature alloys, the alloying of Nb with Ti can enhance the chemically-aggressive resistance of Ti alloys [1].

However, on one hand, the large solubility of O in hcp Ti makes it possible to form a variety of ordered α compounds before reaching the solution limit of oxygen, these compounds are hard to be examined by experimental observations. On the other hand, the addition of Nb into α Ti can introduce a lot of mechanical instabilities, which makes it difficult to capture the phase characterization especially in high Nb composition space.

In this study, we employed a modelling scheme that combines first-principles (DFT) calculations with cluster expansion method and Monte Carlo simulations to investigate the electronic structures, ground-states energetics, atomic interactions and phase stabilities in α Ti-O and Ti-Nb systems.

Methodology

The configurational energy (F_{config}) of the structures (supercells) sampled in the α Ti-O and Ti-Nb systems can be evaluated by DFT calculations by eq. (1) [2], whereas it is impossible and costs too much computational resources if considering all the possible structures across the whole compositional space.

$$H\psi = E_{DFT}\psi \qquad (1)$$

Cluster expansion (CE) method can then be used to predict the DFT energies and capture the effective cluster interactions (cECIs) by searching for crucial clusters, e.g. pairs, triplets and quadruplets, such that the energy of any configurations can be accurately predicted by eq. (2) [3]. In one word, the constructed CE model can represent the energetics of the system in consideration of a specific number of DFT energies, which avoids the tremendous DFT calculations.

$$E(\sigma) = \sum_{\alpha} m_{\alpha} J_{\alpha} \left\langle \prod_{i \in \alpha'} \sigma_i \right\rangle \qquad (2)$$

J_α denotes the cECIs and can be used as Hamiltonian for Monte Carlo (MC) simulations. To get accurate thermodynamics at higher temperatures, the vibrational free energy of each structure can also be calculated with different precision like Debye-Grüneisen model, then another CE can be constructed using these F_{vib} to obtain another set of vECIs which can be added to the cECIs to get the temperature-dependent ECIs (tECIs). When employing the Debye-Grüneisen model, the thermodynamic properties (e.g. heat capacity, Young's modulus) of the ground-states at finite temperatures can be computed from:

$$F(V; p, T) = F_{config}(V) + pV + F_{vib}(V; T) \qquad (3)$$

The information of the ground-states and tECIs is finally imported to the MC simulations as Hamiltonian such that the phase stabilities of the ordered ground-states and disordered phases can be averaged over the varying compositions and temperatures.

Workflow

The core of this study mainly consists of three steps, as shown in **Fig. 1**:

- Enumeration of configurations and DFT calculation.
- Construction of the CE model for F_{config} and F_{vib} respectively.
- Performing MC simulations using CE data (Hamiltonian).

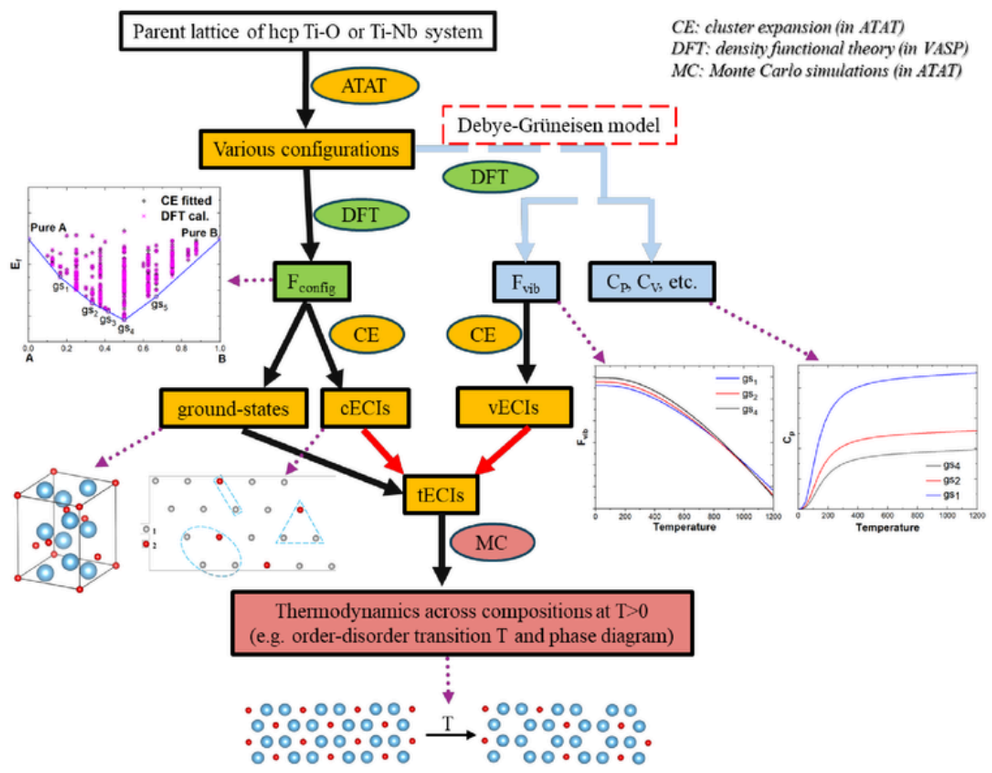
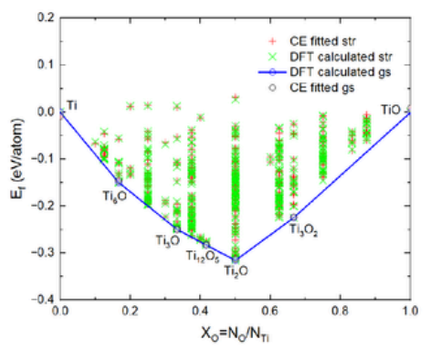


Fig. 1 Workflow of this study.

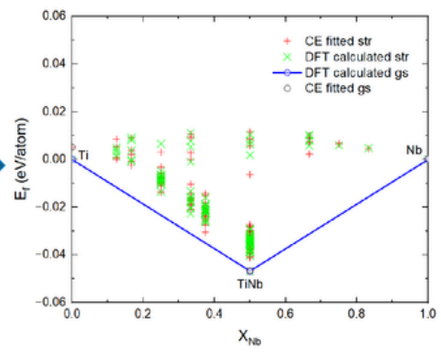
Results

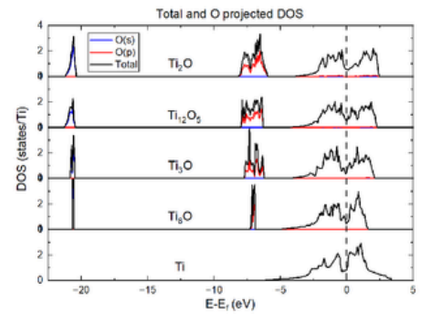
α Ti-O system



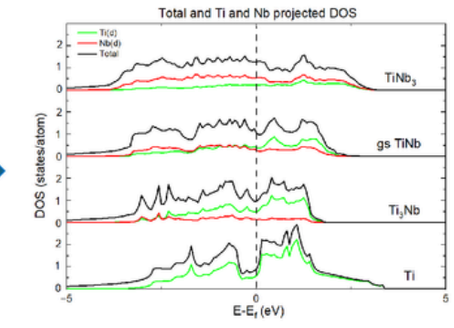
DFT convex hull

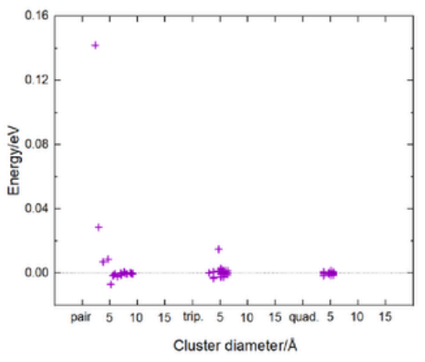
α Ti-Nb system



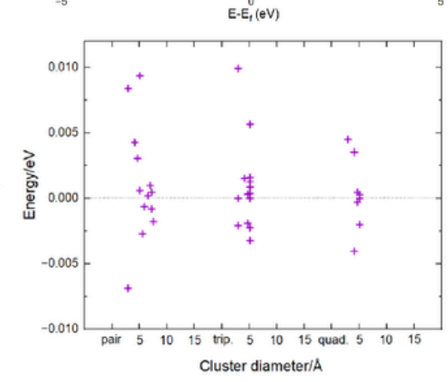


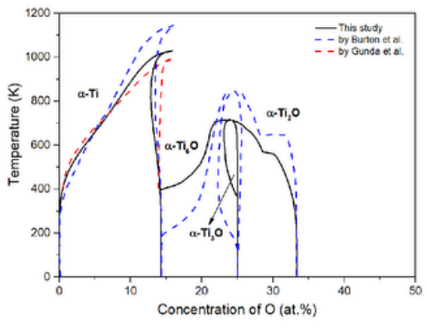
Density of states



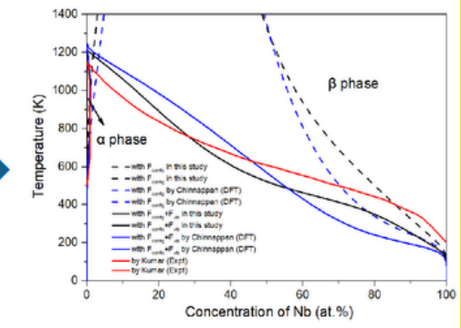


cECIs





Phase diagram



Conclusions

The combination of DFT calculation, CE and MC simulations can be used to study the ground-states characterizations, atomic interactions and phase stabilities for the hcp Ti-O and Ti-Nb systems. This modelling scheme is not limited to these two systems and can be employed to effectively investigate the properties at 0K and thermodynamics at T>0 of any condensed matter systems.

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The 13th BEAR Conference 23~24 April 2024

Next Generation Biodegradable Core Shell Capsules

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Introduction

Aim: Our goal is to develop environmentally friendly microcapsules for pesticides encapsulation, microplastics free, in line with upcoming regulations. We will be focusing on biodegradable capsule chemistry via interfacial polymerization technique and process optimization for scalability via CFD simulations in static mixer.

As agriculture advances, so do environmental concerns like pollution and soil degradation. This project highlights the importance of eco-friendly microcapsules, using biodegradable materials to tackle microplastic pollution[1]. Our focus is on revolutionizing agricultural practices for a sustainable tomorrow.

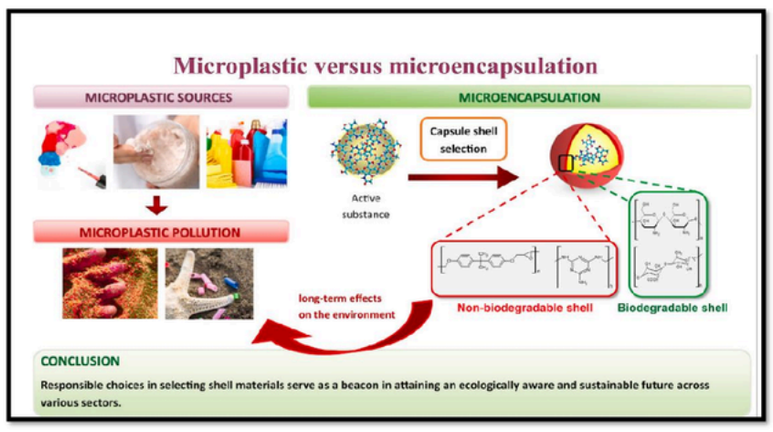


Fig 1 Key role of microencapsulation to avoid microplastic pollution

Overview of the project

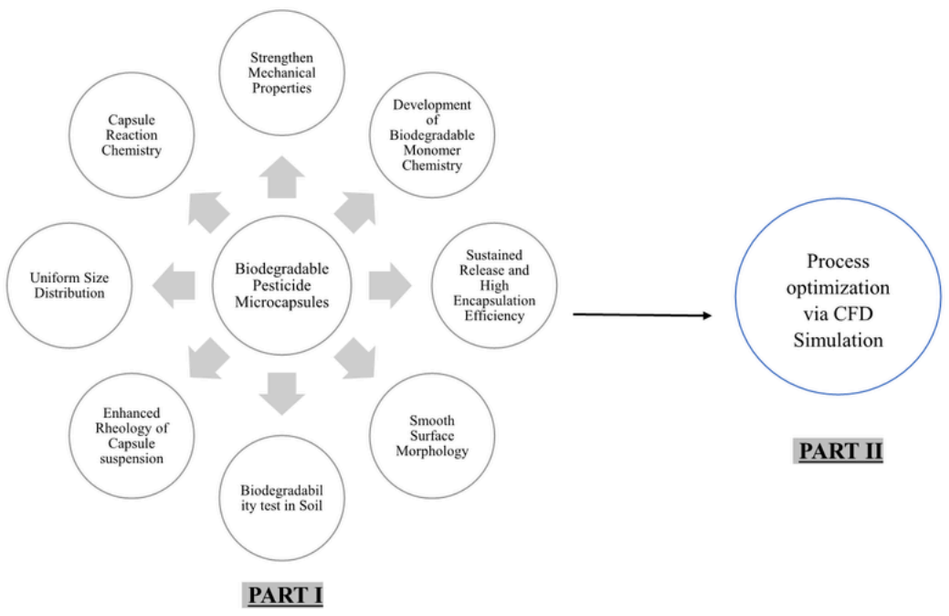
PART I:

- Synthesis of biodegradable monomers and microencapsulation of pesticides promoting sustainable agricultural production
- We carefully select equipment for the polymerization process to cover all bases.

Through organized experiments, we find the best conditions for maximum output and efficiency, setting the stage for large-scale production.

PART II:

- Process optimization through CFD simulation to build a pilot encapsulation rig.



Literature review

- Literature survey found that interfacial polymerization encapsulation (IPE) techniques have been identified as promising methods to synthesis core-shell capsules in the industries due to its reduced environmental impact, enhanced stability, adoptable formulations, compatibility, versatility, scalable methods, and sustainability of pesticides and agrochemicals in modern agriculture[2].
- Several biodegradable polymers prepared till date via IPE are polyesters, PLGA,PLA_PCL modified monomers, polyesterurethanes, polyesterurea, chemically modified polysiloxanes, polyamides, polyurethanes and polysaccharides such as chitosan and cellulose derivatives when chemically modified for interfacial polymerization.
- Key factors for Capsule- biodegradation: a) Labile monomer-linkage: Choose monomers with ester, amide, or ether bonds for easy hydrolysis[5]. b) Degree of Crosslinking: Lower degree of crosslinking to enhance biodegradability. c)Types of monomers: Select renewable sources like lactic acid, with enzymatic degradation-friendly groups. d) Monomer Selection Guidelines: Prioritize renewable, non-toxic monomers, and tailor material properties for specific needs.
- Recently Ghasemlou et al successfully carried out the biodegradability test **(Fig 2)** where reinforcement of polyhydroxy urethane and the presence of cellulose nanocrystals (CNCs) reduced the potential for the soil microbiota to degrade the nanohybrids (ST-PHU-CNC).

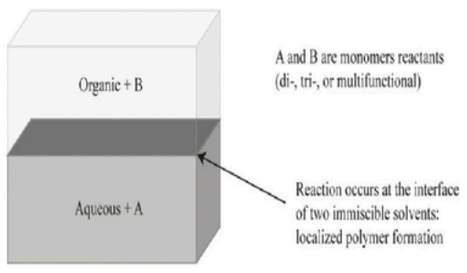


Fig 2 Schematic of interfacial polymerization

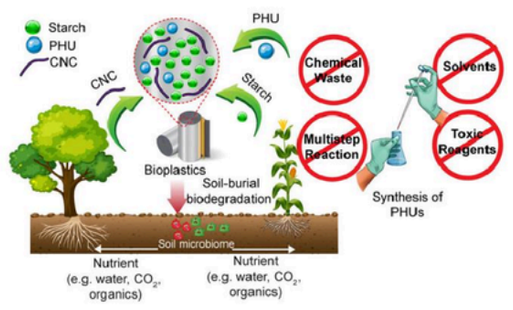


Fig 3 Biodegradation test in soil environment

Preliminary results

CFD simulation in static mixer

- CFD simulations show a strong velocity gradient in the mixer, improving fluid mixing.
- The static mixer induces complex flow without moving parts, leveraging high and low-velocity zones to enhance mixing.
- Cross-sectional views indicates that radial distribution of velocities is crucial to enhance uniform mixing.
- Future improvement: Optimize the mixer geometry to avoid agglomeration and conduct studies at different concentration.

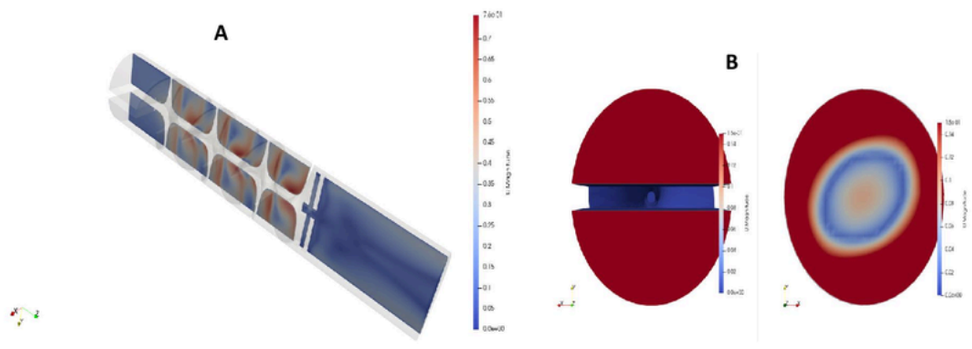


Fig 4 Velocity profile: static mixer CFD simulation (**A**) and inlet and outlet (**B**)

CONCLUSIONS

- ✓ In summary, as capsules contribute to the microplastic waste issue in products like agriculture and other industries, it is crucial to find eco-friendly alternatives. With upcoming international rules to limit microplastic use, it's essential to prioritize sustainable and commercial formulations.
- ✓ Developing biodegradable capsule chemistry with enhanced mechanical and morphological properties, along with high encapsulation efficiency and controlled release formulations are crucial for modern agriculture and promoting a greener environment.
- ✓ It is essential to comprehend the biodegradation mechanism when selecting monomers and functional groups responsible for degradation, as well as adhering to regulations and guidelines during monomer selection.
- ✓ Preliminary simulation results indicates than CFD simulations highlight the static mixer's strong velocity gradient, improving fluid mixing. Static mixers effectively utilize high and low-velocity zones for enhanced mixing without moving parts. Future steps include optimizing mixer geometry to prevent agglomeration and the systematic study based on different boundary conditions such as concentration, temperature, pH, viscosity etc. For further scale up, upon performing CFD simulation based on dynamic meshing inside the stirred tank can be feasible.

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Investigation of high gas flow rates on hydrodynamics in two-phase gas-liquid stirred tanks using Positron Emission Particle Tracking (PEPT)

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2) IFP Energies Nouvelles, Rond-point de l'échangeur de Solaize, BP 3, 69360 Solaize, France

CONTEXT

- Gas-liquid stirred tanks are used in cell cultivation [1] and fermentation processes [2], amongst others.
- Challenges in imaging these systems using optical-based techniques have led to studies being limited to low superficial gas velocities – not industrially relevant.
- We investigate the impact of more realistic gas flow rates and superficial gas velocities on the hydrodynamics of two-phase, gas-liquid stirred tank reactors.

MATERIALS AND METHODS

PEPT

- PEPT is a non-invasive, three-dimensional measurement technique.
- Gamma rays are emitted from a radioactive tracer particle, with radiation detectors recording colinear 'lines of response' (LORs).
- Multiple tracer locations form a three-dimensional Lagrangian particle trajectory, as shown in Figures 1a and 1b.

Figure 1a: 3D Particle Trajectory

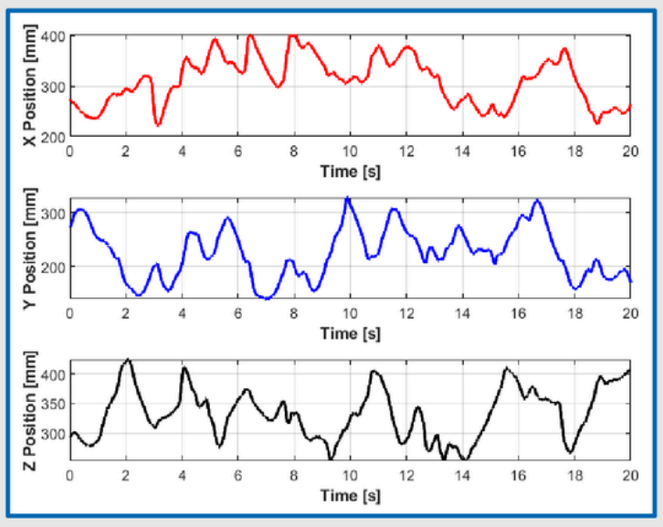

Figure 1b: Sample Trajectories

EXPERIMENTS

- Aqueous Newtonian solution (70% glycerol v/v) (v= 2.81x10^{-5} Pas).
- Two different impeller speeds corresponding to flooded and dispersed aeration regimes:
  - Flooded: N = 190 RPM (Re = 500, Fr = 0.068).
  - Dispersed: N = 530 RPM (Re = 1400, Fr = 0.530).
- Gas flow rates varied between 0.0, 1.6, 3.0 and 5.0 VVM (vessel volumes per minute).
- T = 200mm diameter tank, with a ring sparger positioned centrally below Rushton turbine.

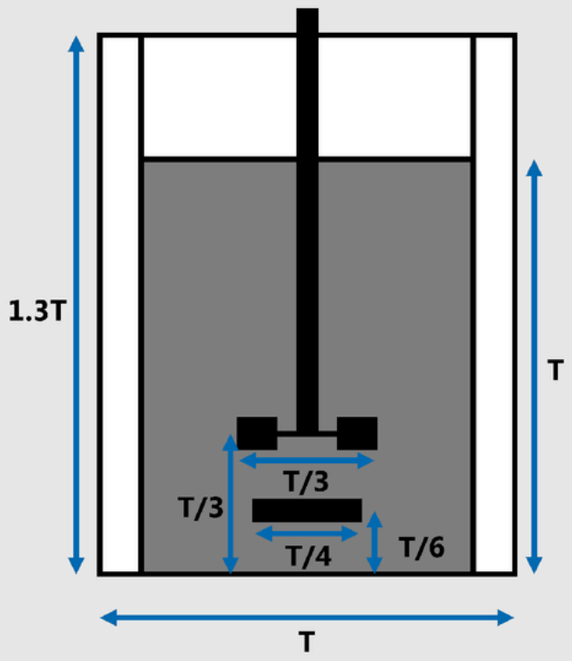

Figure 2a: Tank Schematic

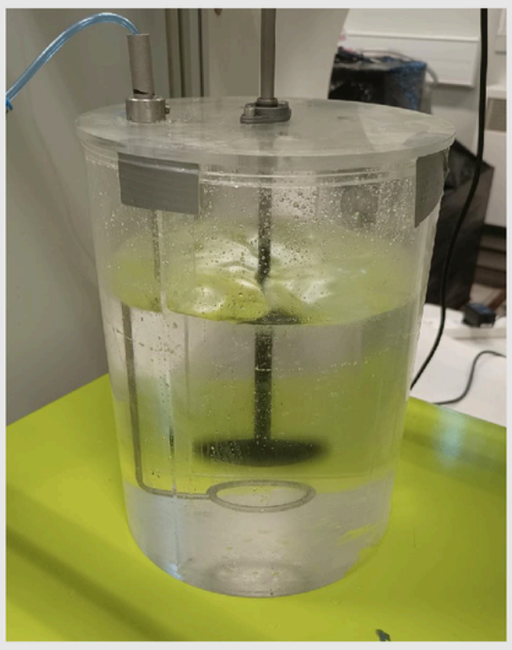

Figure 2b: Tank Setup

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RESULTS

- Data processed using the PEPT-ML algorithm [3]. Post-processing performed using the Up^4 open-source software [4].
- Figure 3 shows the azimuthally averaged velocity scalar fields for the two aerated regimes (both at 5 VVM) and a single-phase base case.

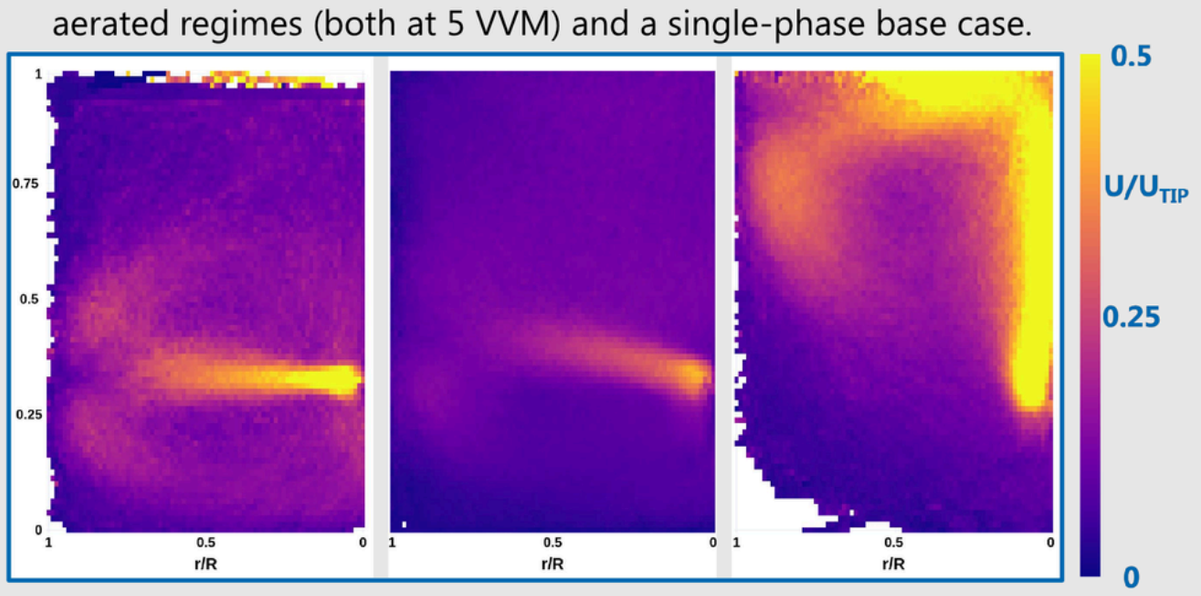

Figure 3a: Single-Phase (Re = 500) | Figure 3b: Dispersed (Re = 1400, 5 VVM) | Figure 3c: Flooded (Re = 500, 5 VVM)

- Figures 3a and 3c shows no commonalities between the flooded and the single-phase case, despite the same Reynolds number. Gas completely dominates the flow. Figure 3b shows the high velocity region becoming more vertical in the dispersed regime, indicating the addition of gas alters the hydrodynamic flow patterns.
- Figures 4a and 4b show the radial variation of velocities at Re = 500 for the single-phase and 5 VVM experiments, respectively. Figure 5a shows the radial variation of velocities at Re = 1400. Figure 5b shows the differing velocities at r/R = 0.33 for all gas flow rates at Re = 1400.

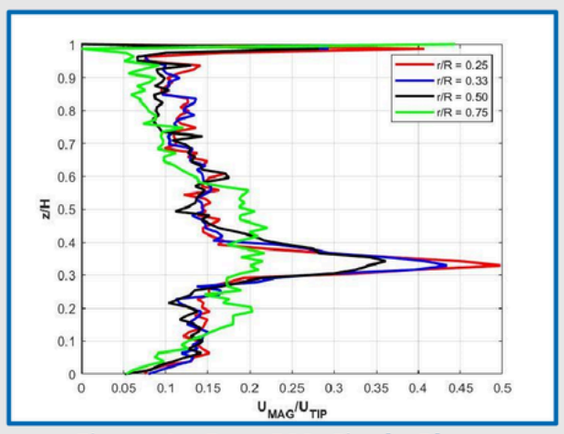

Figure 4a: Re = 500, Single-Phase

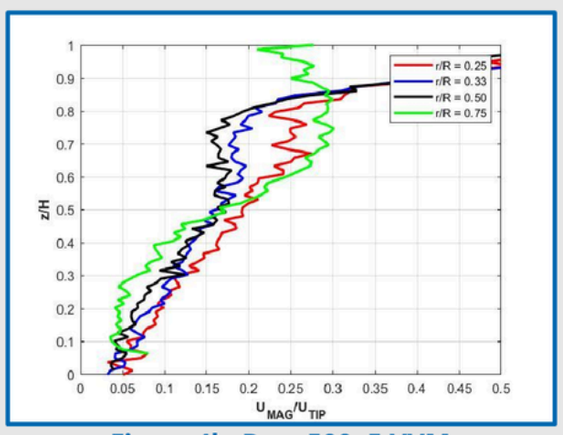

Figure 4b: Re = 500, 5 VVM

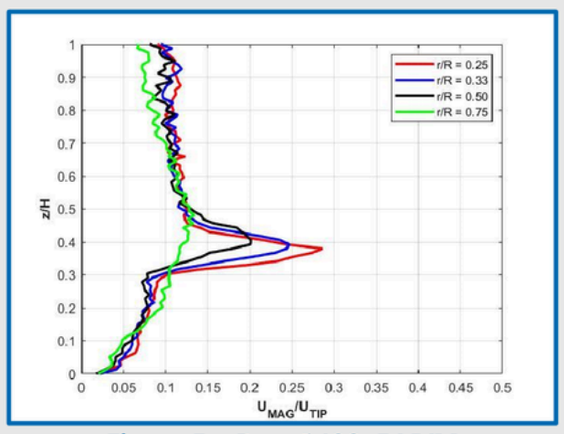

Figure 5a: Re = 1400, 5 VVM

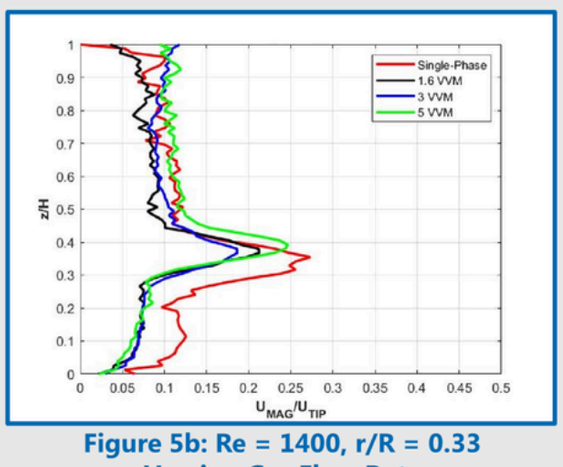

Figure 5b: Re = 1400, r/R = 0.33 Varying Gas Flow Rate

CONCLUSIONS AND FUTURE WORK

- Quantitative flow fields for flooded systems have been determined for the first time. A high velocity plume is observed rising at the vessel axis. Dead zones at the base of the vessel are noticeable in the flooded cases.
- In the dispersed regime, increasing the gas flow changes the angle of the velocity out jet from the Rushton turbine.
- Future experimental investigations will focus on understanding high gas flow rates on non-Newtonian fluids at differing solution concentrations, to understand the impact of viscosity on the dispersion of gas.