UK BATTERY INDUSTRIALISATION CENTRE

The UK's battery manufacturing development facility

Providing scale-up, laboratory expertise, and helping develop skills to support the sector.

We link research and development to mass-manufacture.

Department for Business & Trade

UKRI Innovate UK

UK BATTERY INDUSTRIALISATION CENTRE

Webinar: Coupling Slurry Characterisation with CFD and Machine Learning Reduced Order Modelling as Best Practice for Reducing Slot-Die Coating Defects in Electrode Scale-Up

Dr Helen Walker, Senior Simulation Engineer

Process simulation

Due diligence
Verification of customer designs
Check feasibility and reality of customer claims

Materials, equipment and design verification
Understanding and explaining the limitations of equipment, designs, material and components

Fundamental understanding
Improve our understanding of the underlying physics
Physics-based simulation tells you not just ‘if’ but ‘why’

Time and cost reduction
A reduction in wasted time and scrap material by minimising iterations in design → make → test cycle and reduce ‘dial in’ time on the line

Rapid process optimisation
This could include previously inaccessible Design of Experiments, parametric studies
Facilitate design change and mitigate uncertainties

Process simulation campaign timeline

Modelling and simulation is involved throughout the life of a campaign

- Approximate model inputs
- Initial feasibility assessment
- KICK OFF
- Material characterisation
- Modelling activity
- Inform process parameters
- PRODUCTION
- Data analytics
- Lab work
- Model validation
- Modelling Report

Laboratory activity

Data activity

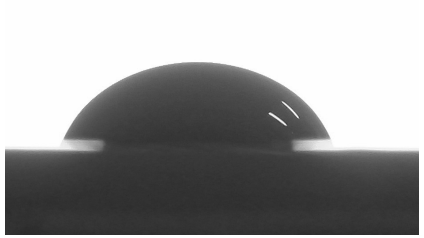
Production

Simulation

Why process simulation at UKBIC is so powerful

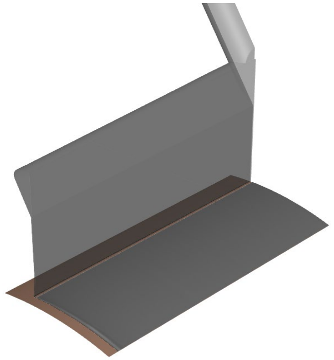
Our simulation offering is unique – with material characterisation, process simulation and advanced data analytics all occurring under one roof

LABORATORY



Advanced material characterisation in laboratory provides the model inputs

SIMULATION

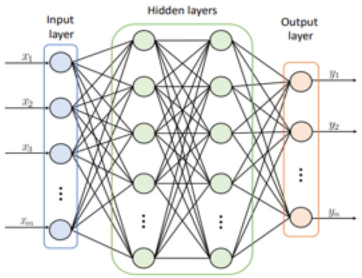


Unique experience in modelling battery slurries and electrode sheets

PRODUCTION

Proximity of simulation engineers to production

DATA



Advanced data analytics on production data to generate data driven models and validate physics-based models

Defects in slot-die coating

Problem

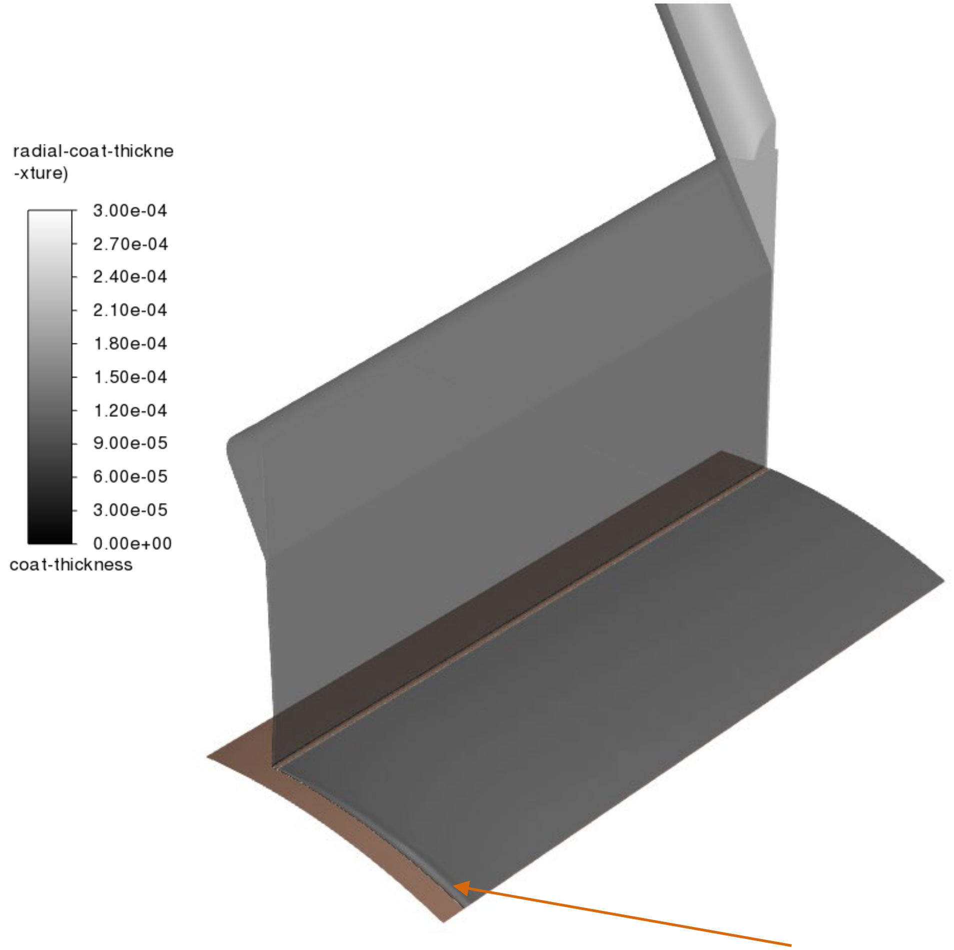
During start-up, significant amounts of time and material can be wasted by determining the optimal process parameters and equipment configuration to achieve coat uniformity and a stable coating window

Objective

Determine slot die set up prior to campaign to achieve coat uniformity (bulk of coating and localised high edges)

Solution

Computational Fluid Dynamics models of slot-die coating of non-Newtonian electrode slurries to predict cross-web uniformity



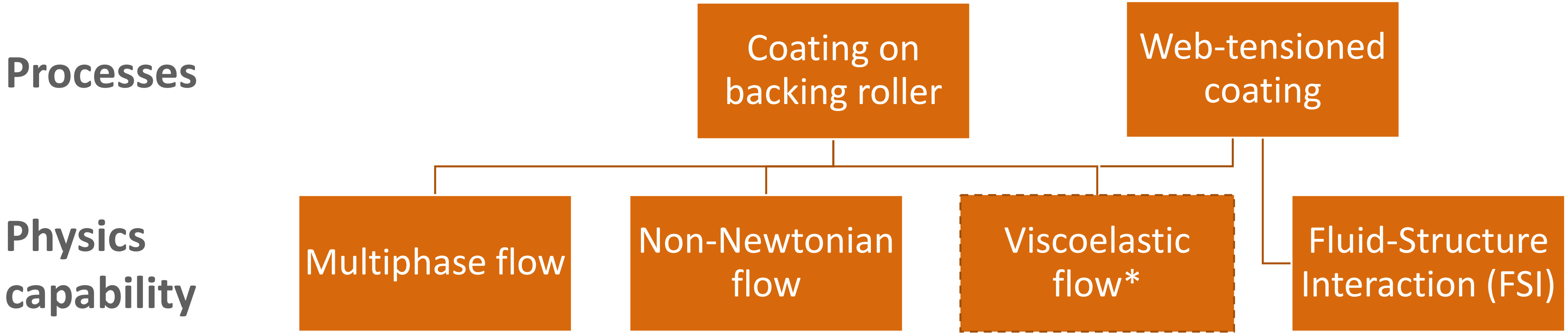
CFD model showing the development of a high edge during anode coating.

Difficulties in modelling slot die coating

Models can be computationally expensive and slow:

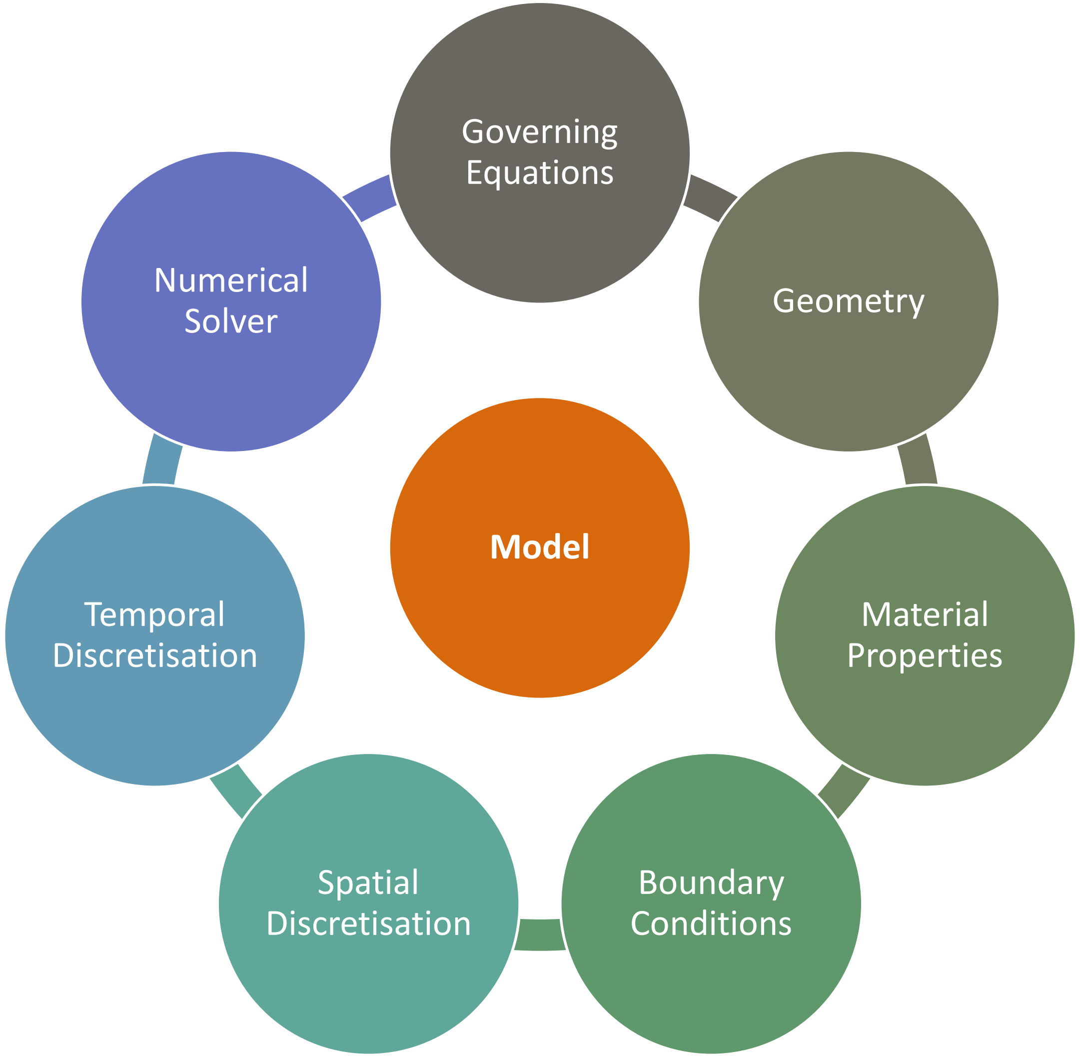
- Highly **complex physics** must be solved simultaneously
- **Nonlinear** phenomena increase solver complexity
- **Large differences in spatial scales** make meshing extremely demanding
- **Unsteady** simulations take far longer than steady-state analyses
- **High-accuracy requirements** for engineering decisions demand finer resolution

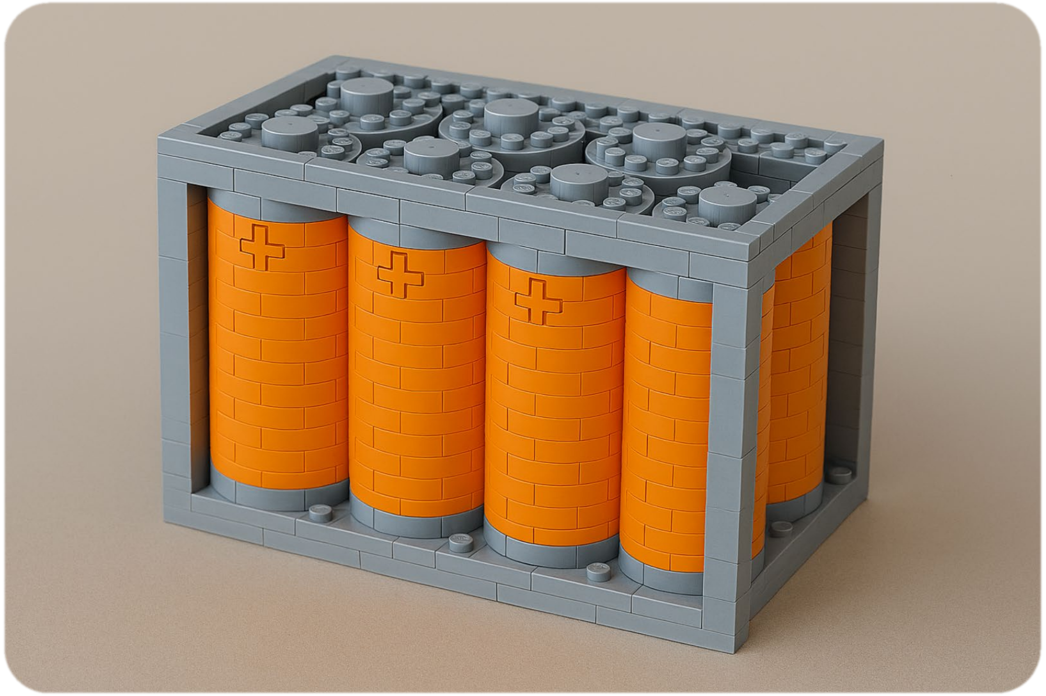
Coating simulation capability for coating



* Dependent on results of elasticity measurements

Background to Multiphysics models

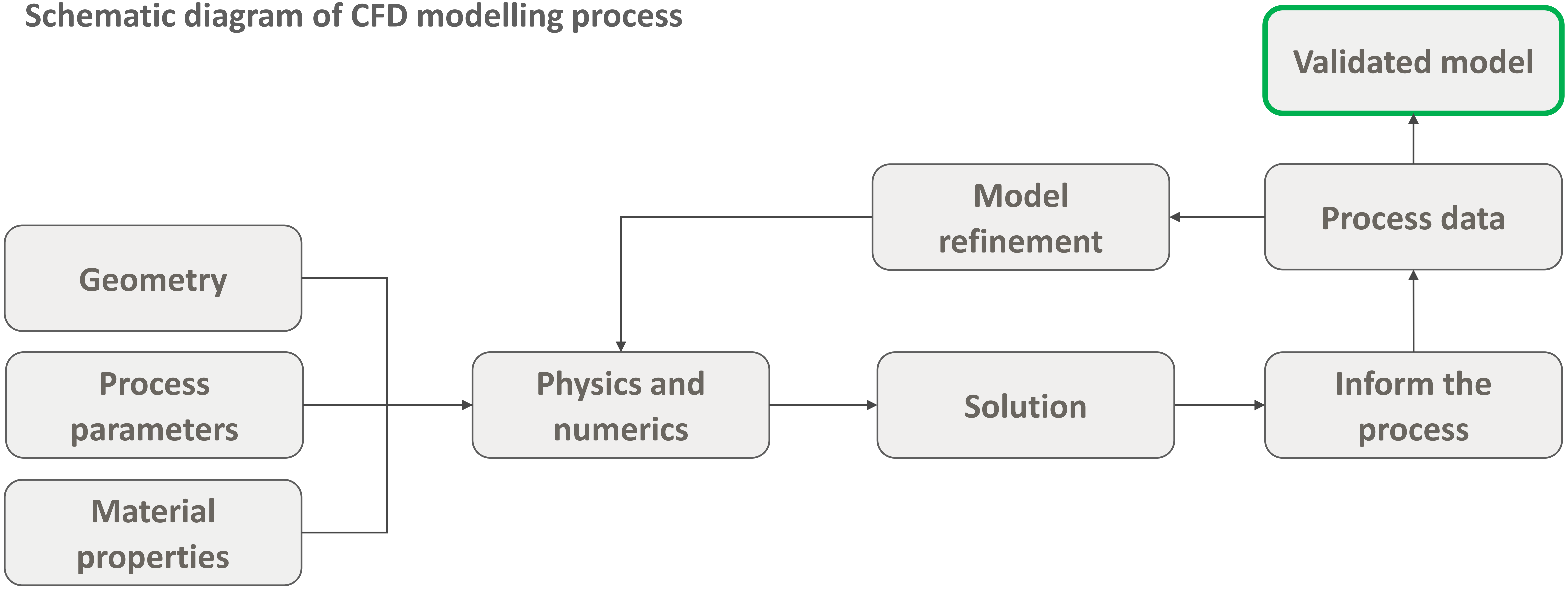




In Multiphysics models, the domain of interest is divided into smaller chunks to be solved independently, then the solution is pieced back together.

The simulation process

Schematic diagram of CFD modelling process



Rheology Industrial Fellowship (PECSO)

Publication: Battery electrode slurry rheology and its impact on manufacturing (Energy Adv., 2024, Advance Article)

Download the paper:

Slurry characterisation methodology
Standard methodology developed for rheology, surface tension and contact angle

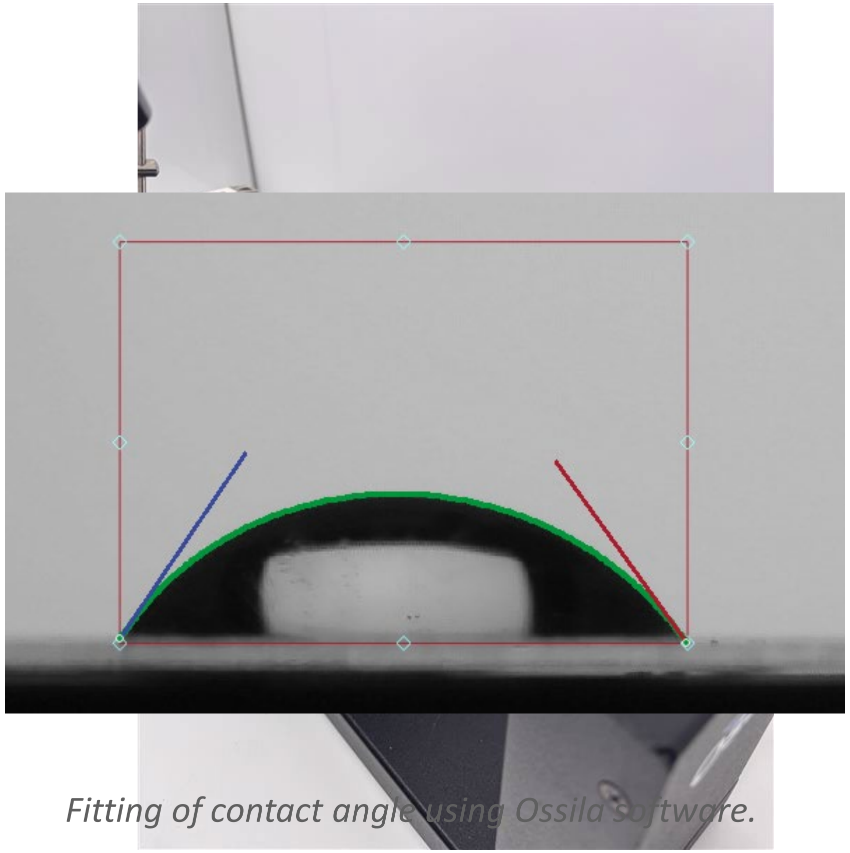
Formulation study
Effect of weight solids and kneading time investigated

Scale-up
220L UKBIC Slurry properties replicated on 1 litre Eirich mixer at University of Birmingham and coated on mini roll-to-roll

Knowledge transfer
Established rheology, surface tension and contact angle analysis at UKBIC to provide inputs to the coating models which are deployed on customer campaigns

Slurry characterisation: contact angle

- Static contact angle of the slurry is measured using a goniometer
- The choice of pipette and droplet size is critical for accurate measurement.
- If the pipette tip is too narrow it produces a droplet depleted in key components
- If the deposited droplet is too large, gravitational flattening and slurry slump can occur
- 10 µL of slurry is dispensed with a 100 µL tip pipette
- An average of 10 readings is taken



Fitting of contact angle using Ossila Software.

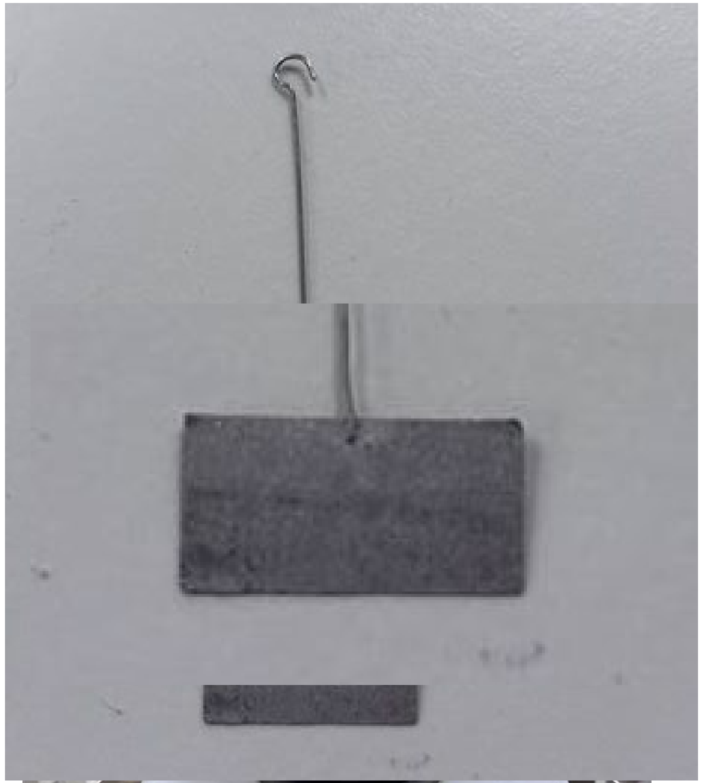
Ossila contact angle goniometer. For slurry analysis foil is taped to a glass slide to create a perfectly flat surface.

Slurry characterisation: surface tension

UKBIC use the Wilhelmy plate method. A platinum plate (for perfect wetting) is typically used.

Challenges

- Tensiometer located in fume hood due to NMP. Some noise when calibrating.
- Cleanliness of plate is critical. Cleaning the platinum Wilhelmy plate after immersion in battery slurry proved challenging due to persistent residue.
- Alternative materials - even disposable - plates can be fabricated as an alternative.



Platinum Wilhelmy plate with slurry residue.

Biolin Scientific Sigma 702D tensiometer used for slurry analysis.

Slurry characterisation: surface tension

The Wilhelmy plate equation comes directly from a force balance at the three-phase contact line (solid–liquid–air interface).

$$\gamma = \frac{F}{P cos(\theta)}$$

Solution

- Glass slide with measured wetted perimeter
- Measure contact angle of liquid on glass slide
- Correct the instrument measurement with

$$\gamma_{act} = \gamma_{reported} \cdot \frac{P_{inst}}{P_{act} \cdot \cos(\theta)}$$

Measurement of DI water using glass plate yielded 72.3 mN/mm. Largest source of possible error will be in contact angle measurement (58.9° over 12 measurements).

Slurry characterisation: viscosity

Standard flow curve

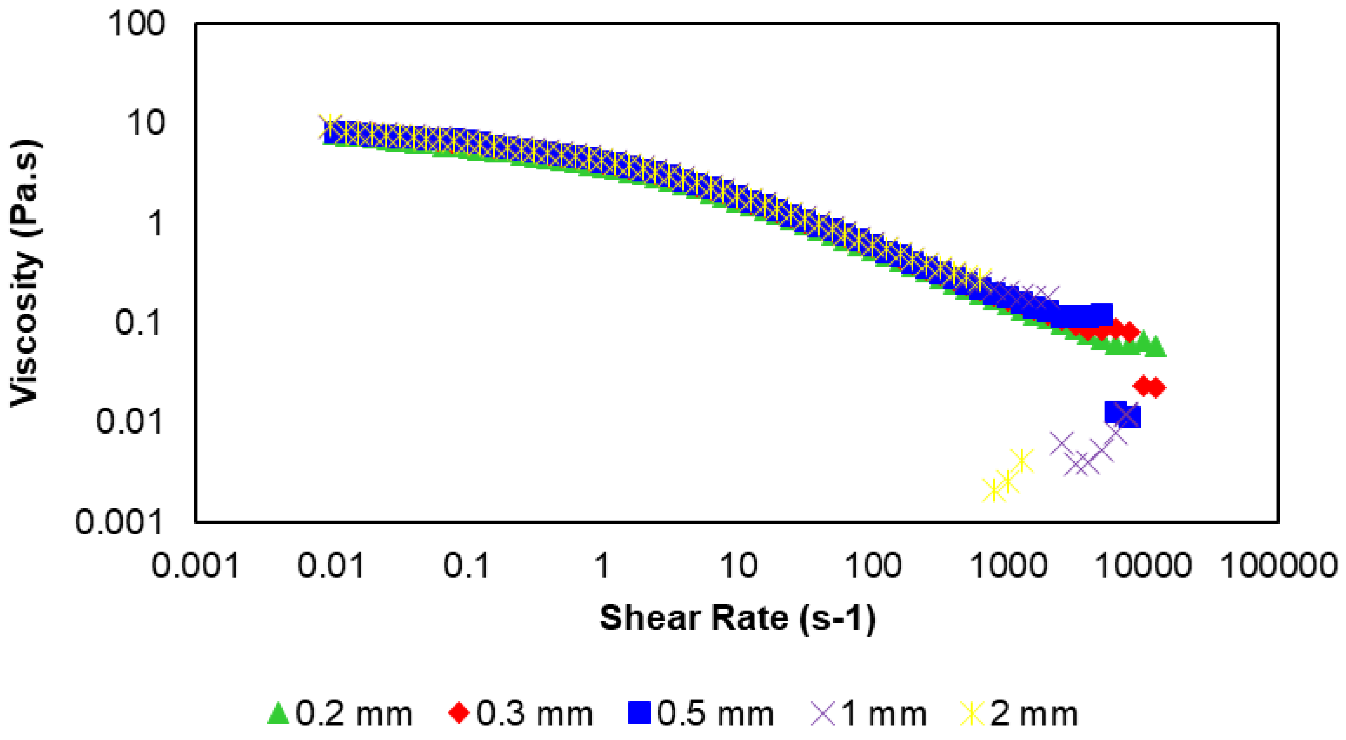
- 1mm gap
- Flow curve 0.01 – 1000 s^{-1}

Extended flow curve

- To push shear rate range run 3 repeats of 0.01 – 10,000 s^{-1} flow curve at 0.2 mm gap
- Discard points which upturn at high shear rates

Model fitting

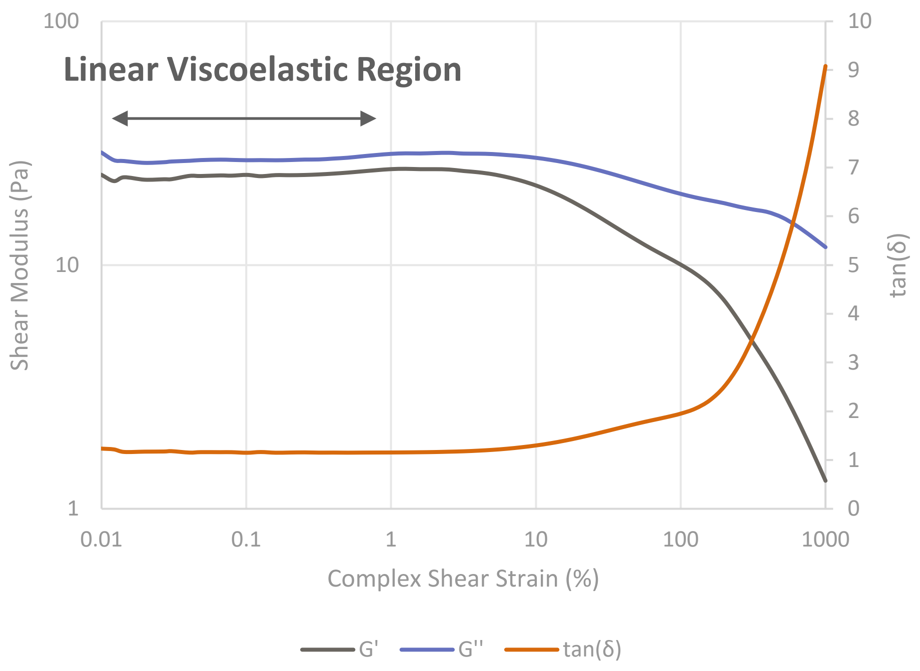
- Most CFD software packages have models for viscosity e.g. Cross, Carreau, Power Law
- The data is fitted to one of these models using least squares approach (**in the log space**)

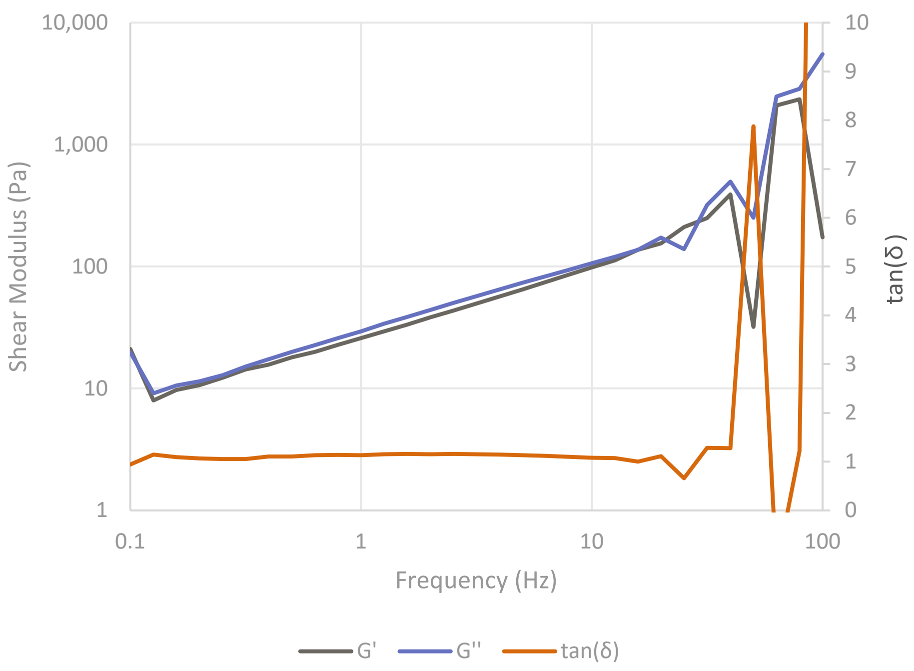


Rheology curves from rheometer optimisation on Netzsch Kinexus Pro+.

Slurry characterisation: elasticity

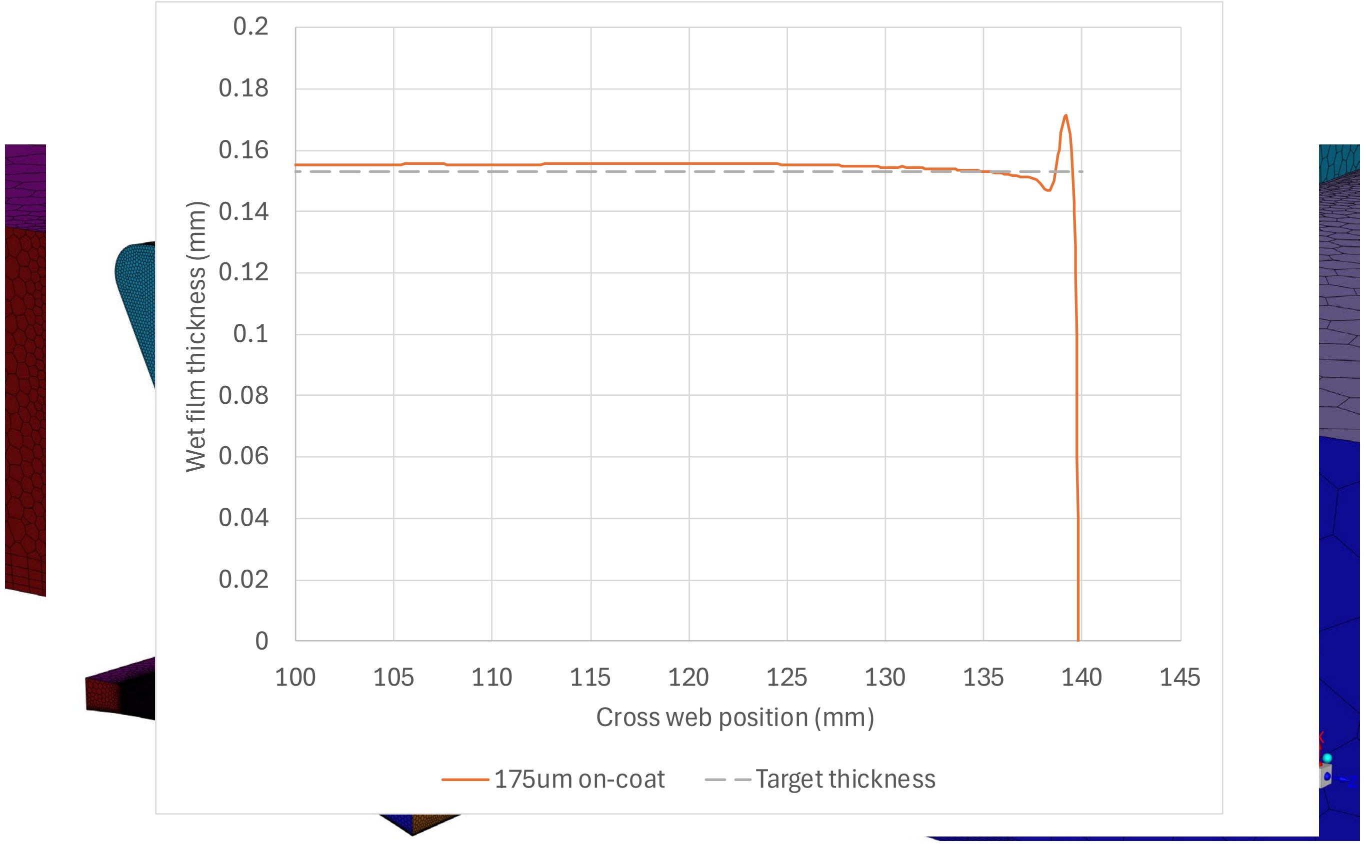
- Amplitude Sweep: 0.01-1000 % strain at 1Hz, 10 points per decade
- Frequency Sweep: 0.1-100 Hz at a strain within LVR (0.1% strain usually fine)
- tan(δ)> 1 largely unproblematic slurry. When tan(δ)~0.5 difficulties arise with pumping



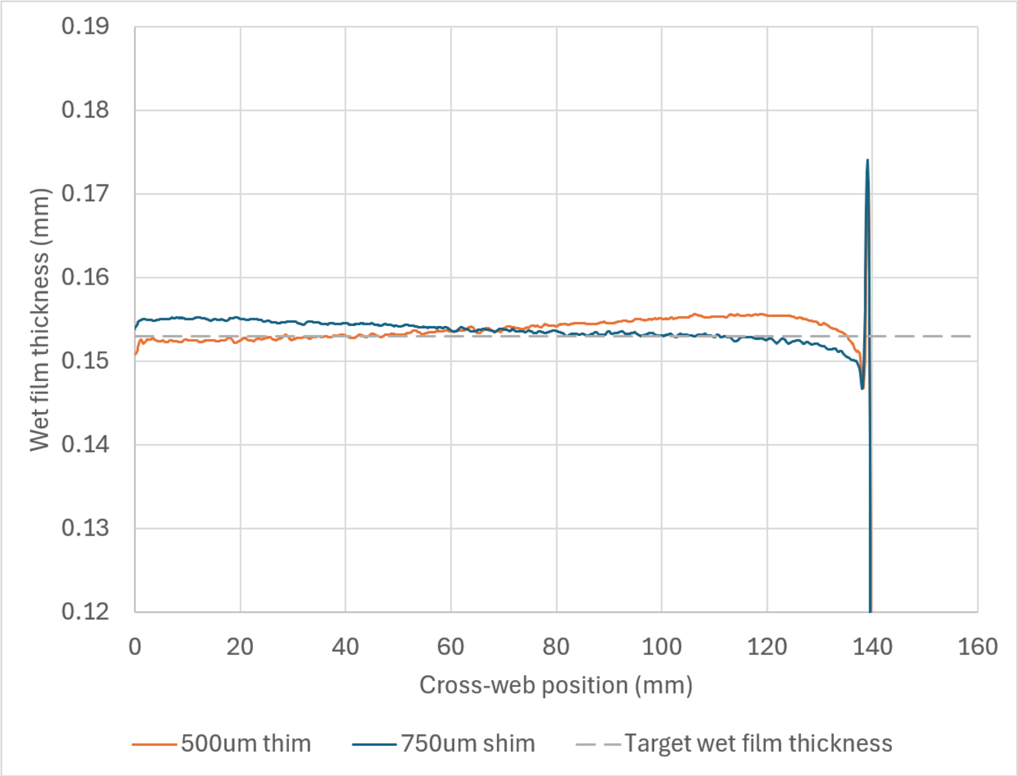


CFD coating simulation

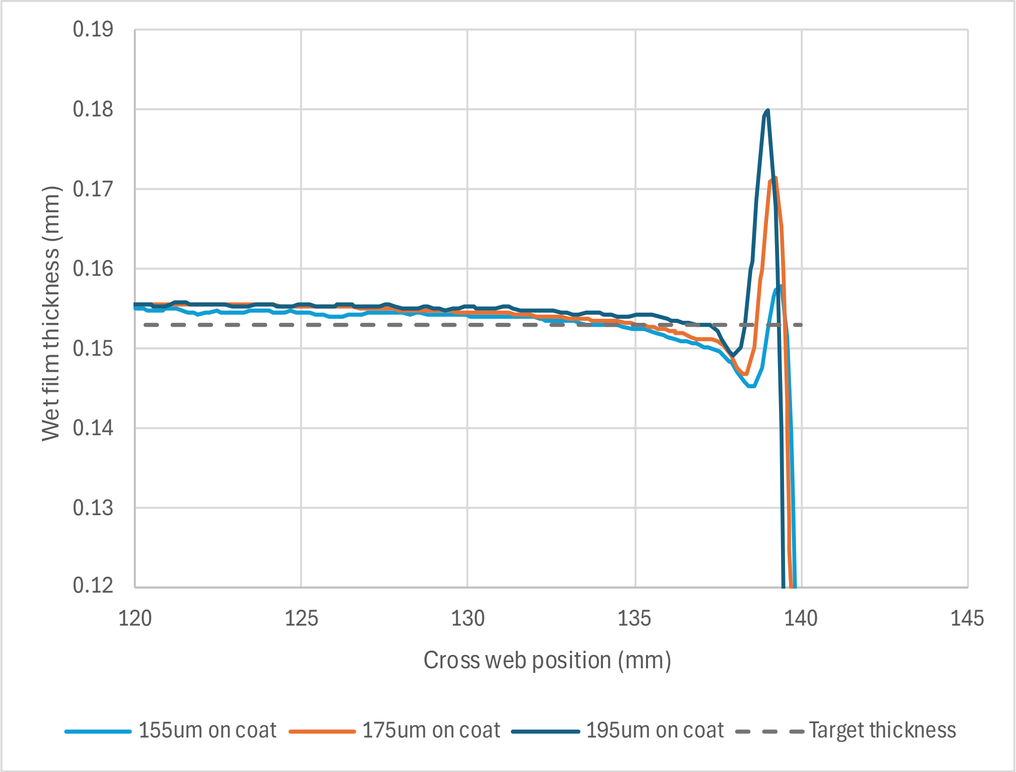
- Exploit symmetry
- Multiphase, Non-Newtonian
- Steady state simulation
- Mass flow inlet and pressure outlets
- The roller is a rotating boundary
- Monitoring quantities of interest for convergence
- Mesh study
- **Runtime 1-6+ hours**



Coating simulation: before scale-up

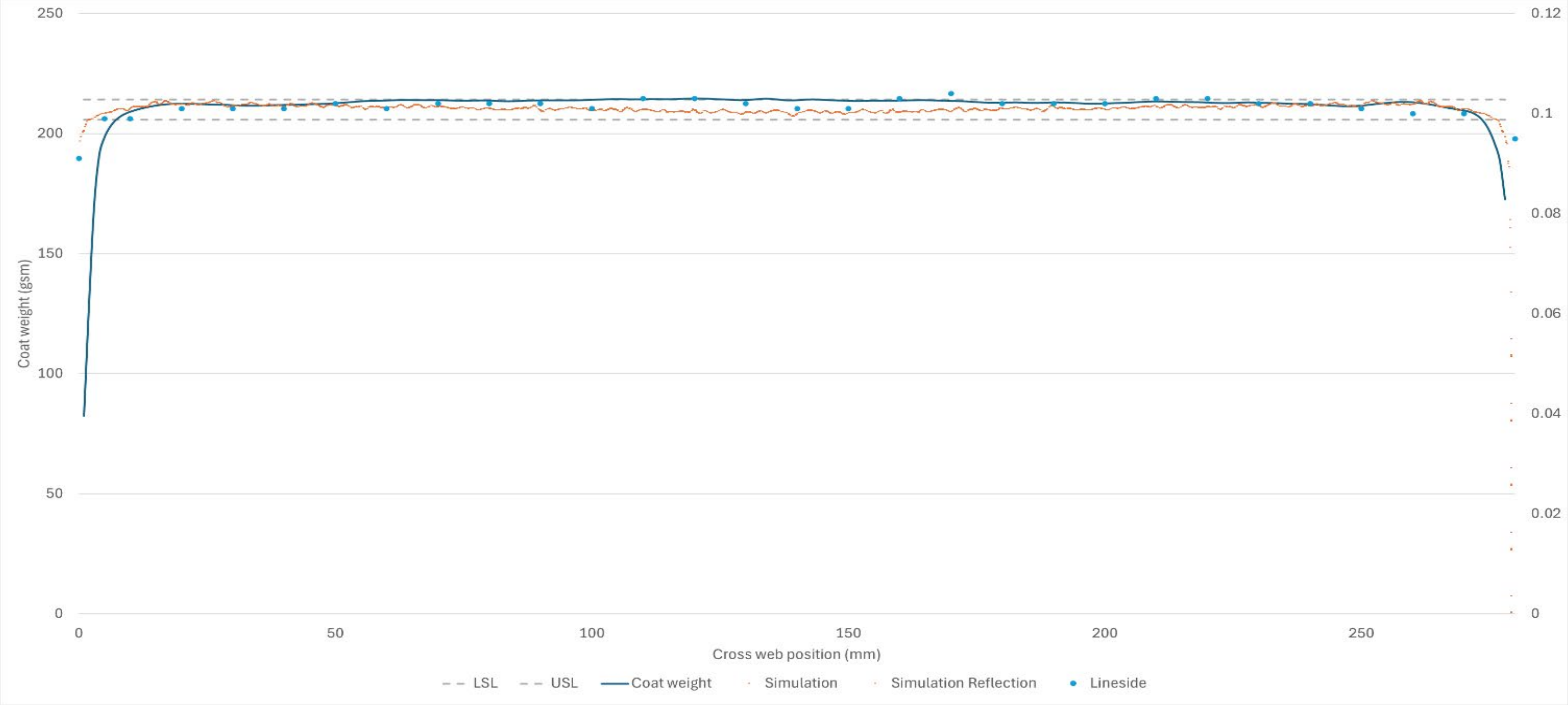


Cross web coat thickness determined by the simulation for different shim thicknesses with 175 µm on-coat position



Cross web coat thickness determined by the simulation for different 'on-coat' positions with 500 µm shim thickness

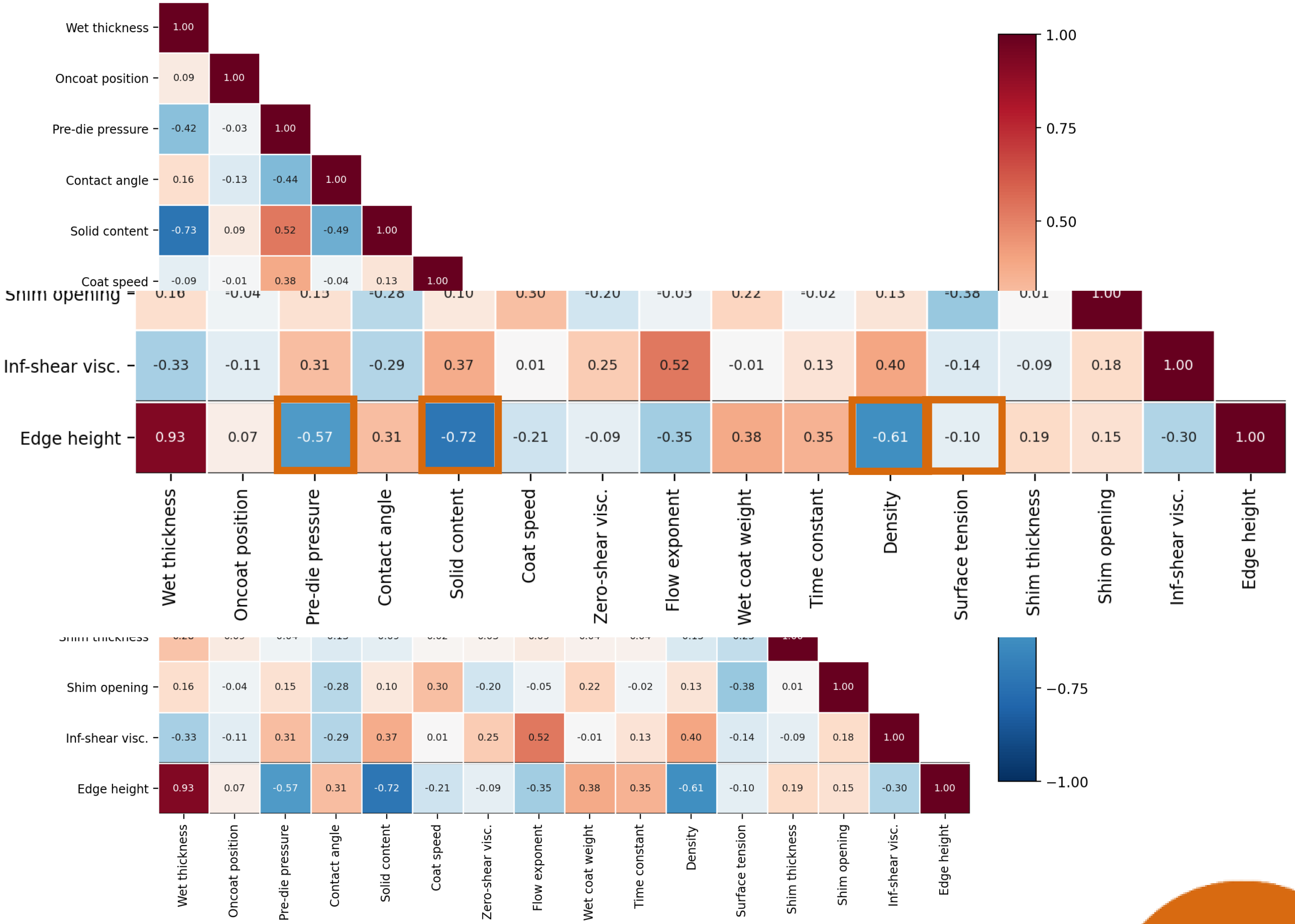
Coating simulation: validation



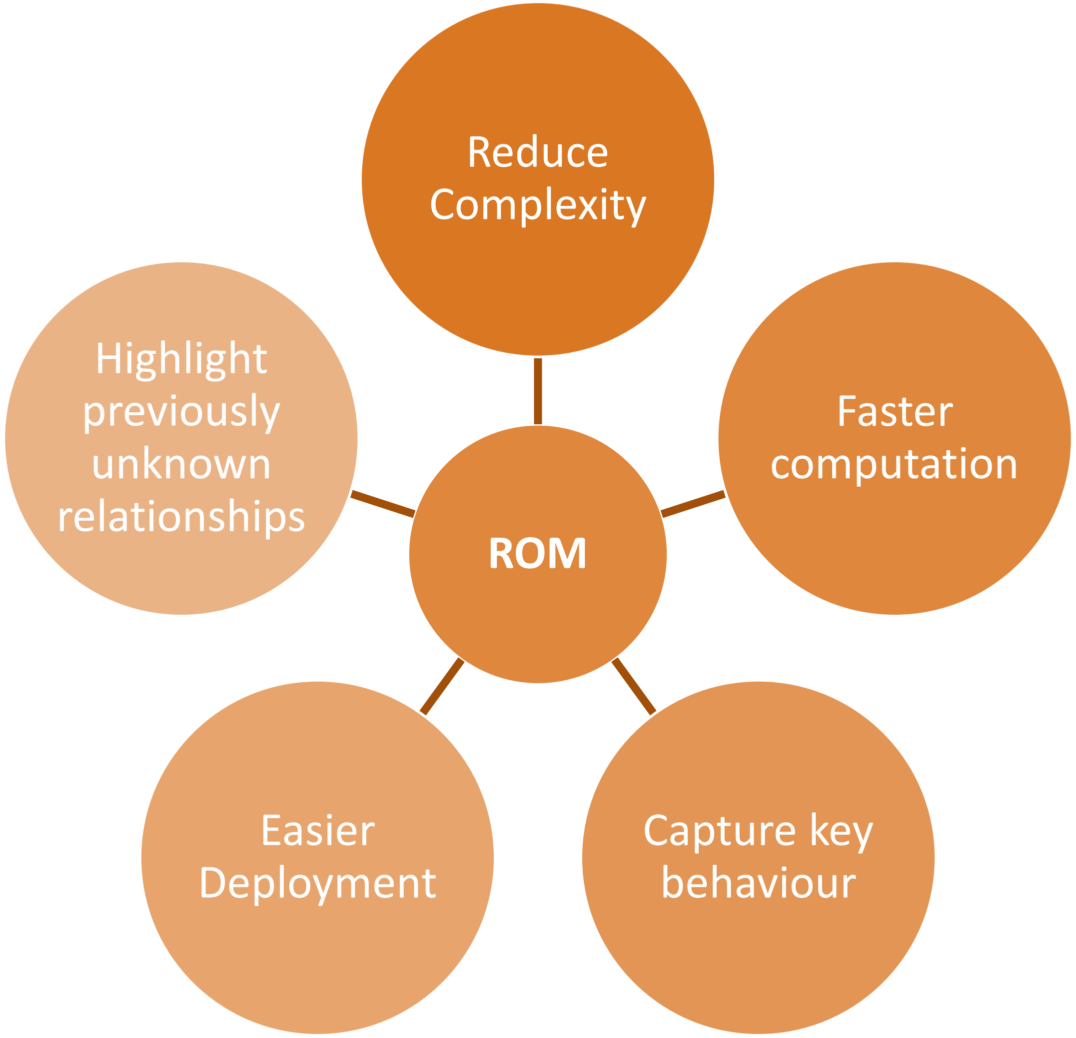
Comparison of simulated cross-web coat web uniformity, inline coat weight measurements and offline thickness measurements

Coating simulation: Statistical analysis

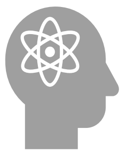
- The dataset (67 simulations) can be analysed to determine the most important factors to coat uniformity
- Pearson correlation can be used to measure the strength and direction of a **linear relationship** between two variables
- We can see which viscosity and process parameters most significantly correlate with edge height
- Caution should be taken since results can be misleading if relationships are nonlinear or confounded, or there is insufficient data



Reduced-Order Modelling (ROM)

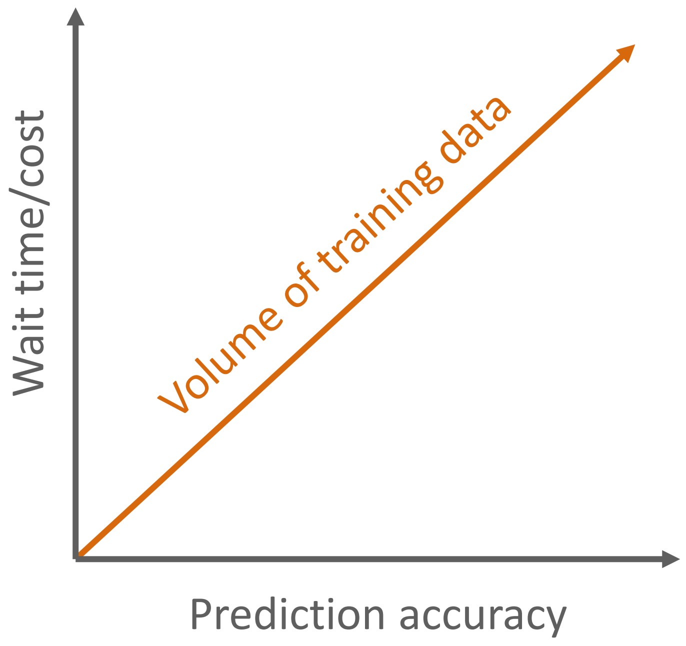


Know before you build



Predict performance

Assess sensitivity



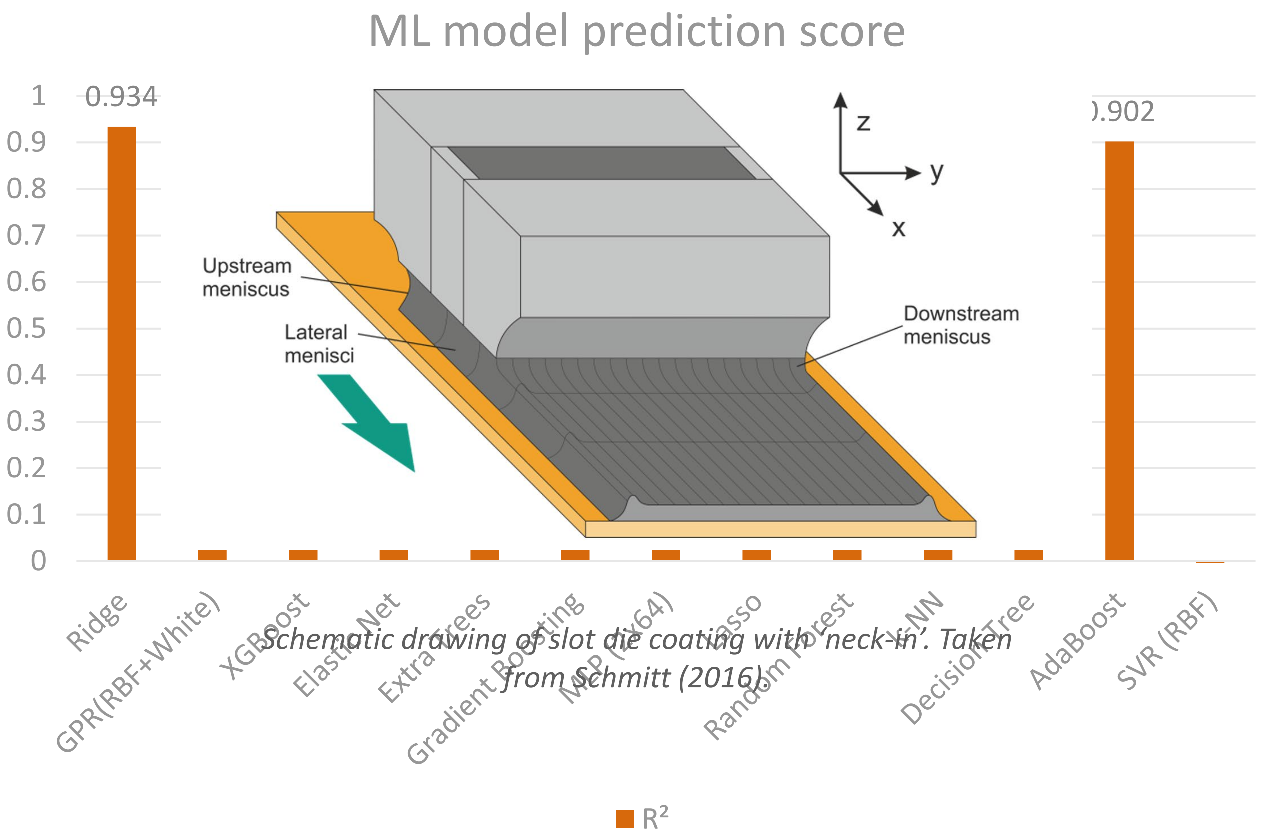
Model comparison and performance evaluation

- Benchmarked multiple machine learning models to evaluate prediction of coating edge height.
- Multiple models were tested to avoid bias, capture unknown relationships, and empirically identify the best-performing approach.

Model types

- Linear: Ridge, Lasso, ElasticNet
- Tree & Ensemble: RF, Extra Trees, Gradient Boosting, XGBoost, AdaBoost
- Others: k-NN, SVR (RBF), MLP, Gaussian Process.

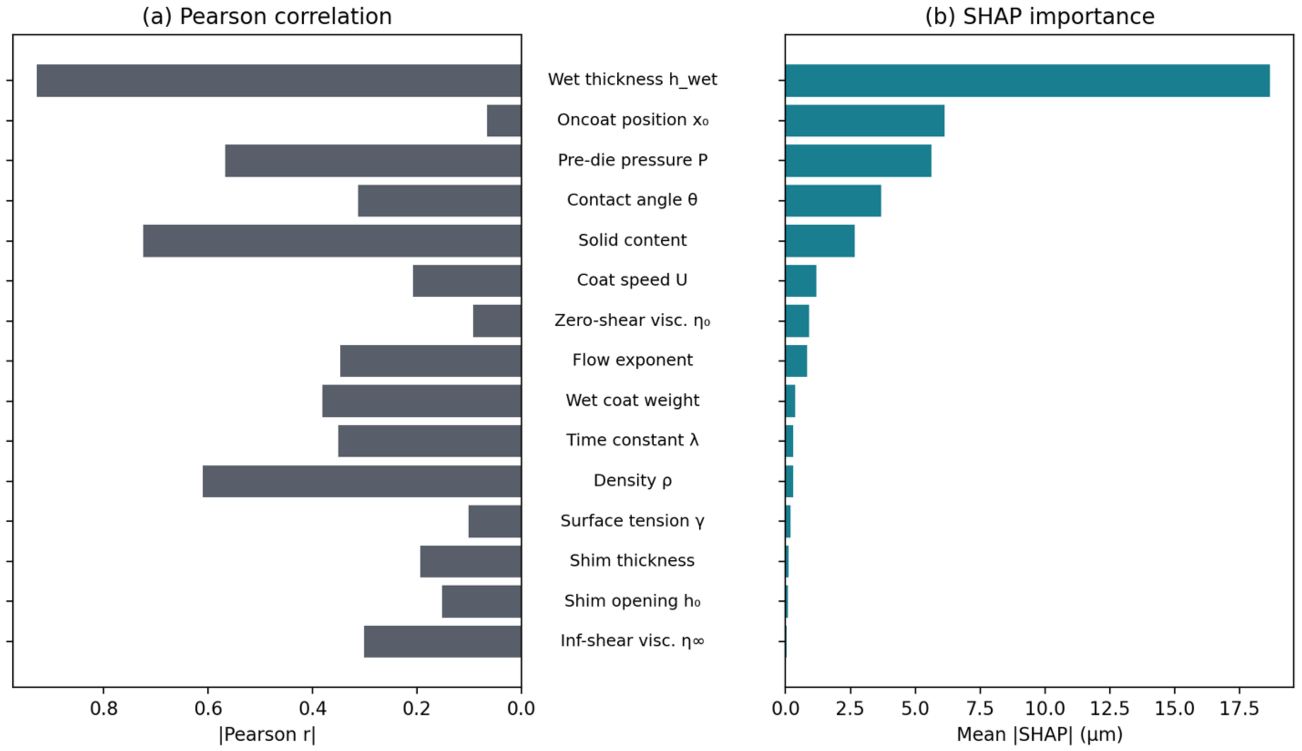
Simple models (Ridge) outperformed complex models.



Schematic drawing of slot die coating with 'neck-in'. Taken from Schmitt (2016).

Feature ranking

- Like Pearson correlation, the Ridge model picks out wet film thickness and pre-die pressure as important factors.
- Now, however, on-coat position is highlighted to be important
- The ML model captures the physical behaviour seen in the CFD simulation
- It evaluates in milliseconds instead of hours, enabling real-time process control



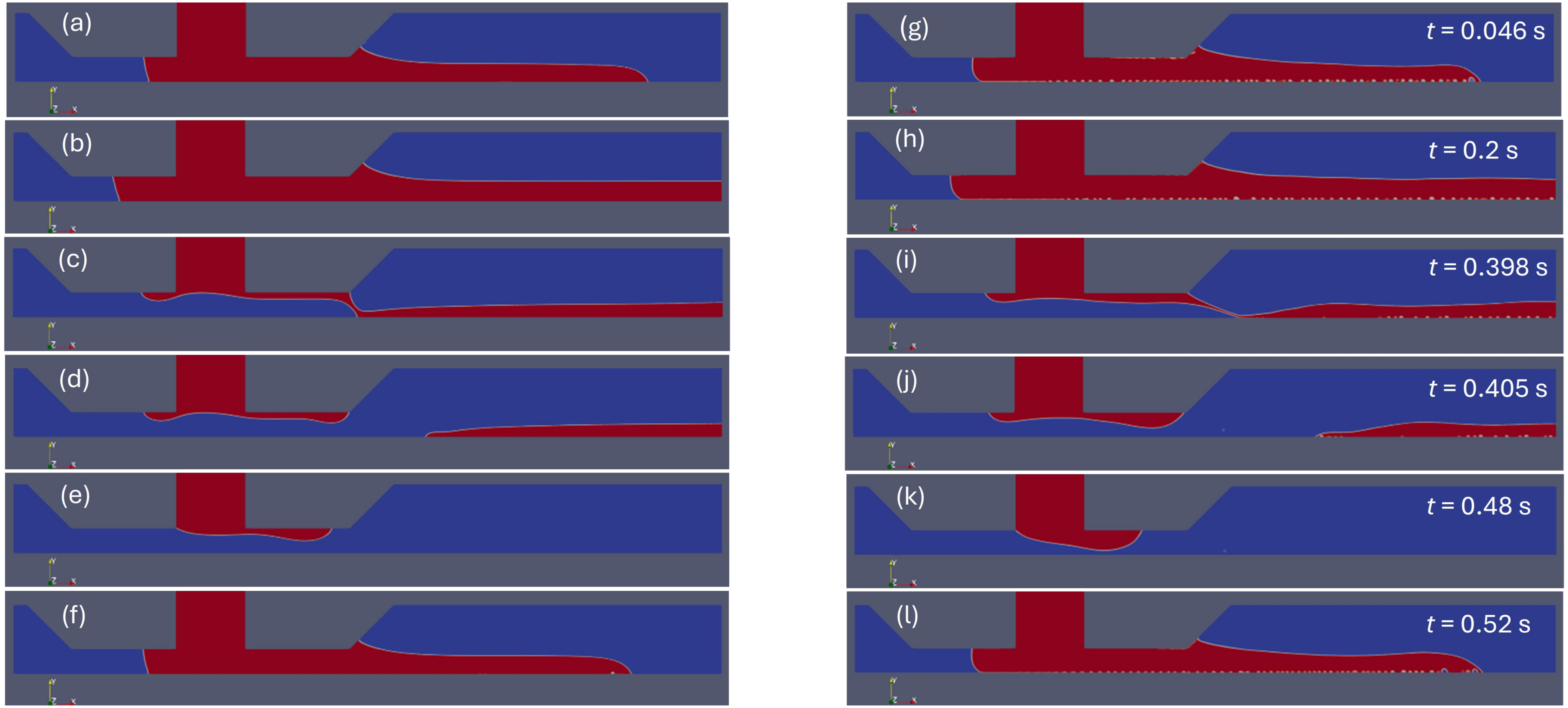
In the Ridge model SHAP (SHapley Additive exPlanations) is the equivalent to R in Pearson regression.

Further development: intermittent coating with viscoelastic fluids

Web speed
U = 5 m/min

Coating gap /
wet film thickness
= 1.20

Non-Newtonian (Cross model) | Non-Newtonian & elastic (Giesekus model (Wi = 50))



Credits: Juan C. Padrino | Giles Richardson
University of Southampton

Conclusions

1. Accurate characterisation of slurry behaviour is inherently challenging; this work has highlighted key considerations and best practices for reliable analysis.

2. CFD modelling provides valuable fundamental insight into slot die coating but can be limited by high computational cost and long run times.

3. With sufficiently large datasets, machine learning offers a pathway to develop reduced-order models, enabling rapid prediction of coating behaviour in future scenarios. The results should be interpreted critically, with the underlying physics in mind.

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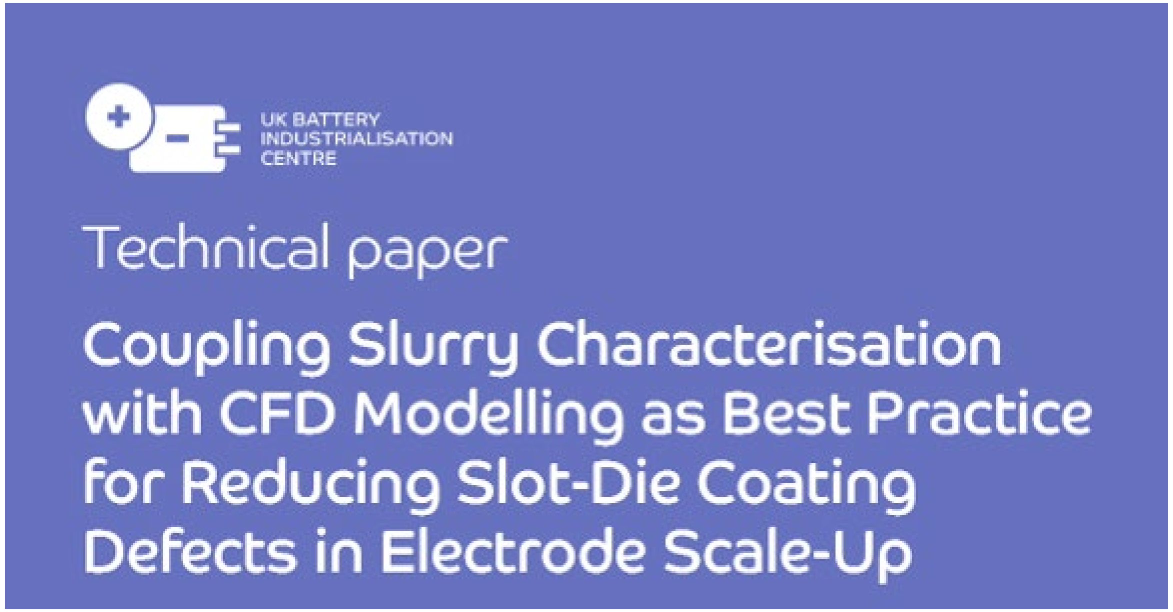
Technical Paper Launch

29 June 2026

- New technical paper with our findings launched
- Also available via our website
  - Webinar recording
  - Webinar slide deck



Question and answer panel

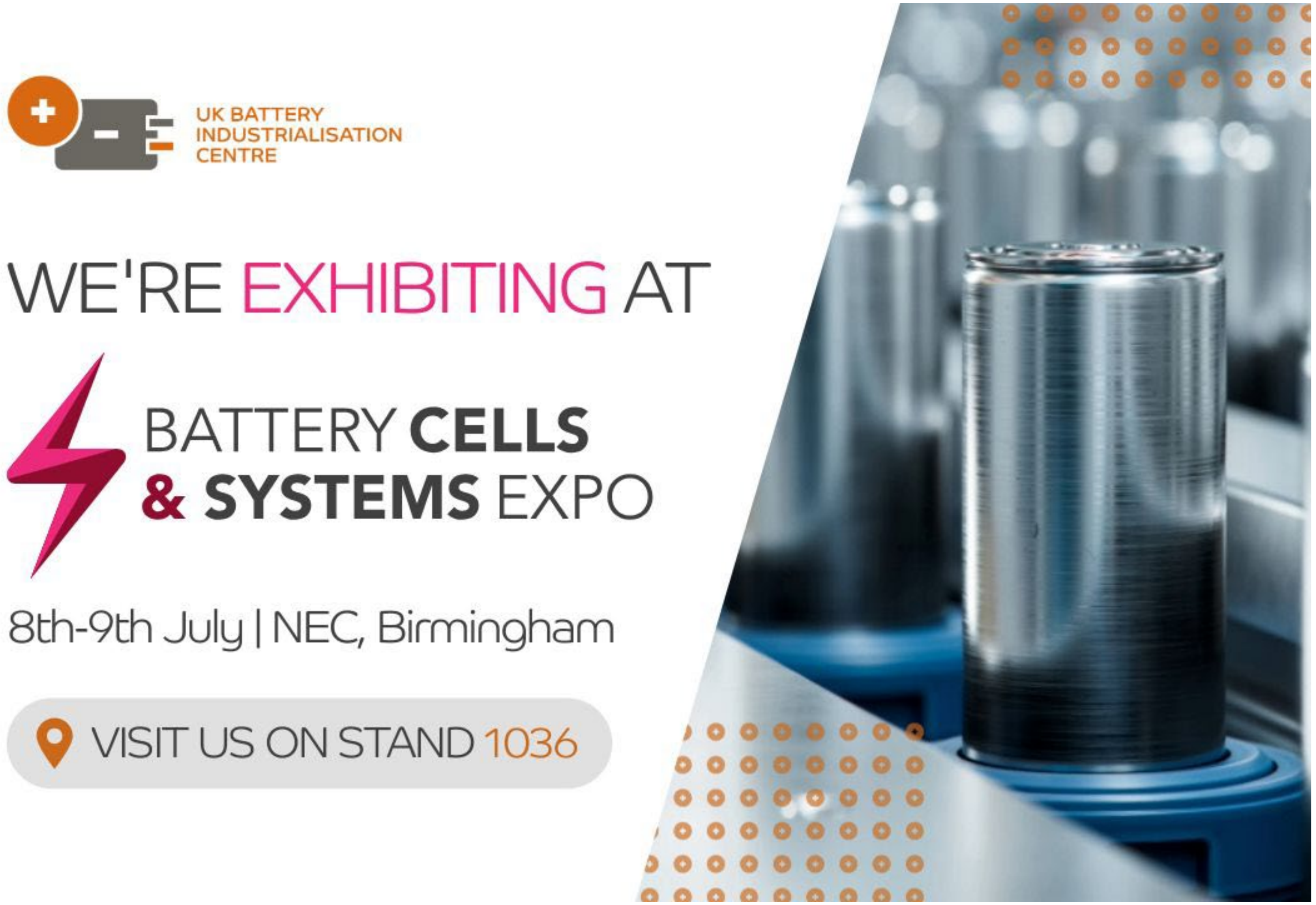
Please use the Q&A function and not the chat function

Dr Helen Walker
Senior Simulation Engineer

Nivedidha Kumaravelu
Data Scientist

Natasha Pines
Analytical Scientist

Come and speak to us



Thank you

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