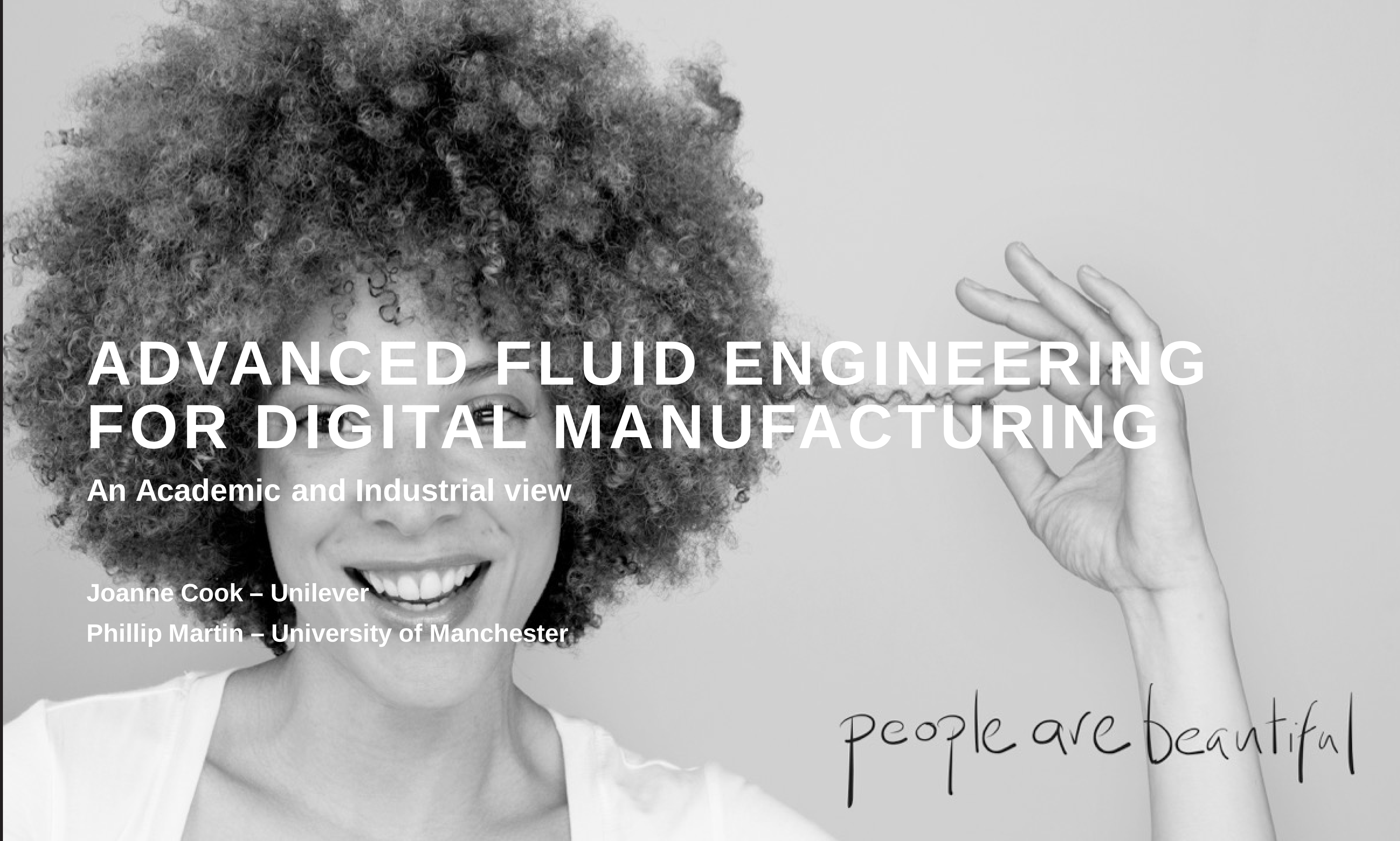
BEAUTY & PERSONAL CARE



ADVANCED FLUID ENGINEERING FOR DIGITAL MANUFACTURING

An Academic and Industrial view

Joanne Cook – Unilever
Phillip Martin – University of Manchester

OUTLINE

Part 1: An Industry View.

Joanne Cook

1. Introduction to FMCG innovation process & challenges
2. In silico ambition
3. CAFE4DM WP2 relevance to Unilever.

Part 2: An Academic View.

Phillip Martin

1. WP1 – simulations.
2. WP2 – structure-property relationships.
3. WP3 – scale up.
4. WP4 – Innovation management and behavioural change

High Volume
Enduring

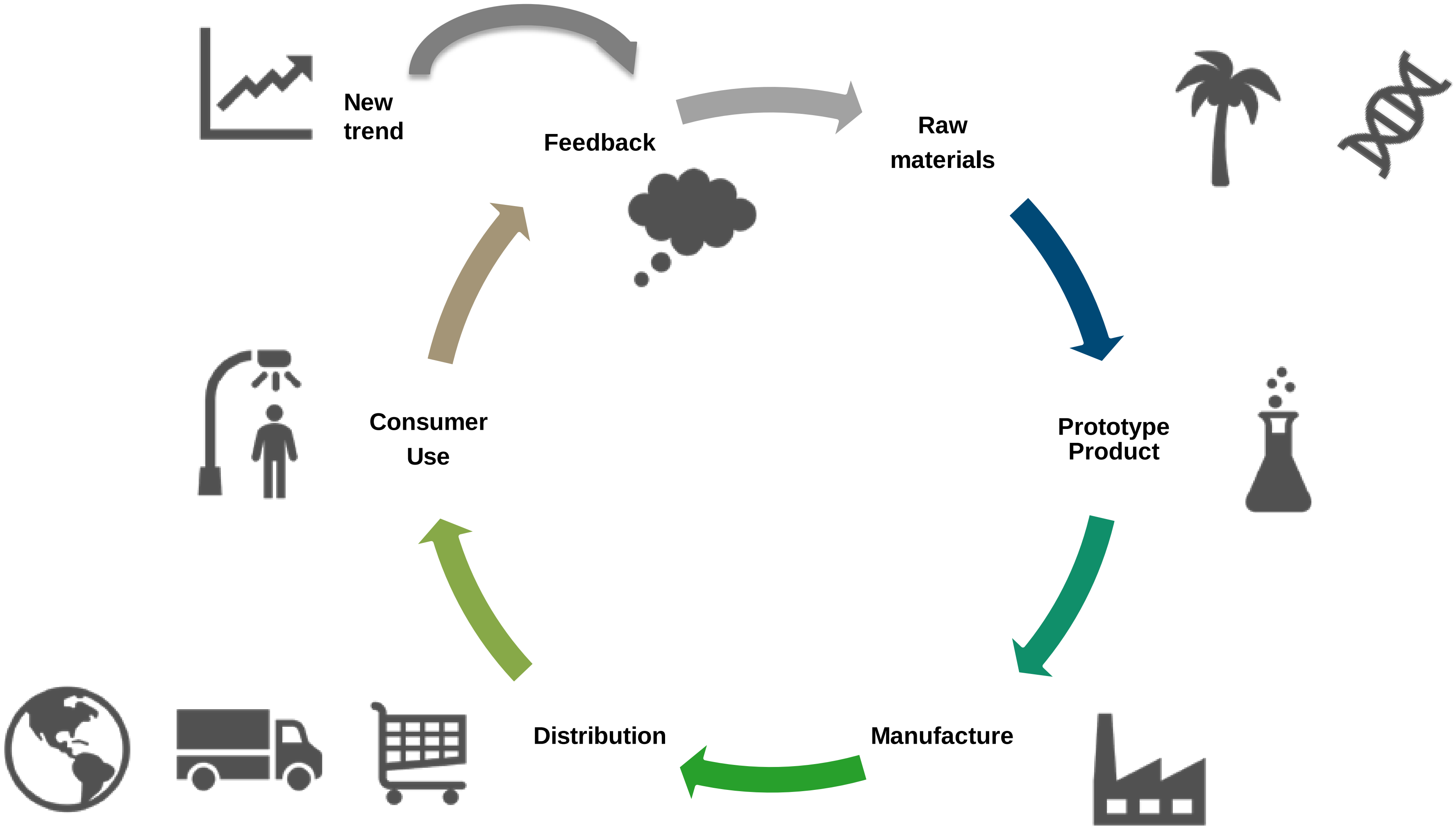
- **Renovation, optimisation**
- **Cost, speed**

Low volume
High turnover

dermalogica
developed by The International Dermal Institute
Living proof.
REN
CLEAN SKINCARE
HOURGLASS
Murad.

- **Trend-led**
- **No surprises ….**

TYPICAL PERSONAL CARE PRODUCT INNOVATION CYCLE



New trend

Feedback

Raw materials

Prototype Product

Manufacture

Distribution

Consumer Use

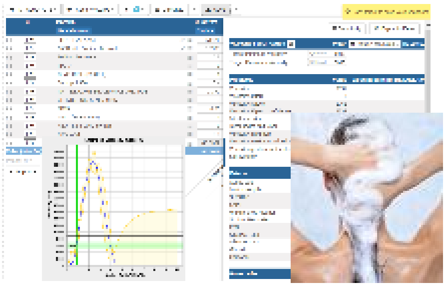
OUR RESULTING DIGITAL AGENDA

DIGITAL PRODUCT ENGINEERING

Suite of models for in-silico formulation and processing

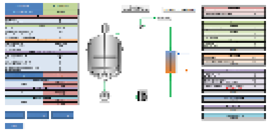
DIGITAL MANUFACTURING

Novel measurements and analysis of process data



Product properties and performance models

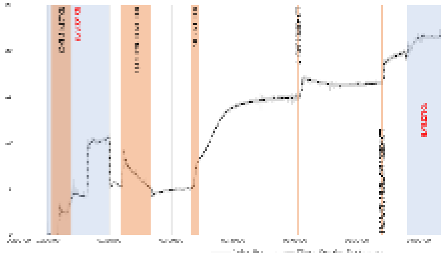
Engineering Calculator



PC Discover + Category

Equipment Performance Calculators


Clear Links and some overlap



Microsoft Business Intelligence

PERCEPTIVE ENGINEERING LTD

POWER BI

pharmaMV

Process data capture and analysis

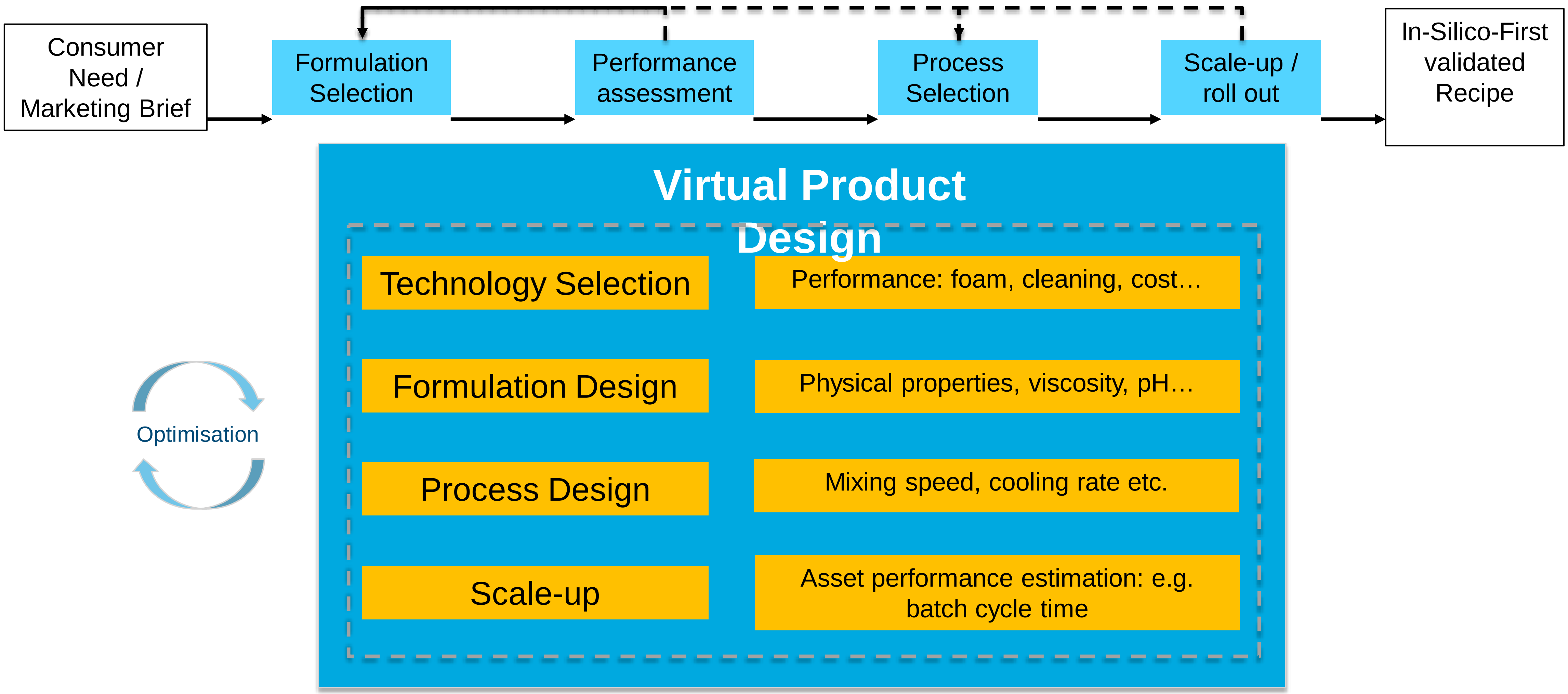
Novel measurements

Expert knowledge in the hands of all formulators and engineers

Supply Chain benefits

AMBITION: IN-SILICO-FIRST RECIPE DESIGN

Simulation & optimisation of product innovation – First exemplar = isotropic liquids



Iterations as required to meet brief

Consumer Need / Marketing Brief

Formulation Selection

Performance assessment

Process Selection

Scale-up / roll out

In-Silico-First validated Recipe

Virtual Product Design

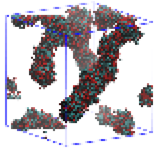
Technology Selection	Performance: foam, cleaning, cost…
Formulation Design	Physical properties, viscosity, pH…
Process Design	Mixing speed, cooling rate etc.
Scale-up	Asset performance estimation: e.g. batch cycle time

Optimisation

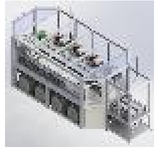
AMBITION: IN-SILICO PRODUCT & PROCESS ‘SCALE-UP’

Expert knowledge in the hands of all product scientists

Microstructure



Mesoscale modelling

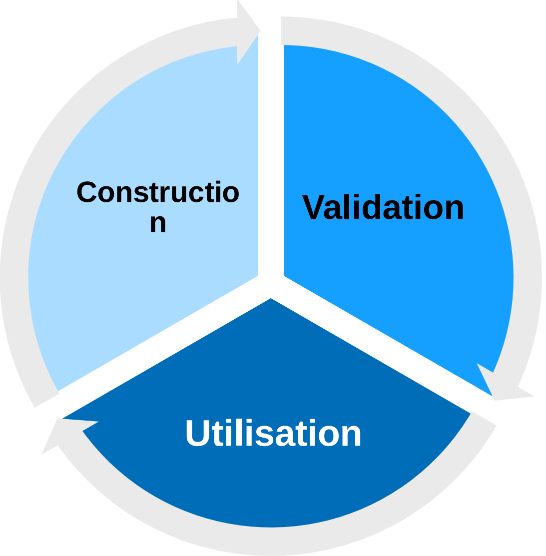


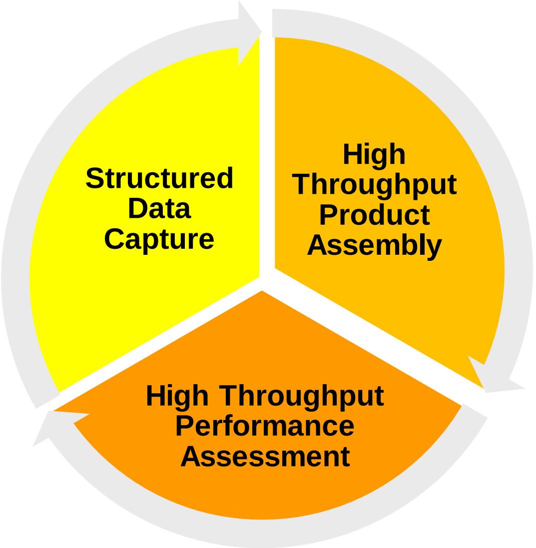
Laboratory automation

Pilot plant

Factory

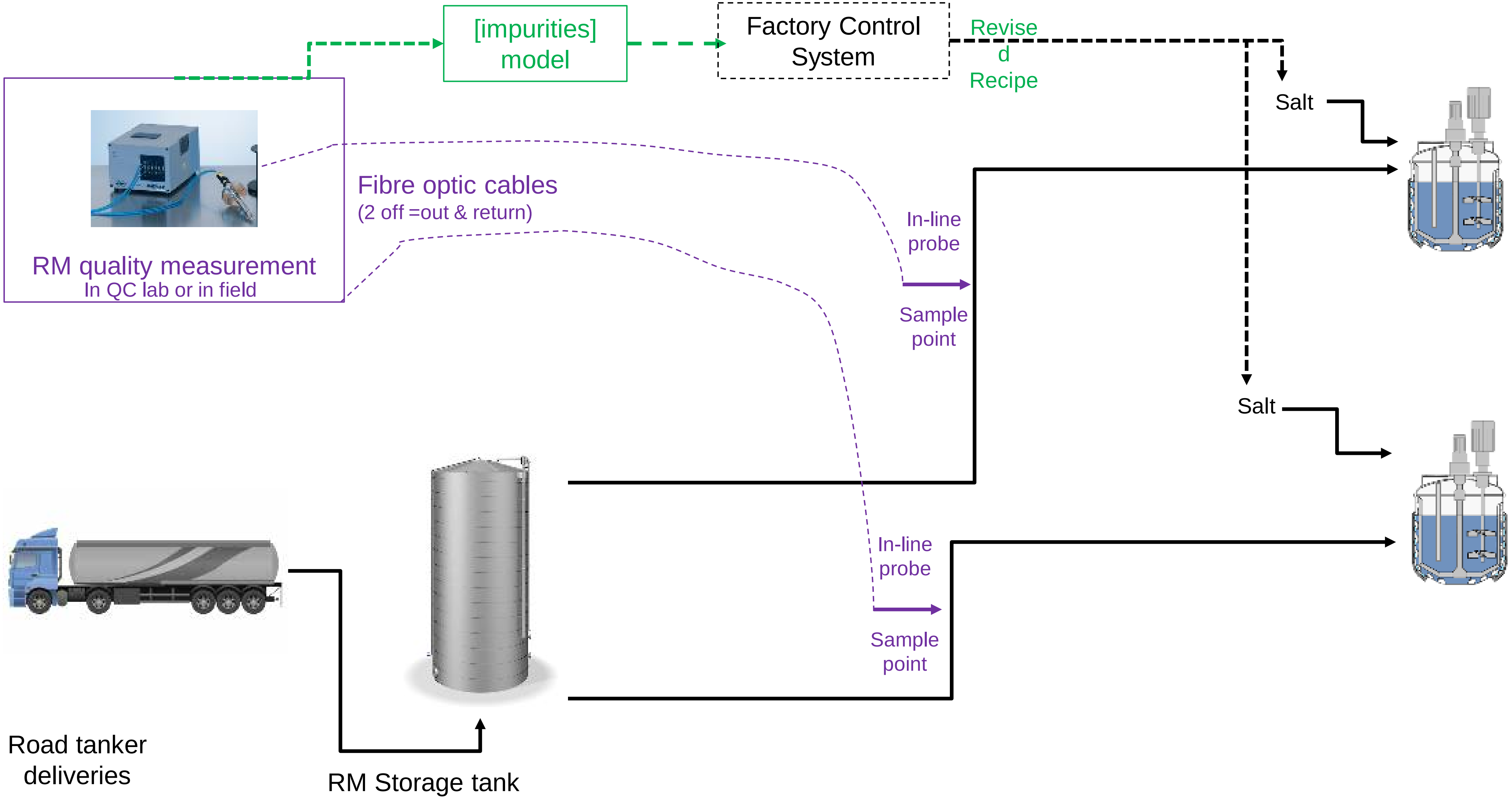
- Linking microstructure to rheology
- Predictive scale up from laboratory to pilot plant to factory
- Accurate scale-up and roll-out over whole supply chain network
- From models to simulations to predictions
- Data generation is the rate-limiting step





AMBITION: QUALITY RIGHT FIRST TIME

FEED FORWARD CONTROL: NO RETROSPECTIVE BATCH ADJUSTMENTS



[impurities] model

Factory Control System

Revised Recipe

Salt

Salt

RM quality measurement
In QC lab or in field

Fibre optic cables
(2 off =out & return)

In-line probe

Sample point

In-line probe

Sample point

Road tanker deliveries

RM Storage tank

AMBITION: PROCESSING TO AN END-POINT

Opportunity to optimise manufacturing

- Current processes are developed empirically guided by off-line quality checks.
- Hypothesis that further optimisation would be possible if product microstructure evolution could be tracked.
- Two approaches:
  1. Identify off-the shelf measurements and validate
  2. Develop new measurements from scratch.

MANCHESTER 1824 The University of Manchester

CAFE4DM

Potential solution

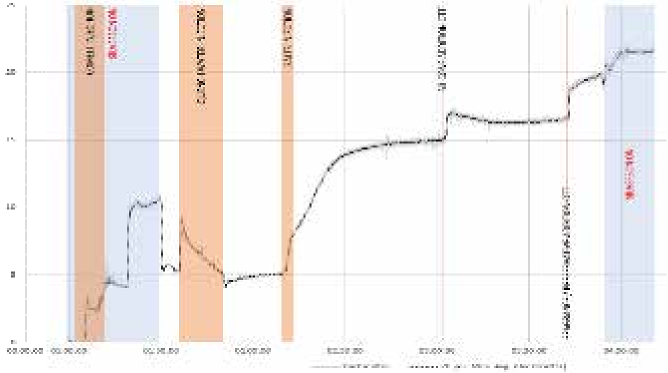
- **In-line measurement technique**

ü Tracks changes in opacity (could be microstructure change), optical properties unique to each mixing step.

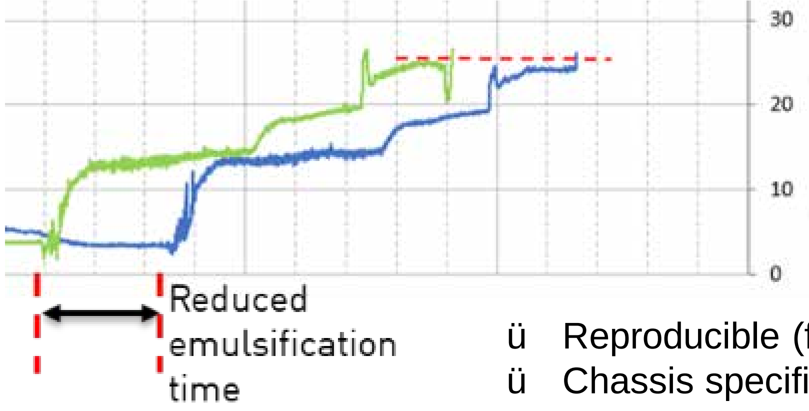
ü Easy to integrate into pilot plant and potentially factory scale.

Validation

Several process steps could be optimised:



Tracked parameter vs. process time in pilot plant trials:



Conventional product batch cycle time

Optimised reduced batch cycle time

Optimised & conventional, same end point

ü Reproducible (features and values)
ü Chassis specific fingerprints
ü PoP for optimising batch cycle time

AMBITION SUMMARY

DIGITAL PRODUCT ENGINEERING

Suite of models for in-silico formulation and processing

DIGITAL MANUFACTURING

Novel measurements and analysis of process data

In silico product recipe design, simulation, optimisation and scale-up

Clear Links and some overlap

Combining advanced sensor measurements with process analytics to enable cost, efficiency & quality benefits

Expert knowledge in the hands of all formulators and engineers

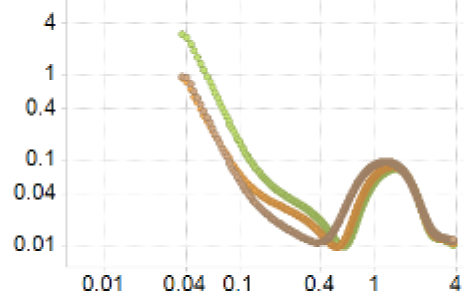
Supply Chain benefits

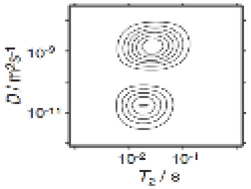
WP2:STRUCTURE-PROPERTY RELATIONSHIPS

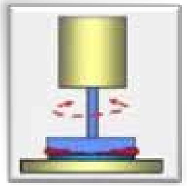
Fuller formulations

Determine the structure

- **Simulated properties (WP1)**
- **Scattering (X-rays or neutrons)**
- **Diffusion NMR**
- **Rheology (steady shear and oscillatory)**

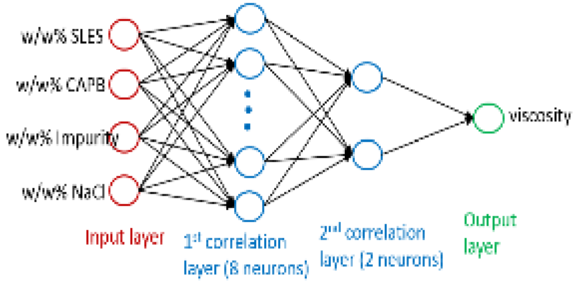


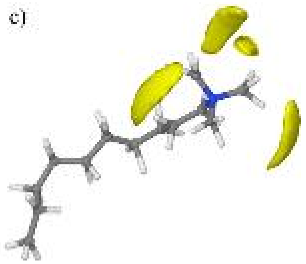




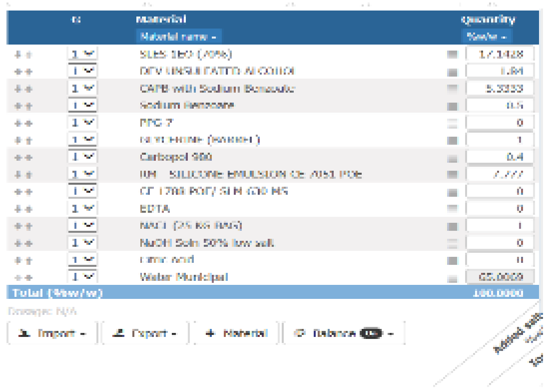
Build predictive or correlative models

- **Machine learning**
- **Group contribution models**



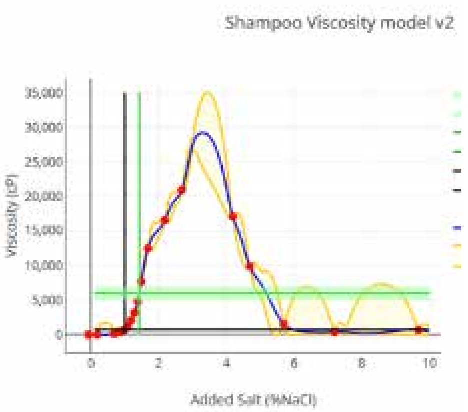


Viscosity prediction available for R&D and SC.



	Material Material name	Quantity %w/w
1	SLES 1EO (70%)	17.1428
1	[illegible]	1.84
1	CAPB with Sodium Benzoate	5.3333
1	Sodium Benzoate	0.5
1	PPG 7	0
1	GLYCERINE (BARREL)	1
1	Carbopol 980	0.4
1	RM - SILICONE EMULSION CE 7051 POE	7.777
1	[illegible]	0
1	EDTA	0
1	NACL (25 KG BAG)	1
1	NaOH Soln 50% low salt	0
1	Citric acid	0
1	Water Municipal	65.0069
Total (%w/w)		100.0000

Dosage: N/A



Structure

Viscosity

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Technical Challenges and Approaches

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1824
The University of Manchester

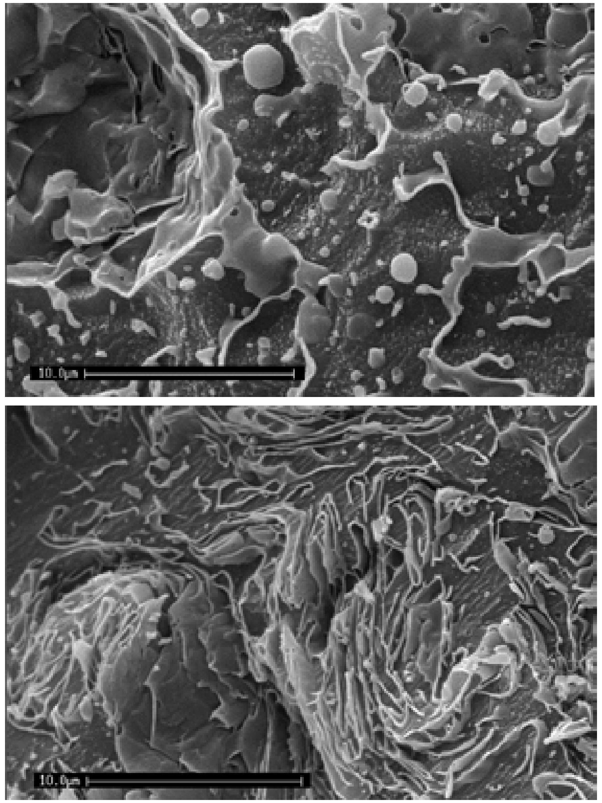
Unilever

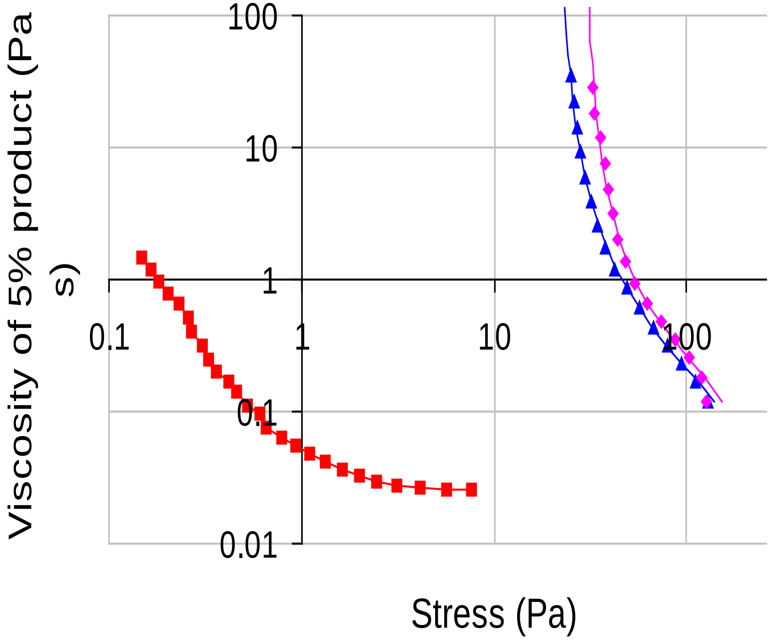
EPSRC
Engineering and Physical Sciences
Research Council

Science & Technology
Facilities Council

UNIVERSITY OF
CAMBRIDGE

ACCELERATING MANUFACTURING: We need to understand how PROCESS INFLUENCES MICROSTRUCTURE



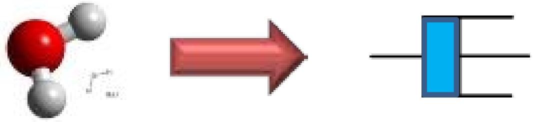


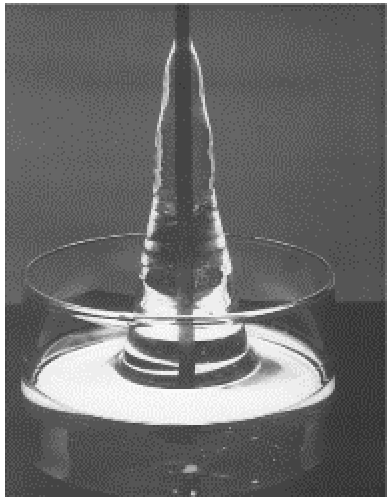
- Same formulation but viscosity differs by order of magnitude - Process design cannot be ignored during product design
- How can we predict properties (rheology) and structure through manufacturing process ?

Modelling challenges

New flow physics with new time and length scales
Competition between scales leads to different macroscopic responses

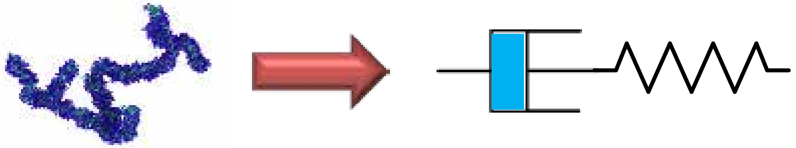
Stir a beaker of (Newtonian) water
Fluid forms a hollow whirlpool





Rheological Phenomena in Focus
By D.V. Boger, K. Walters

Stir a beaker of Polyisobutylene in polybutene
Fluid climbs up the spoon



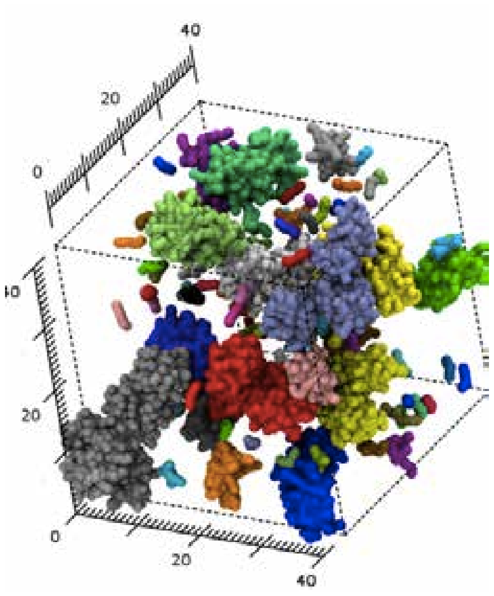
Fluids may respond to ***strain rate*** alone
- Water (Newtonian), Ketchup (shear thinning)

May also respond to ***strain***
- WLM mixtures, polymers, drilling muds....

Many (***many***) different potential models

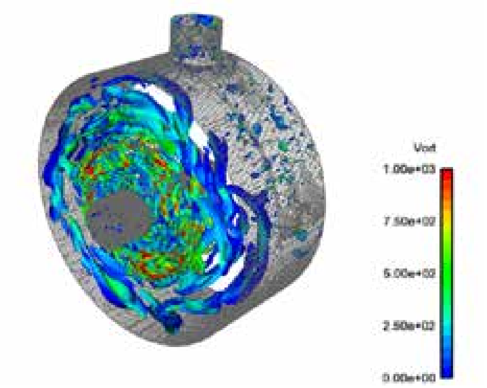
Modelling of complex fluids

Model microstructure Dissipative particulate dynamics (DPD)



Integrate DPD with CFD via constitutive equations

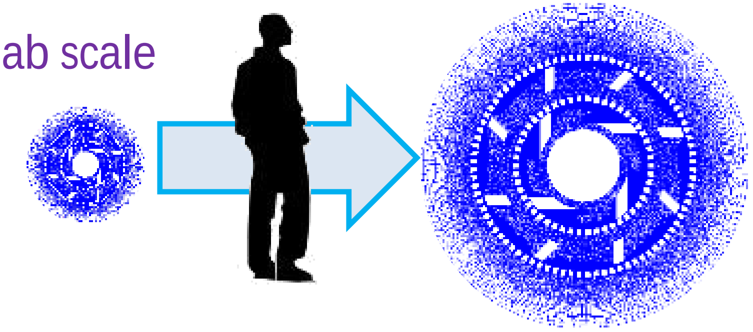
Quantify micelles growth, scission/recombination and surfactant intermicellar rates and branch-point formation free energy and mobility for the basic fluid and multicomponent mixtures



Development of continuum approaches

Viscoelastic computational fluid dynamics (CFD) model

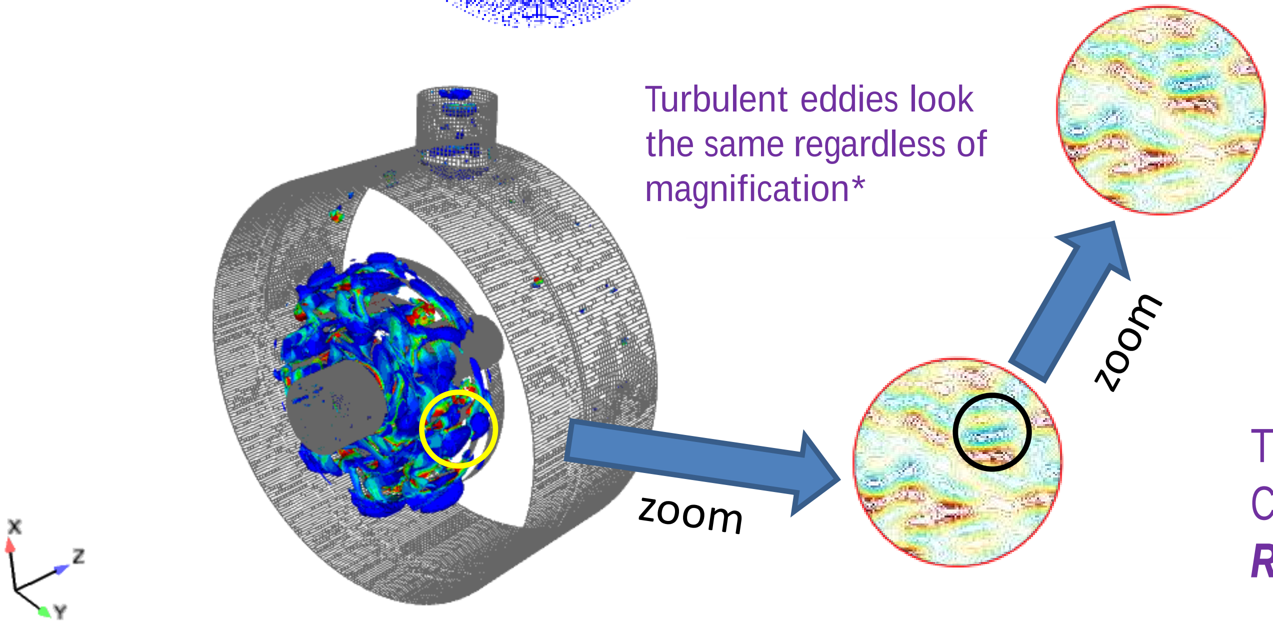
Challenges: (loss of) scale up



Industrial scale

Lab scale

Scale up historically relied on the *scale similarity* of turbulence



Turbulent eddies look the same regardless of magnification*

The turbulence is Characterised by a ***Reynolds number***

Traditional scale up = match Reynolds numbers

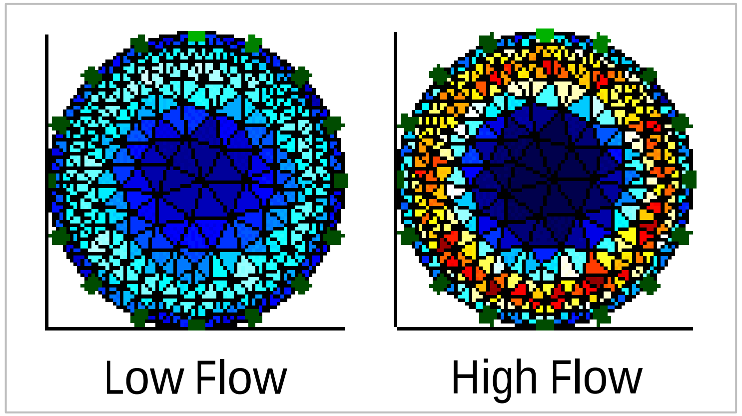
Process Analytics

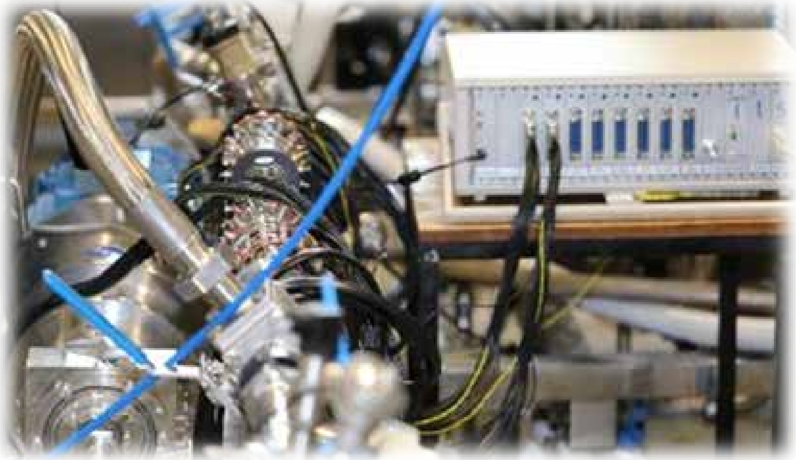
Requirement for accurate, real-time, in-line measurements at pilot and manufacturing scale – current off-line approaches inadequate

Increase capacity by eliminating slow off-line testing

Characterise product batch variability (e,g. between manufacturing sites or due to subtle changes in biosources/local raw materials)

Accelerate engineering design of processes and products through larger more relevant data sets (samples unchanged)

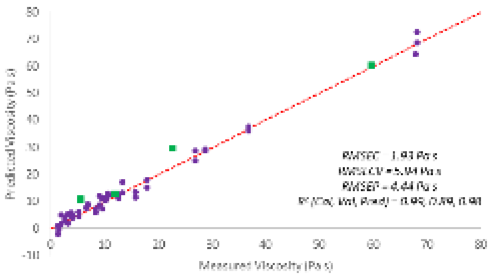




Process analytics - challenges

To provide a suite of in-line techniques to enable the rapid development and manufacture of new products

- Measurement in situ/in-line – how to get probes and sensors in to the vessels or pipes without disturbing the process
- How do we know what to measure?
- Matching accurate off-line approaches
- Moving from correlative approaches to process understanding
- Commercial off-the-shelf instruments often do not exist



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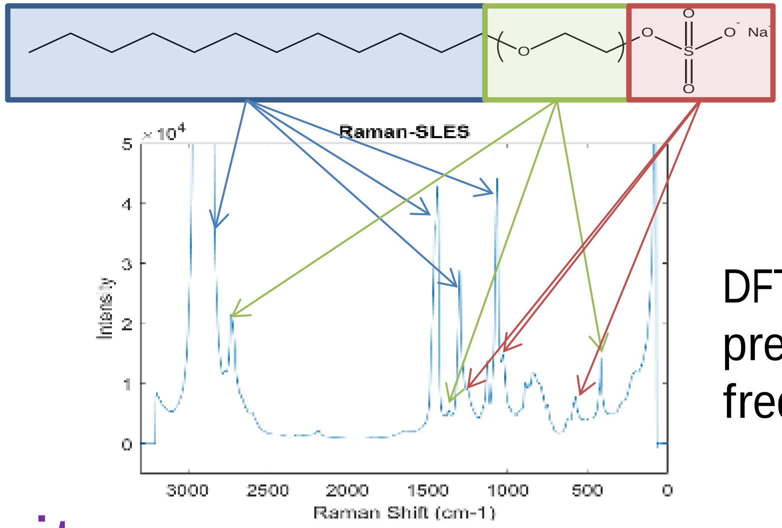
Process analytics - examples

In situ spectroscopy

Determination of SLES quality using spectroscopic techniques for adaptive predictive process control

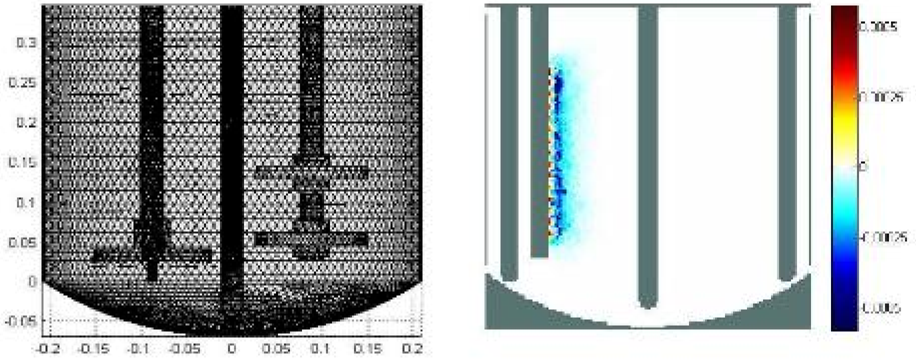


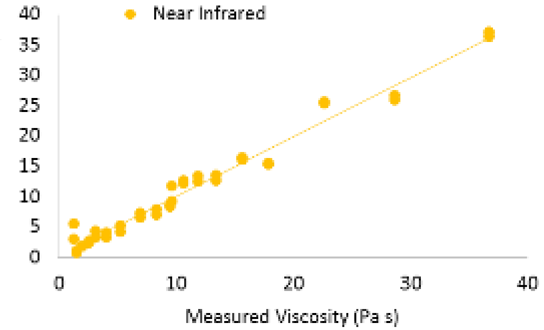
DFT Calcs predict vib freqs

Proxy measurements of viscosity

Near-IR, Mid-IR and Raman in situ spectroscopy

Electrical resistance tomography (ERT)





Partial-least squares regression models

Process Analytics

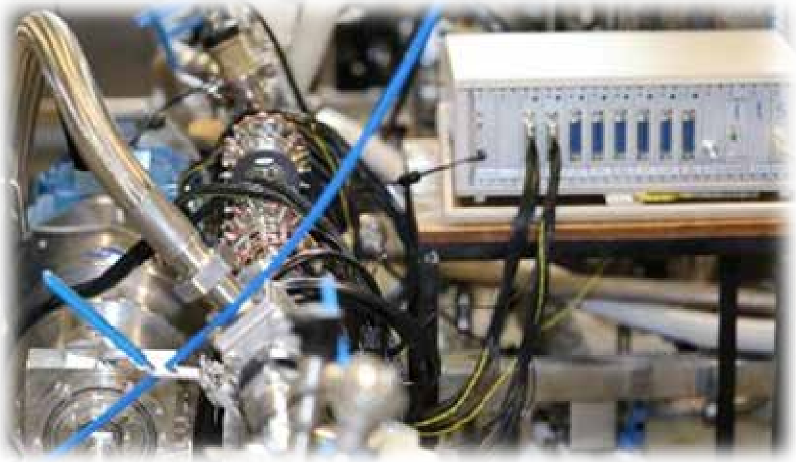
Accurate, real-time, in-line measurements at pilot and manufacturing scale.

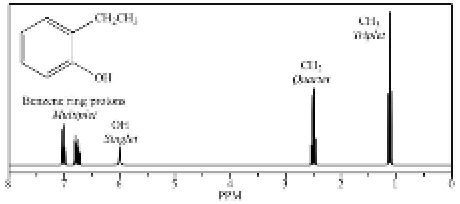
Sophisticated process analysers and low cost sensors

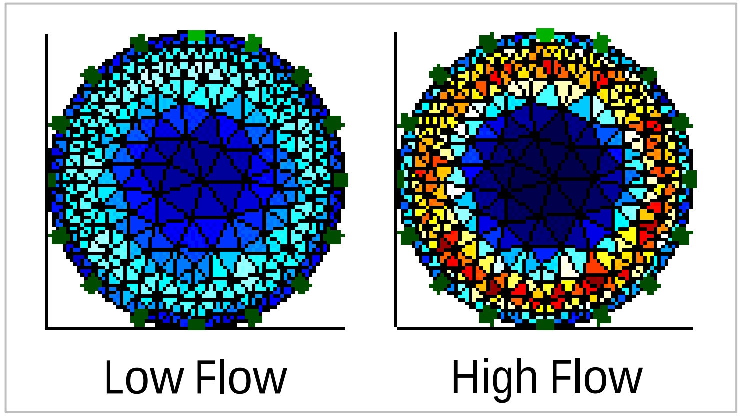
Validation of virtual process models

Measure critical parameters in manufacturing process

Big data







Low Flow

High Flow

Electrical Resistance Tomography (ERT)

Innovation Management and Behavioural Change

How to promote behavioural change within this new digital environment?

How can leaders can use digital information to make better, quicker decisions?

How to use *data visualisation techniques* and *data mining* to enhance knowledge sharing?

How to enhance the adoption of these technologies and facilitate the radical change in organisation and process of innovation within the company which is required for this new digital workflow?

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Thank you