# Digital in (CPI) Formulation


## Mark Taylor

Manager High Throughput, Informatics and Modelling


# Overview

**Brief introduction to CPI**

**CPI Digital Strategy**

**Digital Toolset & Infrastructure**

**Digital Design – Modelling, HTE**

**Smart Factory**

**So what's in it for me (you) ?**

**We help companies to develop, prove, scale-up and commercialise new products and processes**

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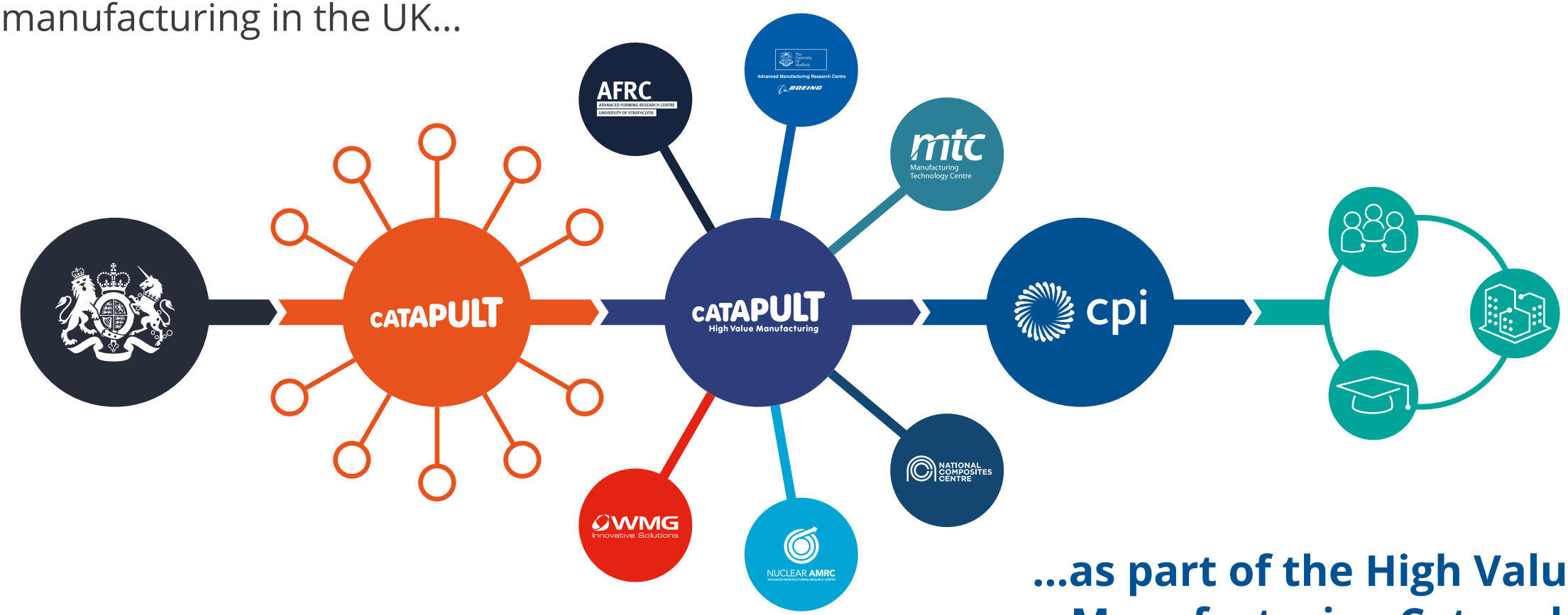
Supporting the growth and development of advanced manufacturing in the UK...




**...as part of the High Value Manufacturing Catapult**

# We help deliver, de-risk and accelerate...


# ...your concepts into successful products

# ...enabling companies in high value markets

Pharmaceuticals

Medtech

Agritech

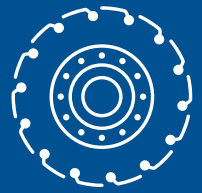
Food, drink and nutraceuticals

Fast-moving consumer goods

Logistics and packaging

Electronics

Energy



Automotive

Aerospace

Speciality chemicals and materials

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Biotechnology

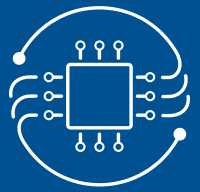
Biotherapeutics

Formulation and materials

Pharmaceutical processing

Photonics

Printed electronics



Flexible hybrid electronics

Digital

# ...with our expertise and core capabilities

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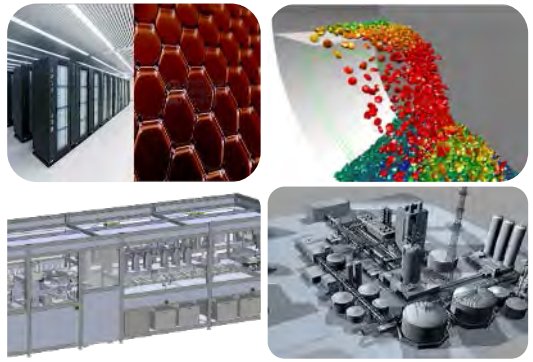
# CPI's Digital Strategy and Key Competencies

- What enables us to do our job better (faster, cheaper)
- What enables us to serve our customers better

- Enhancing our Operational Efficiency
- Building and Applying Capability and Expertise
- Developing a Digital Culture

## Digital Design

Modeling and Simulation of products and processes, Predictive Design,

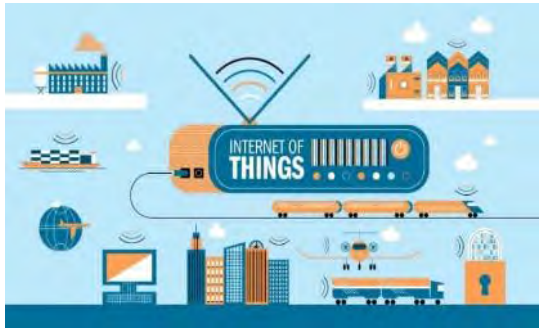


## Smart Factory

Digital Twin, Advanced process control, Smart Equipment & Robotics

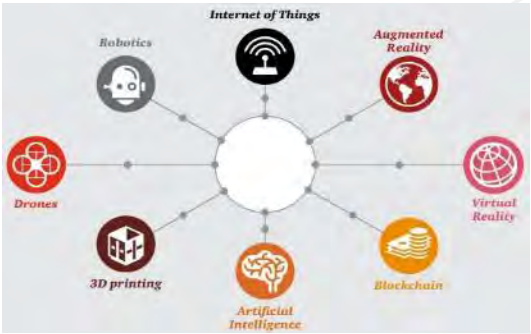
## Smart Connected Devices

Smart Packaging, Wearables, MedTech devices, Connected Supply Chain




## Digital Toolset

Infrastructure, tools and mindset




**Formulation, Biologics, Industrial Biotechnology**

**Medicine Manufacturing Innovation Centre**

**Electronics**

# Digital Toolset

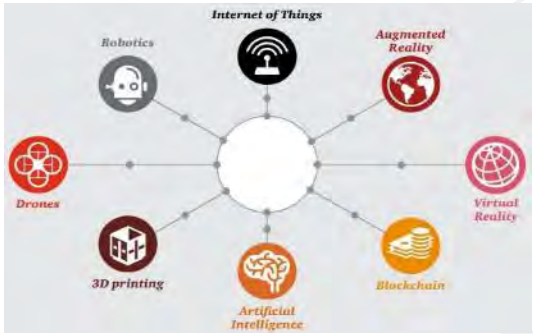
- ELN & lab data
- Structured data capture
- Controlled data analysis

| Digital Design | Smart Factory | Smart Connected Devices | Digital Toolset |
|---|---|---|---|
| Modeling and Simulation of products and processes, Predictive Design, | Digital Twin, Advanced process control, Smart Equipment & Robotics | Smart Packaging, Wearables, MedTech devices, Connected Supply Chain | Infrastructure, tools and mindset |



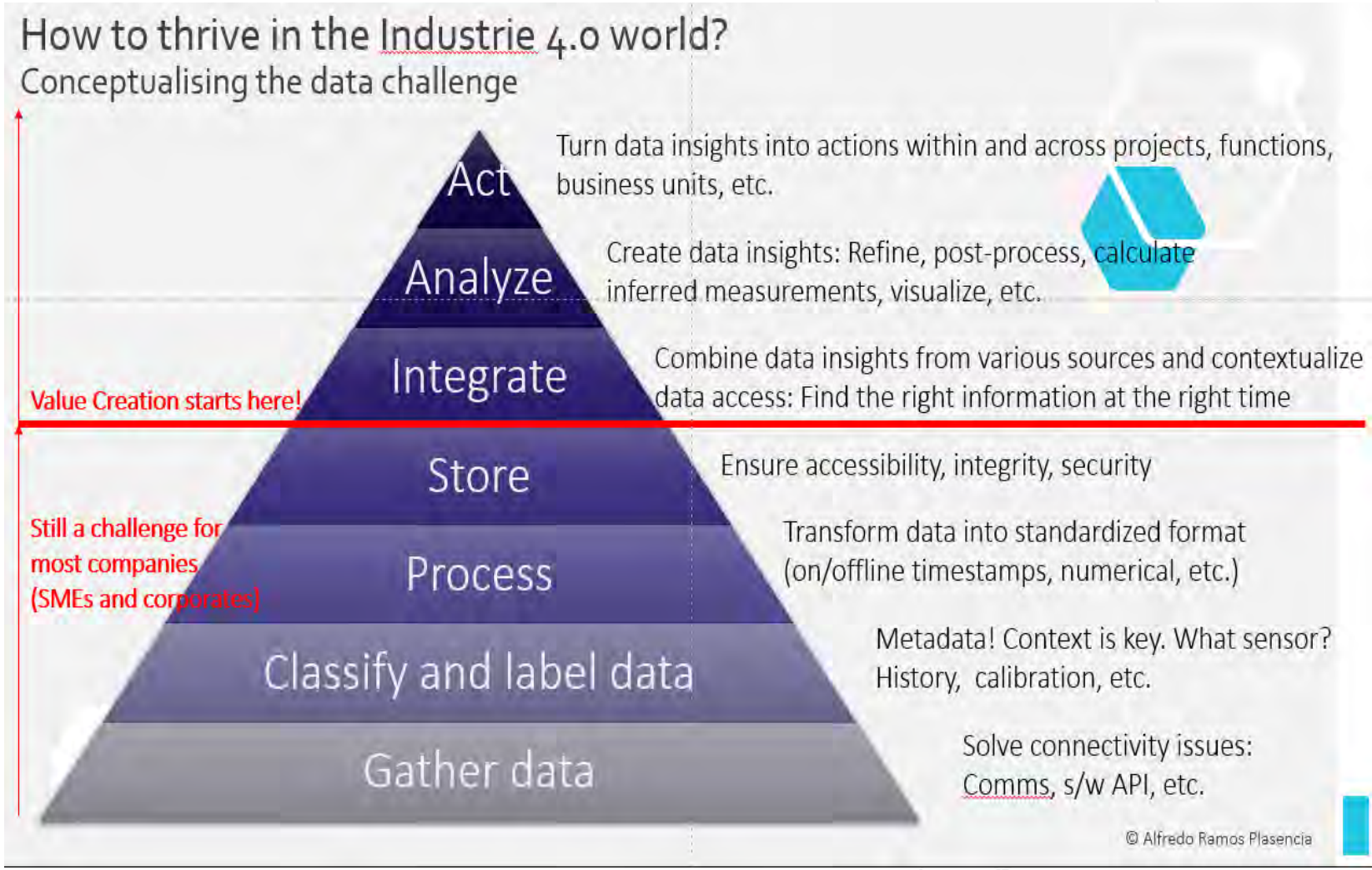




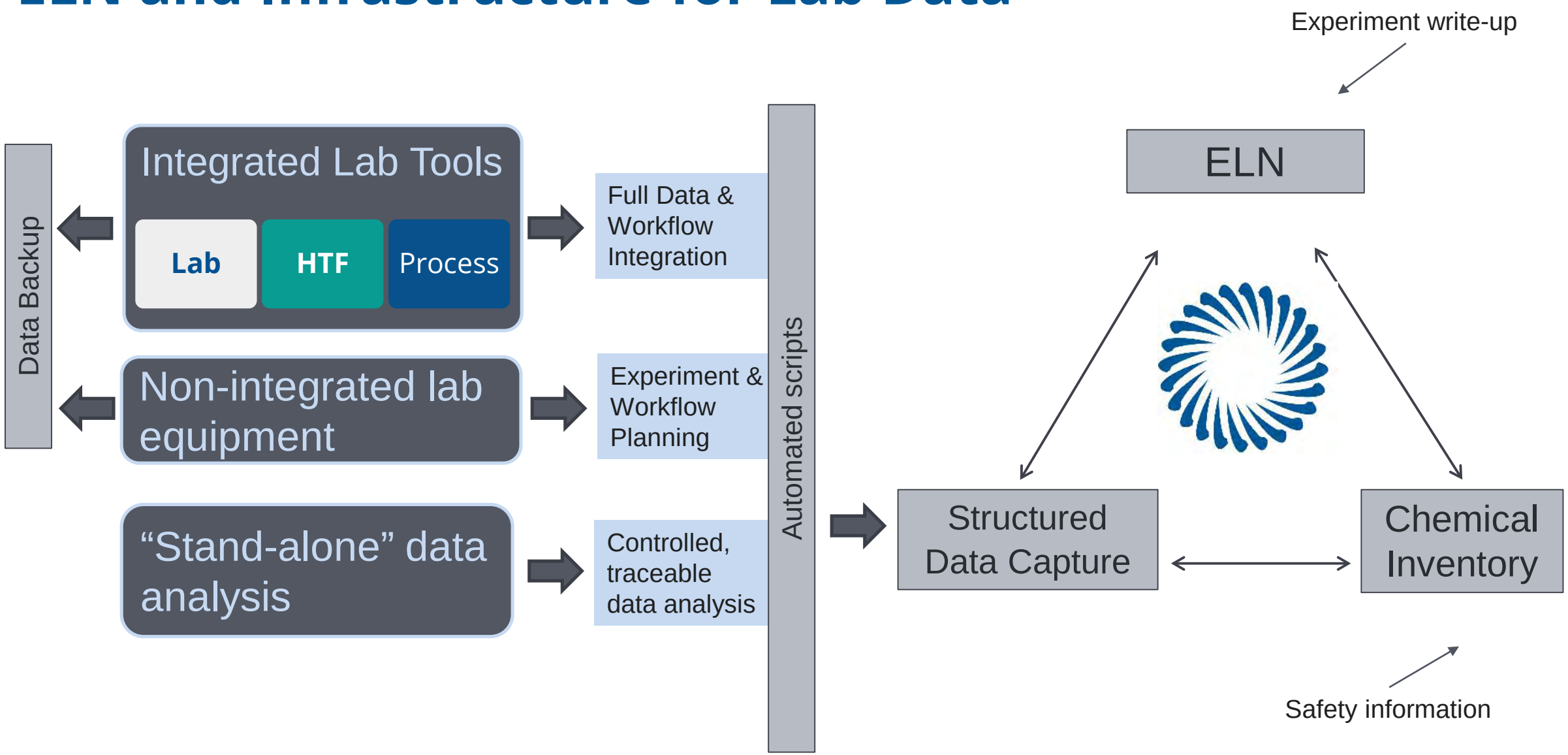
# Digital Toolset


By Androidmarsexpress - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=93026655




*With thanks to Alfredo Ramos*

# ELN and Infrastructure for Lab Data



# Structured Data Capture - Integration with HTE

Input parameters → Log file input to Chemspeed → Run Experiment → Runlog file uploaded to Integration → View standardised analysis → Validate data and save to EKB database → Pull data back into ELN for experiment write up

**Input Parameters**

Ingredients

## Method Comments:

Chemspeed Formax integration

## Planned Parameters

| Parameter | Fixed Or Variable | Value |
|---|---|---|
| Planned Vessel Temp (°C) * | Fixed | 67 °C |
| Planned Vessel Pressure (mBar) | Fixed | |
| Planned Stirring Rate (rpm) * | Fixed | 1000 |
| Stir Mode * | Fixed | Low |

## components

| Parameter | Component 1 | | Component 2 | | Component 3 | |
|---|---|---|---|---|---|---|
| | Fixed? | Value | Fixed? | Value | Fixed? | Value |
| Container (Value) * | ☑ | Edenor K 12-18 MY(C0( | ☑ | Ethanol(C000703) | ☑ | Lutensol® AO 7(C0007 |
| Dispense Type (Value) * | ☑ | Gravimetric | ☑ | Gravimetric | ☑ | Gravimetric |
| Dispense Weight (g) * | ☐ | 5 of 5 | ☐ | 5 of 5 | ☐ | 5 of 5 |
| Dispense Volume (mL) * | | | | | | Add |
| Required Temp (°C) | ☑ | 25 °C | ☑ | 67 °C | ☑ | 67 °C |
| Required Vortex 1 (rpm) * | ☑ | 1000 | ☑ | 1000 | ☑ | 1000 |
| Required Vortex 2 (rpm) | ☑ | 300 | ☑ | 300 | ☑ | 300 |
| Vortex Time (Mins) * | ☑ | 20 | ☑ | 20 | ☑ | 40 |

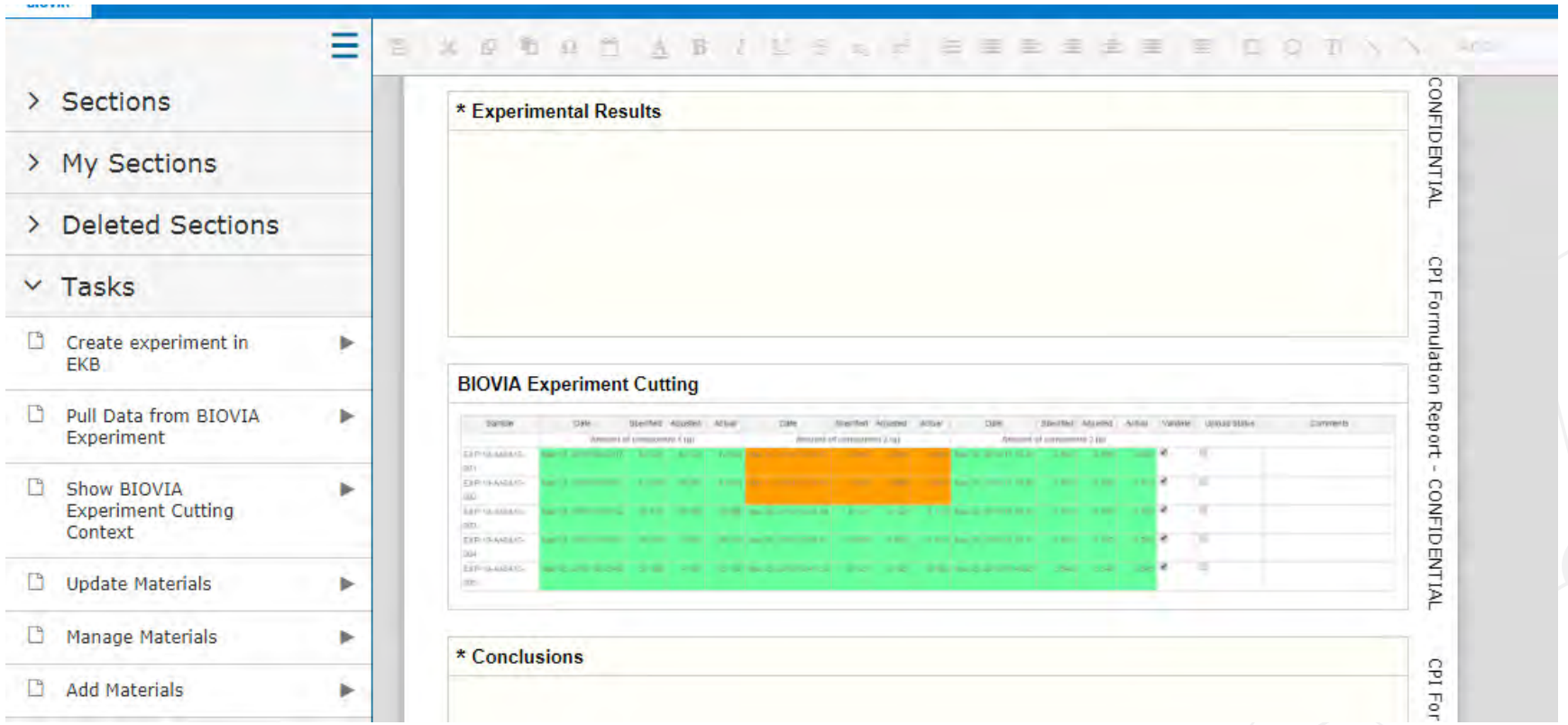
* Required Field
* Validation Rules Apply (hover mouse on parameter for details)

Recalculate Parameters

Save Details

# Structured Data Capture - Integration with HTE

Input parameters → Log file input to Chemspeed → Run Experiment → Runlog file uploaded to Integration → View standardised analysis → Validate data and save to EKB database → Pull data back into ELN for experiment write up



# Controlled Data Analysis



Standardised and automated data analysis methods

Saves data in structured format in searchable database

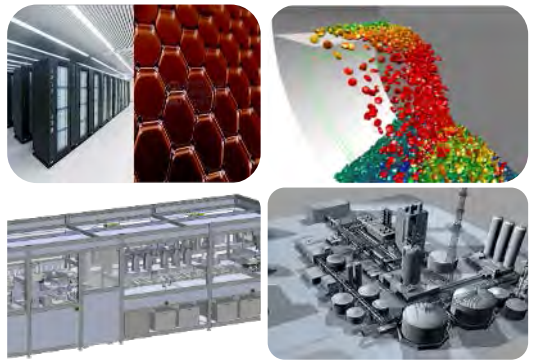
Use cuttings tool to return this analysis to the ELN

# Digital Design

- Modelling & Simulation
- Automated & High Throughput Experiments

**Digital Design**

Modeling and Simulation of products and processes, Predictive Design,



**Smart Factory**

Digital Twin, Advanced process control, Smart Equipment & Robotics



**Smart Connected Devices**

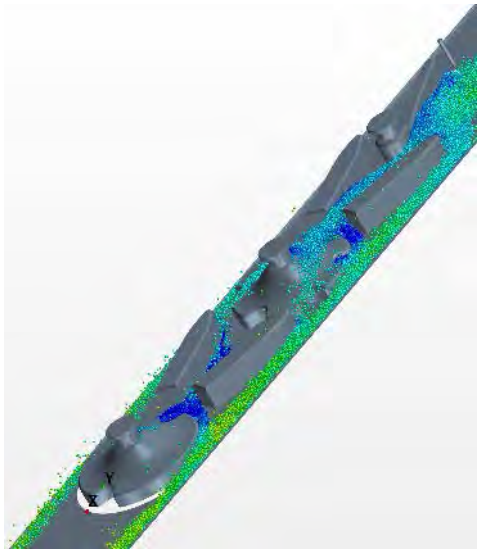
Smart Packaging, Wearables, MedTech devices, Connected Supply Chain

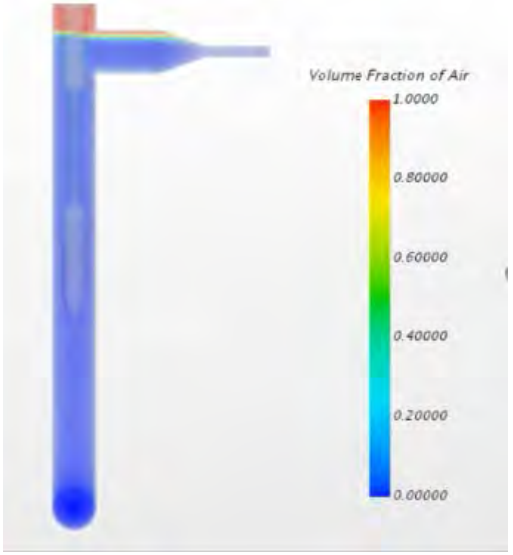


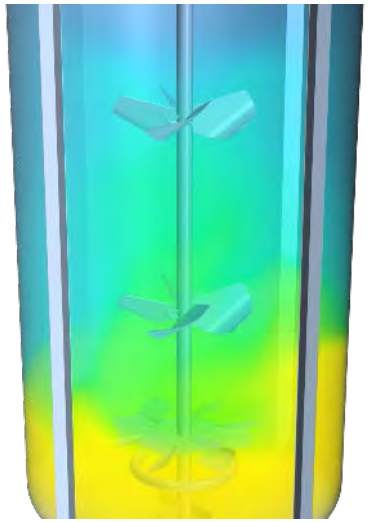

**Digital Toolset**

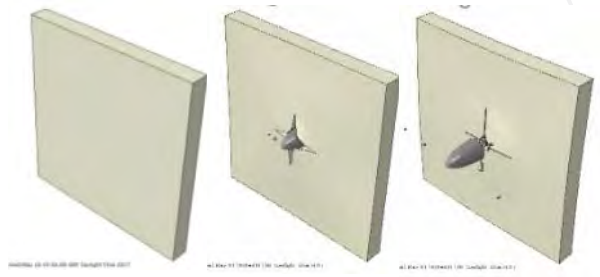
Infrastructure, tools and mindset

# Modelling & Simulation







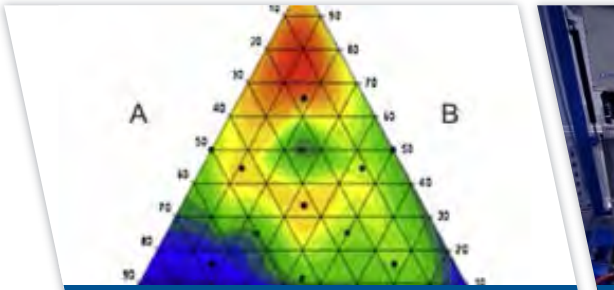
**Designing granular flow for PAT**

**Optimising flow around viscosity probe**

**Impeller design for batch reactor**

**FEA for mechanical properties**

# Versatile High Throughput Capability




Design

Make

Screening and Automated Characterisation

Application and Final Formation

## SECTOR WIDE COVERAGE FOR

Paints and Coatings

Home Care

Personal Care

Pharmaceuticals

**Supported by integrated informatics infrastructure**

# Capability and Upgrades

## CURRENT SWING

### Making simple formulations

Make and mix of simple formulations. **Broad category use:** for low viscosity liquid formulations eg. inks, home care, drinks, and agrochem.

**CAPABILITY**

- Dispense of mobile and viscous liquids; high shear homogenisation
- *Viscous liquid transfer, screw capping, heating, shaking, dispense of solids*
- *2 x increase in sample capacity*
- *Access hood (safety upgrade for solvent use)*

## CURRENT FORMAX

### Make and measure broader formulations

Make, mix and inline measurement of complex formulations (including time resolved processes). **Broad category use:** eg. reactive coatings, inks, batteries, home and personal care, food, adhesives, and composite resins.

**CAPABILITY**

- Dispense of all materials including molten waxes
- Heating, shaking vessels, Screw capper, vacuum
- In line measurement (rheology, NIR, PSD, pH, camera)
- Make or measure – not both simultaneously
- *Access hood (safety upgrade for solvent use)*
- *2 x capacity expansion of samples*

## SEPTEMBER 2020

### Capacity step change in making complex formulations

Parallel preparation/process understanding of multiple complex formulations for offline testing. **Broad category use:** across whole formulation sector.

**CAPABILITY**

- 4 x increase in capacity vs current Formax.
- All dispense capabilities, with expanded number of different materials
- Measurement carried out off line
- Free up current Formax to allow greater use as in line measurement platform

# Smart Factory

Testbeds for
- Model-based Process Control
- Process Digital Twins
- Sensor / PAT development

*"The smart factory is a flexible system that can **self-optimize performance** across a broader network, **self-adapt** to and learn from new conditions in **real or near-real time**, and autonomously run entire production processes."*

https://www2.deloitte.com/us/en/insights/focus/industry-4-0/smart-factory-connected-manufacturing.html

**Digital Design**

Modeling and Simulation of products and processes, Predictive Design,



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Digital Twin, Advanced process control, Smart Equipment & Robotics

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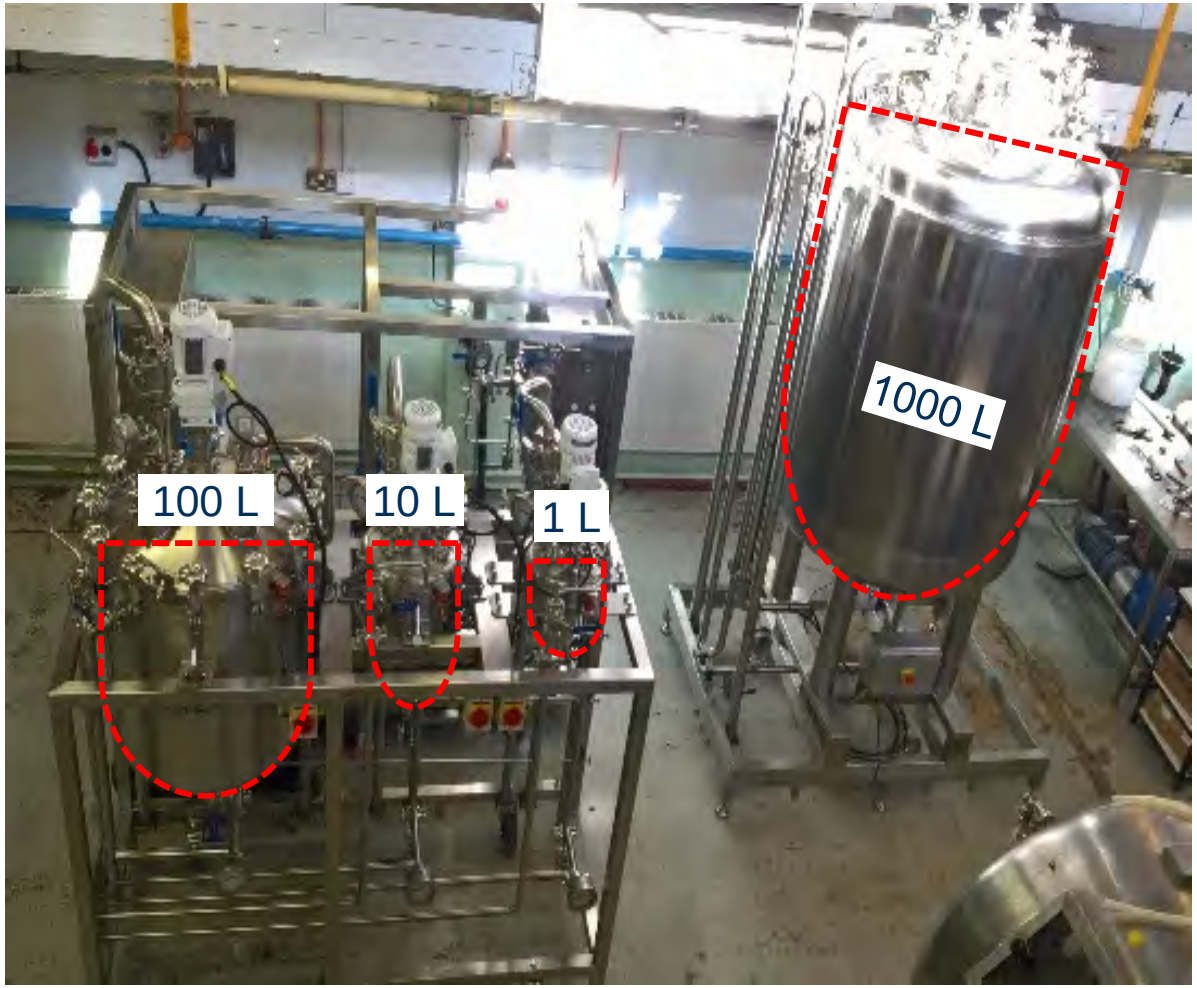
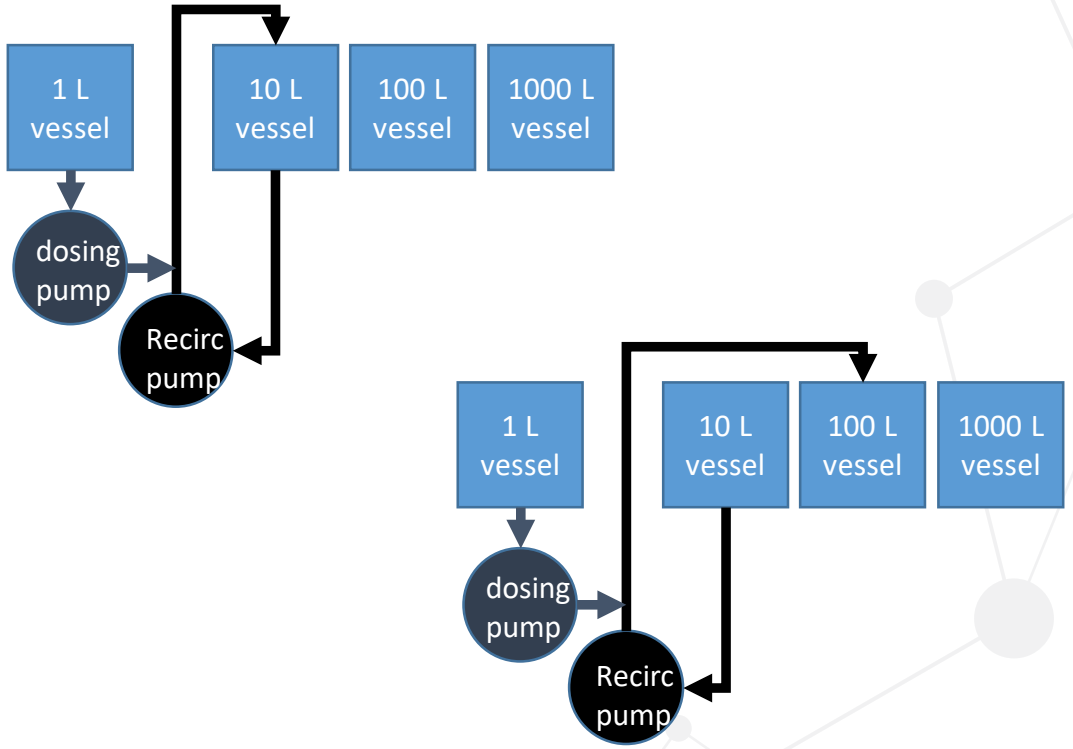
**Digital Toolset**

Infrastructure, tools and mindset

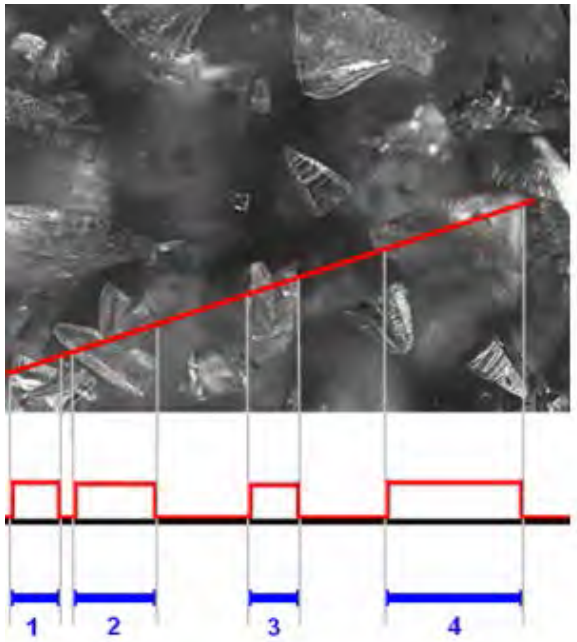
# Testbed 1 - Complex Liquid Processing & Scale-up




## Test Bed for Innovation in Liquid Formulation Manufacturability



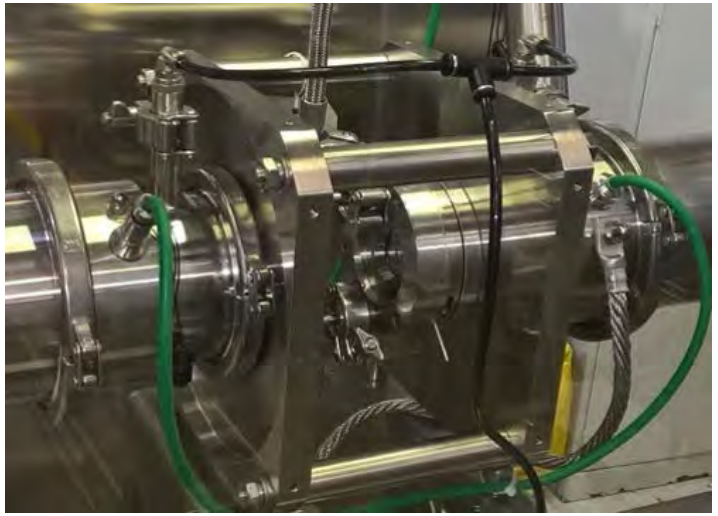
# PAT




**FBRM (particle size) and Particle Viewer (microscope)**

Chord length distribution and micrographs

FBRM measurement range : 0.5 to 2000 um



**Insitec ( laser diffraction )**

Quantitative PSD requires RI model

Low concentration (or dilution)

Measurement range 0.1-2500 um

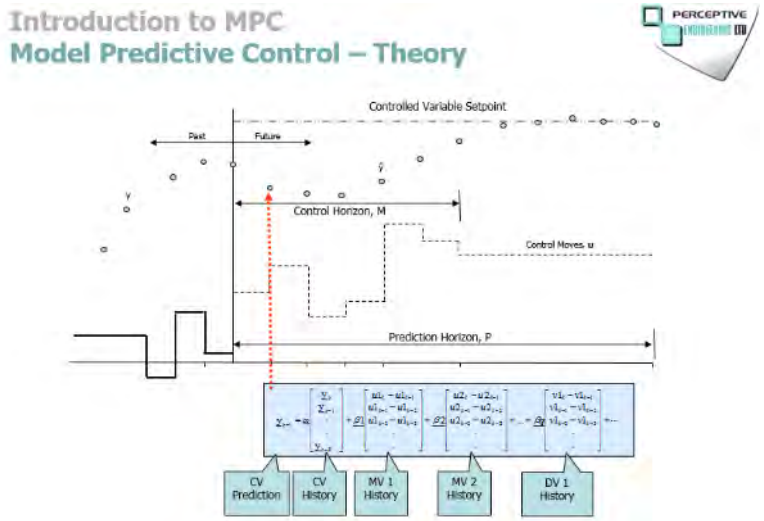
**In-line Viscometer**

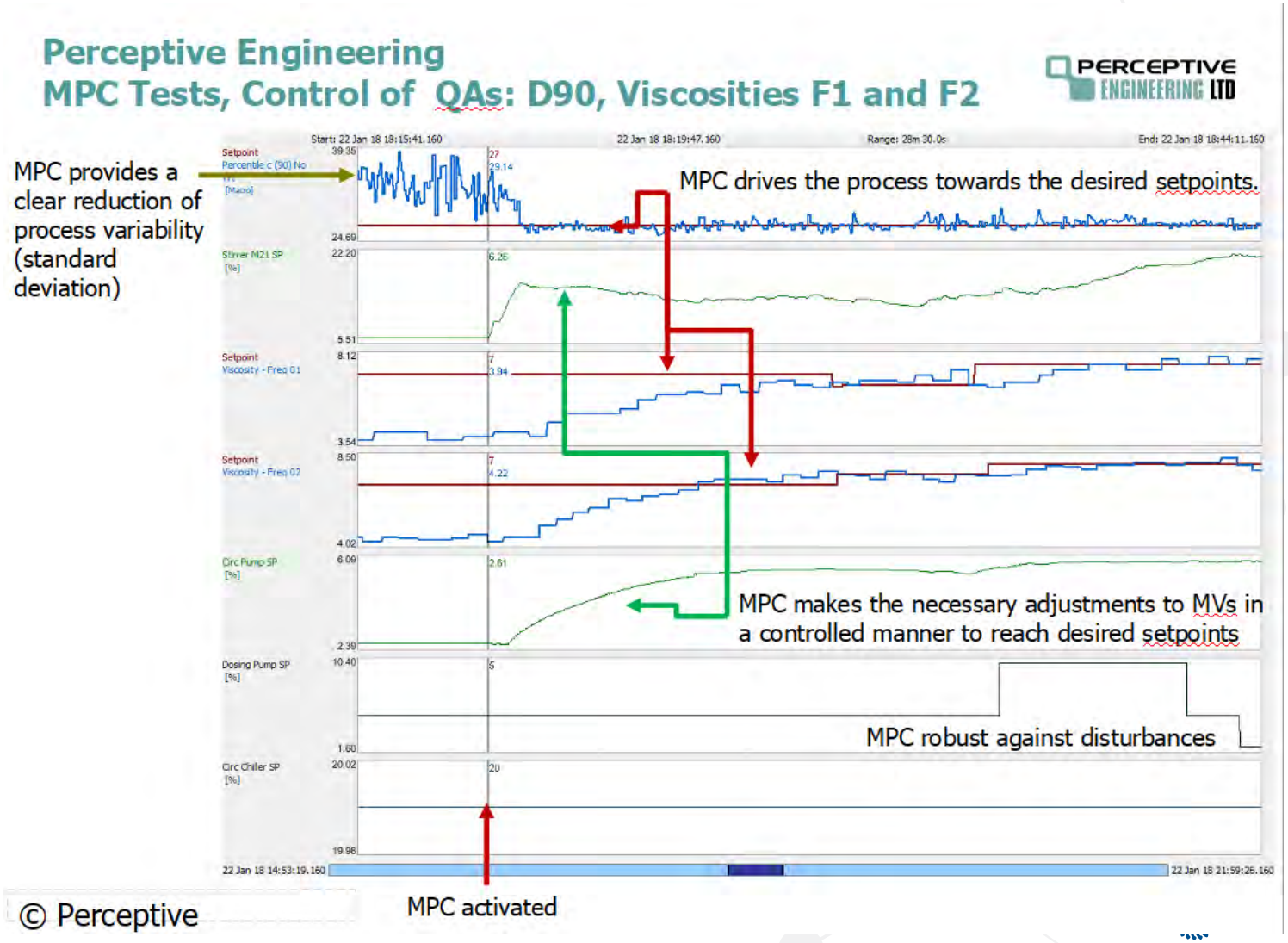
Operates 250 and 2500 Hz

Good understanding of flow field required for optimum results

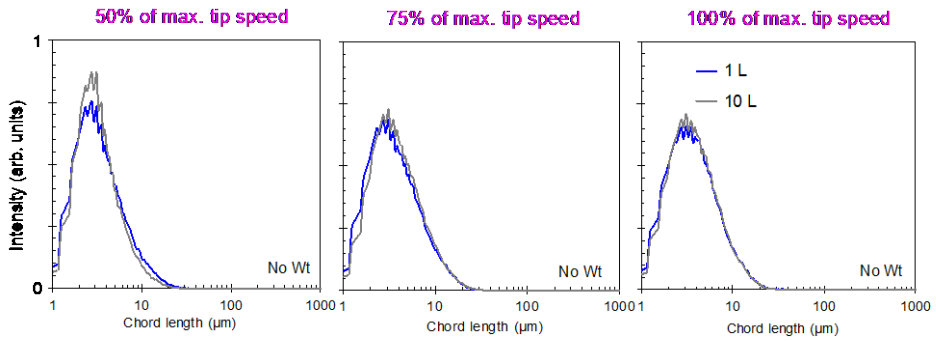
Range 1-100,000 cP

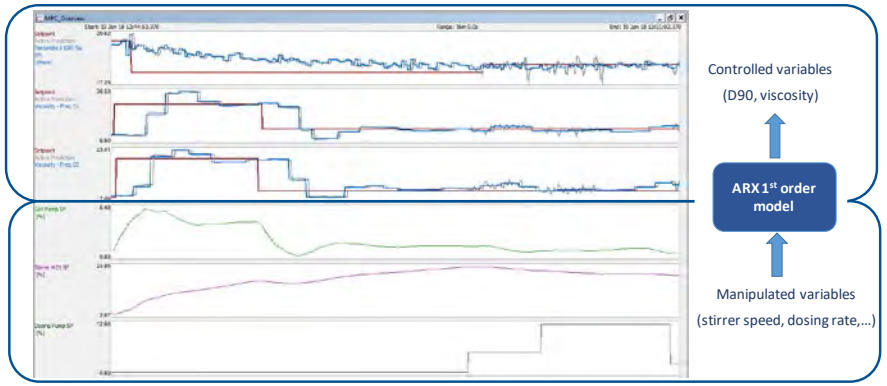
# Model Predictive Control

# Scale-up from discovery to pilot




## Test Bed for Innovation in Liquid Formulation Manufacturability

De-risk innovation by testing new manufacturing & sensor technologies at pilot scale prior to any capital investment

Rapid and robust process scale-up through smaller scale learning

Scaled-down formulation capability to efficiently test effect of re-formulation

Establish manufacturing control schemes – adjust process parameters in real time to narrow specification tolerances / limit off-spec product

# Testbed 2 - The twin screw granulator & PAT

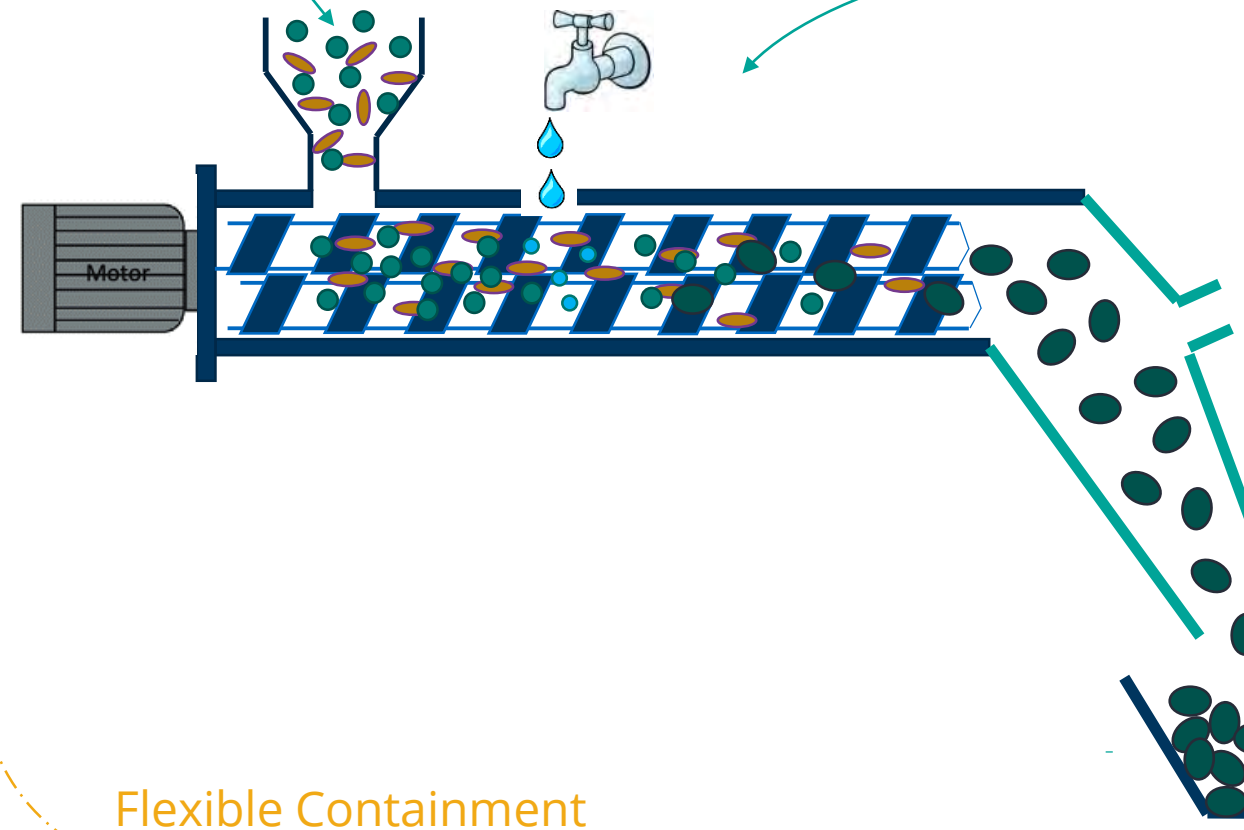
Characterisation

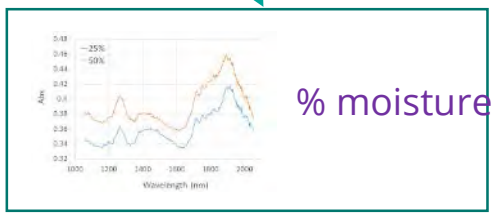
Model System API1
Formulated Blend

Advanced Process Control

Control Models

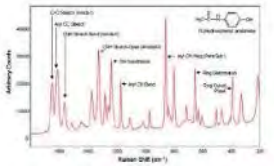
Calibration Models



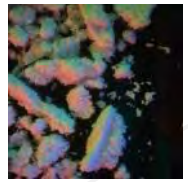



% moisture

PAT Probes



% API



PSD

Wet Granules

Dryer

Tablet Press

Dissolution Bath

Flexible Containment

Increase UK productivity in the manufacture of granulated products and to trial new manufacturing technologies

cpi

www.uk-cpi.com

# Testbed 2 - The twin screw granulator & PAT


## Multieye

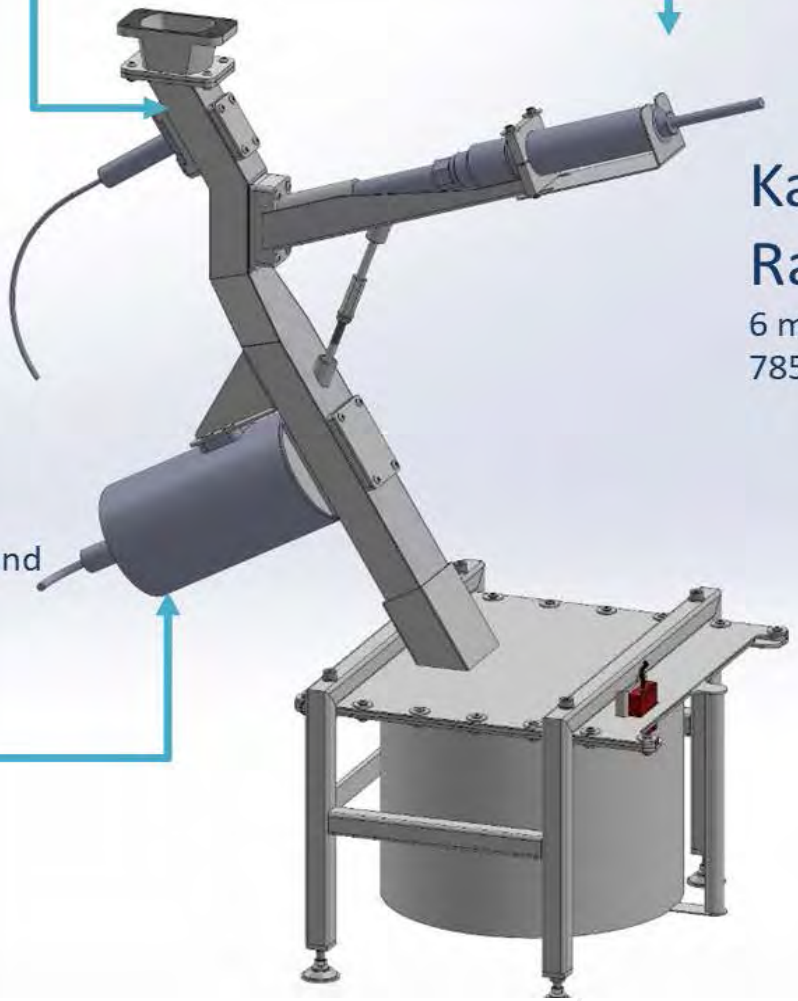
NIR probe from (Innopharma)

## Eyecon 2

Particle Size Distribution and shape analysis from (Innopharma)


## Kaiser Phat Raman probe

6 mm spot size and 785 nm laser



Increase UK productivity in the manufacture of granulated products and to trial new manufacturing technologies

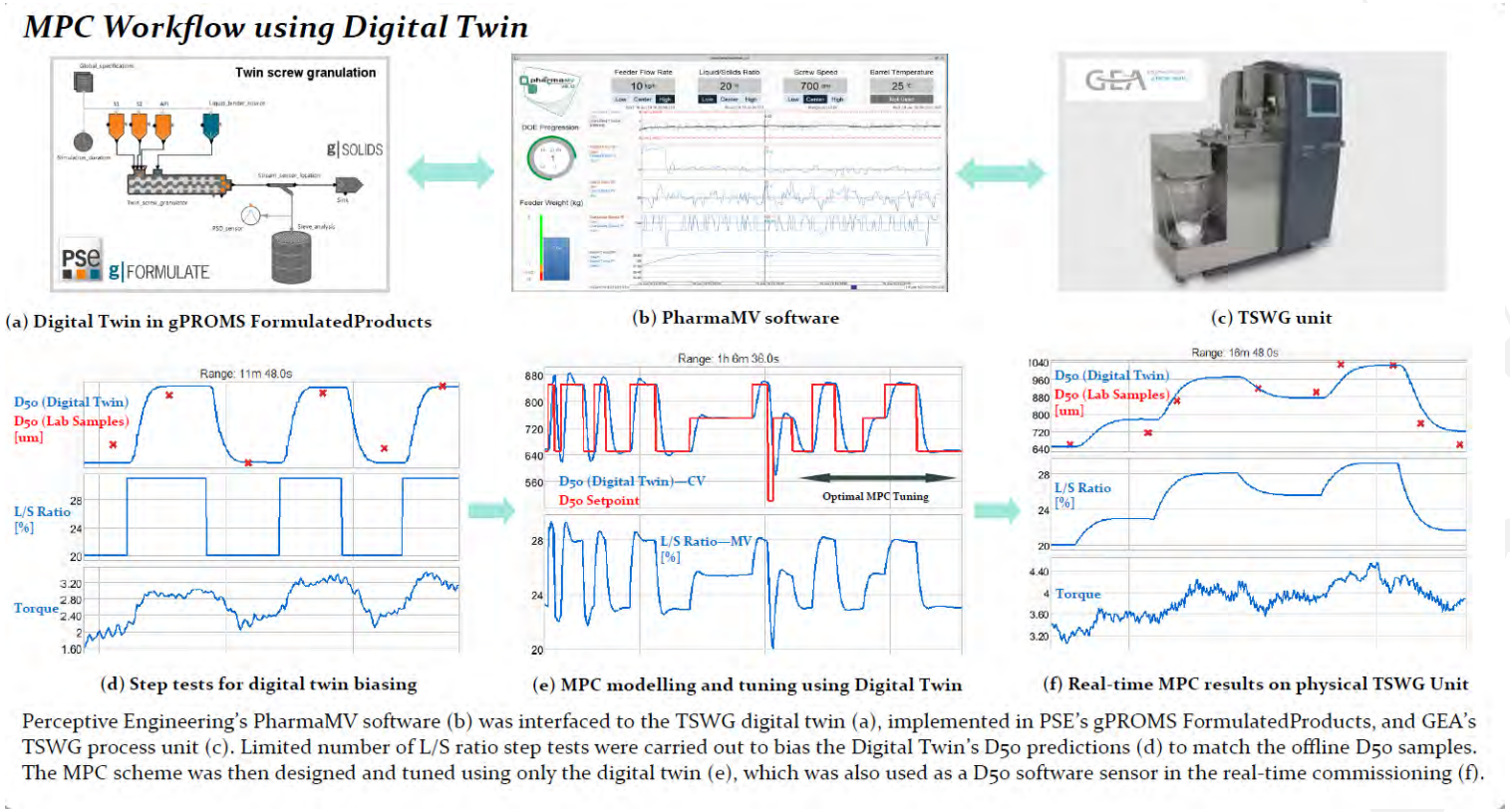
# Use of Process Digital Twin

An MPC Advanced Process Control system designed in-silico using a mechanistic model

The MPC and mechanistic model were transferred to a TSWG unit and used to predict and control PSD D50 in real-time

MPC scheme developed and tested in three trials with less than 10 kg of powder

Demonstration of how a mechanistic model can be used as a process digital twin to speed up controller design and reduce the experimental effort and cost




Perceptive Engineering's PharmaMV software (b) was interfaced to the TSWG digital twin (a), implemented in PSE's gPROMS FormulatedProducts, and GEA's TSWG process unit (c). Limited number of L/S ratio step tests were carried out to bias the Digital Twin's D50 predictions (d) to match the offline D50 samples. The MPC scheme was then designed and tuned using only the digital twin (e), which was also used as a D50 software sensor in the real-time commissioning (f).

# Acknowledgements


## Digital Strategy

Graeme Cruickshank, Anand Pogul, John Carroll

## Digital Toolset

Rachel Findlay, Alfredo Ramos

## Digital Design

Alex Smith, Kristi Potter, Paul Dooling, Lynn Donlon, Adam Todd, Jodie Clark

## Smart Factory

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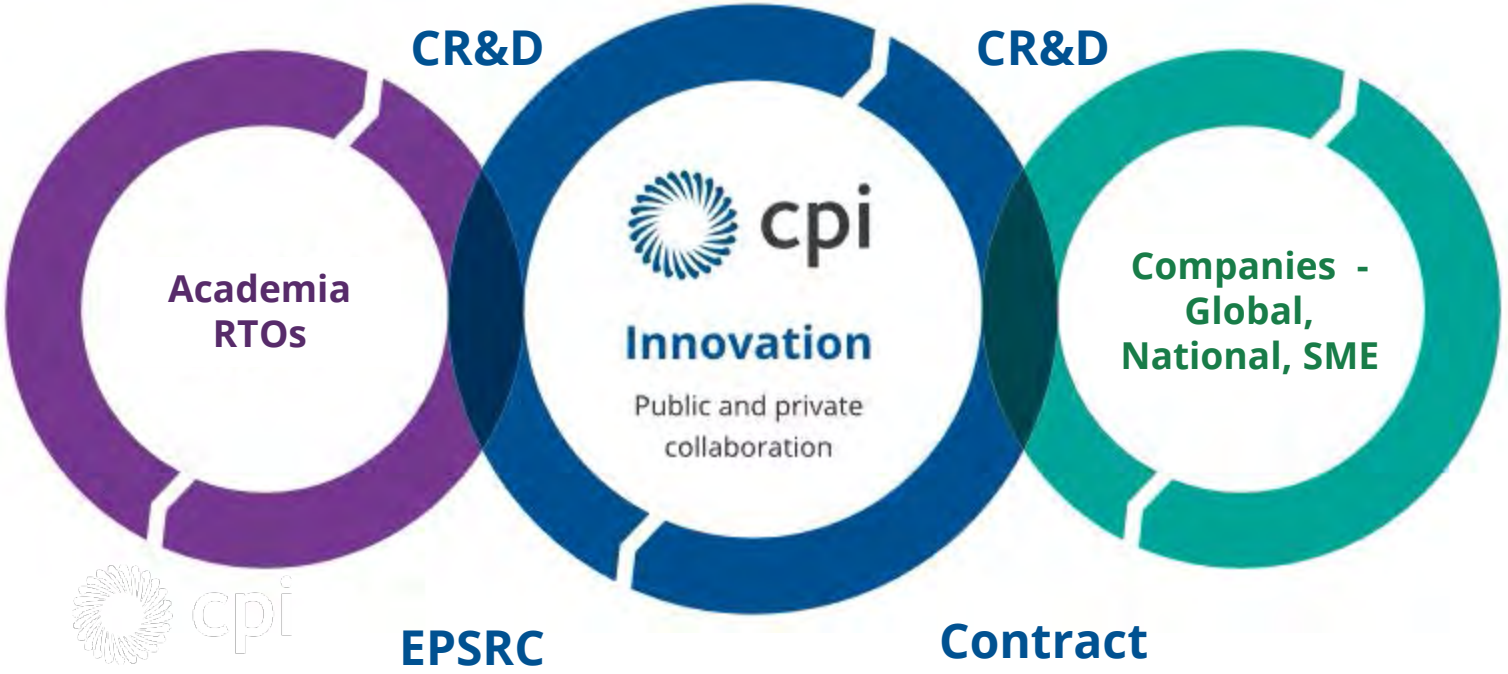
# So what's in it for me (you)?

ERDF
- ForTAmP - https://www.uk-cpi.com/fortamp
- PROSPECT



# Thank you

For more information visit **www.uk-cpi.com**

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