



# The National Formulation Centre





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Technical Strategy Director, Formulation; CPI

# Formulation (Integrate to Deliver Surprising Benefits)



Formulation, the creation of multi-component, multi-phase products, is an **enabling capability** 

Creating value through intricate microstructures and powerful ingredient synergies

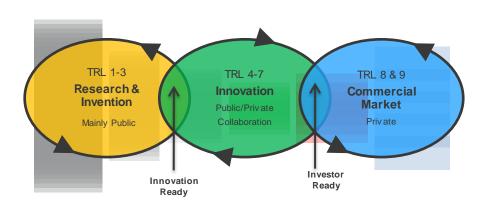
Underpins many **sectors** in our economy and **high-value manufacturing** industries globally.

The formulated products market in the UK is worth around £180 billion per annum with a potential for companies in emerging overseas markets of around £1,000 billion per annum



# UK Formulation Industries Connecting the Ecosystem



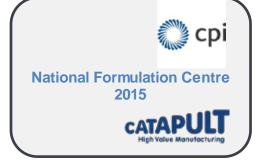




EPSRC

Engineering and Physical Sciences
Research Council

Future Formulation of
Complex Products 2015





# The National Formulation Centre - Overview



Create value for UK-based companies through formulation science by enabling bigger, cheaper or faster innovation

**Productivity from value-creating strategic alliances** with industry and the wider UK formulation eco-system (inc SME/supply chain and Knowledge Base (Academic) partners)

Create and use an **industry-led portfolio of advanced capabilities**. Sweat the UK assets by best harnessing current capabilities and then plugging any critical gaps identified

Sustainability from enduring access and application of advanced capabilities

# Formulation Lighthouse Vision 2030



**Productivity** and **Simplification** in Innovation by Predictive Design

Ultimately created **autonomously**, from selflearning, IoT connected systems

> **MORE ROBUST** UNDERSTANDING OF **COMPLEX SYSTEMS** TO ENABLE MODEL **DEVELOPMENT**

- SOLIDS
- LIQUIDS



- INNOVATION FFFICIENCY
  - PRODUCTIVITY
  - R&D SIMPLIFICATION



**AUTONOMOUS LEARNING WITH** SYSTEMS IOT ENABLED TO FORMULATE AGAINST REAL **NEED/CONDITIONS** 



**DEVELOP TRULY** 

**DELIGHTFUL PRODUCTS IN FUNCTION AND DESIGN** (STEM TO STEAM)

CuppaTea







**CURRENT ART OF** 

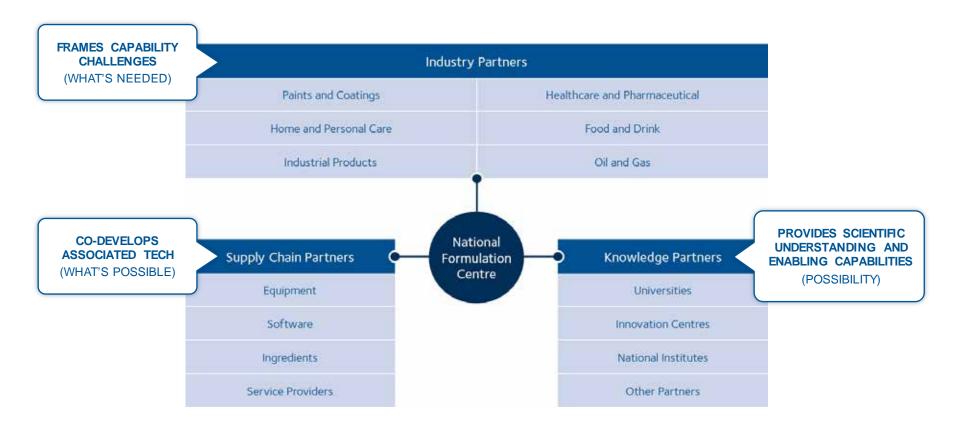
**FORMULATED** 

**PRODUCTS** 



# Structure – Activating the Innovation Eco-system





# Potential for UK Leadership in a Global Capability Race



| Past      | 2014                  | 2017                                  | 2020 | 2025                | 2030 |                         |
|-----------|-----------------------|---------------------------------------|------|---------------------|------|-------------------------|
| Empirical | Semi-empirical        | Predictive (Sub-systems)              |      | Predictive (System) |      | Formulation<br>Maturity |
| Data-poor | Data-rich             | Information-rich                      |      | Knowledge-rich      |      | Knowledge<br>Intensity  |
| "Experts" | Fragmented<br>Systems | Connected Systems / Data<br>Standards |      | Closed-loop Design  |      | Knowledge<br>Capture    |

### **CPI National Formulation Centre**

Transforming formulation from art to science, faster

- Transformation potential through advances in enabling technologies such as informatics, modelling, measurement and sensors (Telemetry), and automation robotics
- Faster progress through integration model

# Capability Themes to Work Against

Revalidated by Industry Steering Group (ISG)



# **Predictive Designs**

### **Faster Innovation**

Faster, more reliable approaches to get to ideal formulation design

## **Radical Effects**

## **Bigger Innovation**

Unexpected synergistic effects to deliver bigger/disruptive benefits

# Manufacturability

## **Process Innovation**

Optimised, reliable system to guarantee ideal formulated product delivery

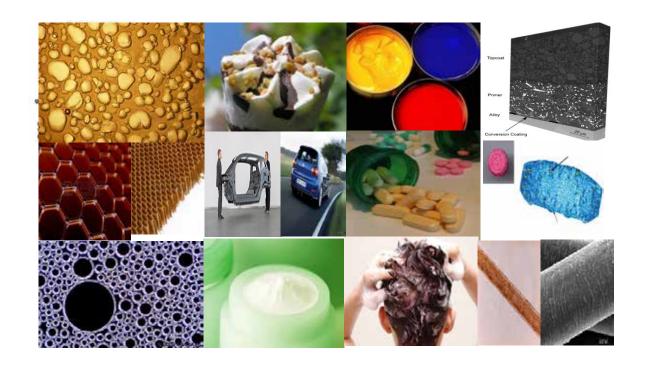
# **4IR Capable**

## **Innovation Enabler**

Critical foundational component for knowledge management and connectivity

# Formulations operate at different length & time scales to deliver required functional effects

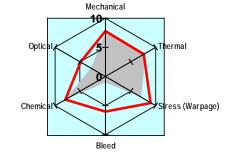




# Formulation and Product Development

#### **Functional Properties**

Mechanical, Surface, **Electrical, Optical, Thermal** Chemical, Biological, Sensory



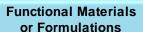
**Final Form** 

**Primary** 

Structure

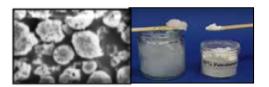
**Increasing comlpexity Secondary** Structure

Material in End-Use











# Functional Requirements - Coatings

## **Appearance**

Colour, texture, opacity

## Stay Clean

Antibiofouling, antibacterial, appearance

## Thermal Management

Heat protection, efficient energy coupling

#### Structural / Mechanical

Anti scratch, non cracking etc.

#### **Protective**

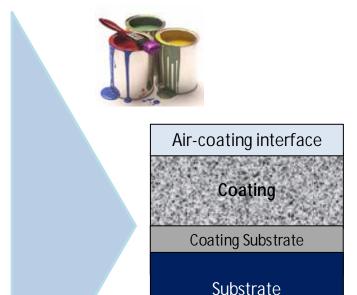
Anti corrosion, packaging, chemical resistance

## Electrical / Magnetic

EM, shielding, transmission

## **Extended Durability**

Light Stability, weatherability





## **Uncured Coating Properties**

Rheology

Wetting behaviour, surface tension Shelf life, colloidal stability

Thermal stability

Appearance

Reactivity, cure behaviour

## **Surface Properties**

Light reflection

Hardness

Scratch resistance

Friction/surface roughness

Repellent properties

**Erosion resistance** 

## **Bulk Coating Properties**

Opacity

Colour Flexibility

Barrier

Chemical resistance

Environmental resistance

## **Coating Substrate Interface**

Adhesion

Durability

Anti corrosion

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# Microstar: Microfluidic Platform for prediction of stability and rheology of complex fluids



# INTEGRATED LIQUID STABILITY AND RHEOLOGY PREDICTION TOOLKIT

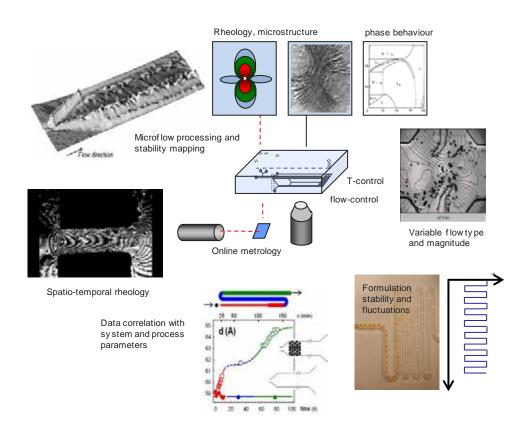
- Novel micro-flow methods for rapid screening of phase and metastability with relevant process variables
- Accelerated ageing tests; structural/dynamic metrology
- Cross-sector open-access test rig (Research Infrastructure)

# PHASE BEHAVIOUR/STABILITY MAPS OF COMPLEX MODELS AND REAL-WORLD SYSTEMS

- Generic open-learning
- Company-specific private-learning

#### **PARTNERS:**

P&G, BP, Imperial, Durham



# PROSPECT: Proving of Real-wOrld Scalable

PrEdiCtive Tools / Technologies



#### LIQUID SCALE-UP LEARNING LOOP

Simple, flexible, multi-scaled rig to screen/trial sensor and control scheme technologies

#### ASSOCIATED MODEL LIQUID FORMULATION

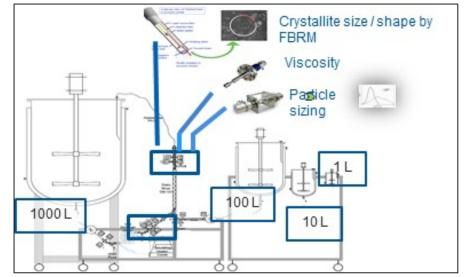
Enables closer to real-world studies - complex material structures and properties.

#### PLATFORM TO IDENTIFY PROXY MEASURES

To enable cost efficient and operator friendly process sensing upgrade – cheap, 24/7, widely adopted, info-rich sensing.

#### **PARTNERS:**

Birmingham, Leeds, Edinburgh







# Implementation of Particle Models for Industry





















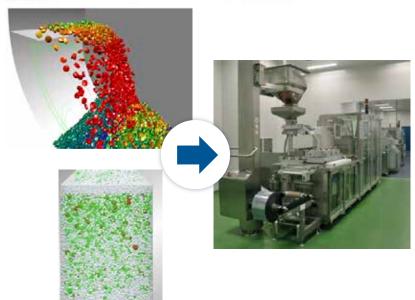
Currently major capability gap to transfer models from Academia to Industry.

#### METHODOLOGY AND FRAMEWORK FOR TRANSLATING MODELS TO INDUSTRY

Wet granulation case study which will fit as a tool within CPI- Chariot granules facility

#### METHODOLOGY /BEST PRACTICE GUIDE AND SUPPORT NETWORK CAN BE APPLIED TO OTHER MANUFACTURING PROCESSES

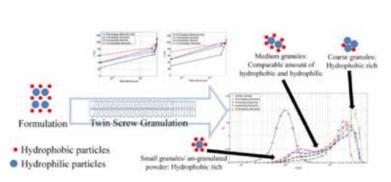
- Driving step-change modelling adoption
- Complement commercial vendors
- Creating UK hub for model commercialisation and in-slico development



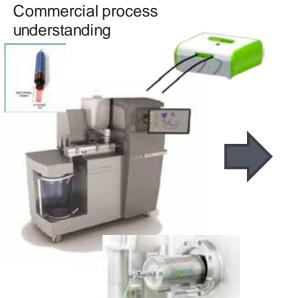
# Innovation Knowledge Flow



Mechanistic insight, modelling, analytical and process innovation



Yu et al; Int. J. Pharm. Sci. 475(1-2) (2014) 82-96



CPI Test Bed

Commercial Process
Development

Commercial control strategy



Pharma & CMO
Commercial
Manufacture

Academia

Discovery & Understanding

# Formulation - What next?



By 2020, 7.7 billion people will be online, 6.1 billion will have smartphones, 200 billion things will be connected to the Internet, and everyone on earth will have one thing in common.

## **Drivers**



Increasingly Digitally enabled world



Reatime Feedback on Product Performance



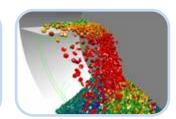
Increased Personalisation



Sustainability/ Regulatory



Computer Designed molecules & materials



Need for Predictive Models to rapidly get to best formulated candidate systems



Integration of
Characterisation and
HTE formulation for
verification of
candidate formulation
performance



Digitally enabled flexible manufacturing

Tuesday, 30 May 2017

# Dynamic Adaptive Product Design: Formula design to real world performance: Automotive Lubricants



## **Product Model**





Real time
Monitoring learning real
conditions















# Digital Engineeringand Manufacturing Leadership Group

1 December 2016

















# **The Working Groups**







Implementation





Skills, Work and Society



Cyber-Security and Legal Aspects



# The Real Challenge for Formulation Product Development & Manufacturing

- Data Space is vast not tractable even with HTE
- Need Predictive Models that allow rapid selection of candidate systems
- Information about ingredients and their relevant chemistry/material properties is linked to formulation data
- Experiments are designed to reveal fundamental science and inform models
- Informatics is used to recognize clues hidden in the data that contain real learning
- Discovery properties are scalable into flexible manufacturing processes
- We make a conscious effort to move the state of the art forward in a way that adds real value to companies and the way they approach formulation