Innovation 4.0 - Digitalised R&D in the chemical sciences

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About Us

Innovate UK KTN exists to connect innovators with new partners and new opportunities beyond their existing thinking – accelerating ambitious ideas into real-world solutions.

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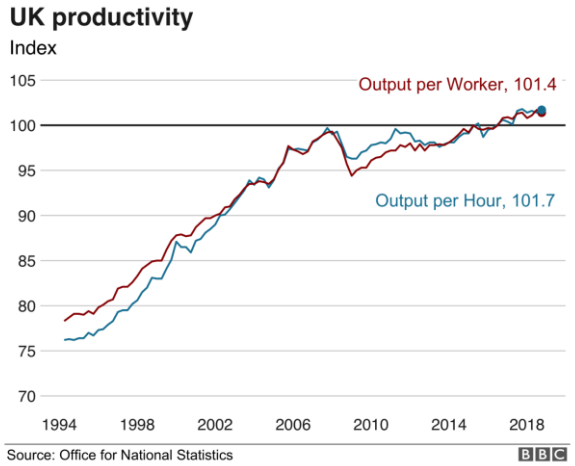
Background

- Digitalisation is a “megatrend” for various industries including chemicals, materials, pharma and formulation – “Industry 4.0”
- A large amount of reference material and literature is available for Industry 4.0 as applied to manufacturing activities
- Less available is reference material specifically addressing the Industry 4.0 opportunity for lab-based R&D and scale-up activities
- Innovate UK KTN is socializing the concept of “Innovation 4.0” to carve out this particular opportunity in lab-based R&D
- One tool we have developed to help in this regard is a Digital Maturity Framework for R&D (co-developed with the Materials Innovation Factory, University of Liverpool)
- This framework we hope will make it easier for R&D organisations to understand the opportunity, define their ambition and develop tailored digitalisation roadmaps



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Outline

- Innovation 4.0 Challenges
- Digital Maturity Framework
- Innovation 4.0 playbook
- IUK M&M team “Reimagining Materials and Manufacturing” vision
- Resource Efficiency for Materials and Manufacturing (REforMM) funding
- Funding through CLIMATES
- Funding related to ”AI solutions”
- Funding through the KTP scheme
- Funding through Smart Grants

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Challenges in R&D digitalisation

1. R&D Companies are at various stages of a digitalisation “journey”, and each journey is unique to that company (although there is some commonality in the workflows, processes and technology used). The appetite for digitalisation also varies depending on the awareness of what is available and achievable and the attitude to risk.
2. Companies do not have a central source of info or guidance when it comes to digitalisation. Many R&D managers use a mixture of internal expertise, external contacts in academia, consultancies and known solution providers. This fractured approach may be reducing the scale and speed of digital adoption.
3. It is challenging to demonstrate the benefits of digitalisation and build compelling business cases that can drive adoption. Becoming more digital requires capital expenditures (physical kit, software, and staff training) and hence strong business cases for change. IT departments tend to be risk averse and senior management often prioritise short and medium term payoffs.

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Challenges in R&D digitalisation

4. There are high-level challenges that cannot be fully addressed by individual companies (e.g. standards for data production and storage, centralised quality-controlled curation, data sharing etc.). R&D companies appear to be relatively open to the idea of common databases as long as competition concerns are addressed, but this requires a separate organisation to host and manage it.
5. Some technologies need to be developed and adapted for increasingly complex materials and products. This will require a multitude of collaborative effort between R&D companies and solution providers.

Digital Maturity Framework for R&D

LEVEL	Physical experiments	Virtual Experiments	Analytics
Level 0	Experiments are run by hand, with conditions and results recorded by hand or written to local data files which remain distributed on individual machines or notebooks. Only simple office software & file storage methods are used.	Minimal, if any, use of simulation and modelling techniques for generating an understanding of the material/chemical/formulation properties.	No deployment of AI or ML methods on data. Only simple offline analysis tools are used. Design of Experiments (DoE) methods are underutilised.
Level 1	Direct Digital Capture of information from manual workflows to a secure repository. Experiments are run by hand, but conditions and results are automatically recorded and stored in a central, secure repository, allowing enhanced access. (IoT, data loggers, sensors, integrated lab notebook systems).	Some use of simulation and modelling techniques for understanding the material/chemical/formulation properties, but manually executed and/or conducted on a project-by-project basis. No direct integration with lab data.	Simple, ad-hoc DoE methods used to inform experiment planning.
Level 2	Automated Lab Robotics with Experimental Data Management. Execution of high frequency, time consuming tasks with high reproducibility.	Simulation and modelling techniques integrated with high fidelity, robotically generated lab data	AI and ML methods deployed on the high quality robotically generated datasets for enhanced insight and experiment planning.

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Digital Maturity Framework for R&D

LEVEL	Physical experiments	Virtual Experiments	Analytics
Level 3	Highly integrated workflow management. A seamless blend of digital data capture, lab robotics, simulations and flexibly deployed significant computational resources. Physical and virtual experiments are conducted in a single workflow.		AI and ML methods are informing the experimental direction but the human researcher is still in ultimate control of the workflow, defines the end-point and provides validation input.
Level 4	Algorithmic control of Closed-Loop workflows. Autonomous control for Discovery, Optimisation, and Routine Testing. Application of 'reasoning AI' methods in formulating hypotheses and designing, and executing, physical and/or virtual experiments. Research questions are posed by humans, but the experimental workflow is created and executed entirely by AI and lab robotics.		

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Innovation 4.0 Playbook

- Explanation of the benefits of digitalization
- Digital Maturity Framework
- Case Study

https://iuk.ktn-uk.org/news/innovation-4-0-playbook-for-chemical-sciences/

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Relevant updates and programmes

https://iuk.ktn-uk.org/reimagining-manufacturing/

Next generation materials to reduce emissions and energy consumption (includes light weighting, material substitution, materials for circularity etc)

- Computer simulation and modelling, AI/ML, and high throughput virtual and physical screening of materials

Smart design for resource efficiency and through-life value using effective design methods

- Computer simulation and digital twinning of processes on-plant coupled to lab scale experimentation and digitally enabled supply chain

Resilient supply chains of sustainable feedstocks with visibility, co-locating waste and emission streams

- If feedstock variability, or transition, requires product redesign/formulation, digitally mature R&D can handle this much more easily

High value production for high quality products with minimal material waste

- The value of materials is in their performance/cost ratio – digitally mature R&D can do a much better job of optimizing this

Longer in use and reuse to minimise material use and waste, practicing complete traceability and using new value retention processes

- Again, this could be used as a design parameter, using AI/ML to optimize the material properties towards this end, and use computer simulation and modelling to perform predictive assessments of longevity

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Funding through REforMM

Funding competition

Resource efficiency for materials and manufacturing: CR&D

UK registered organisations can apply for a share of up to £12 million for ambitious collaborative R&D projects to support UK materials and manufacturing organisations to become significantly more resource efficient.

Competition opens: Friday 31 March 2023

Competition closes: Friday 26 May 2023 11:00am

Simultaneous demonstrations of how UK materials and manufacturing will become more resilient or technologically advanced are encouraged.

Your proposal must improve resource efficiency and reduce carbon emissions

You must focus on two or more of these five core areas:

- materials for the future economy
- smart design
- resilient supply chains
- world-class production
- longer in use and reuse

https://apply-for-innovation-funding.service.gov.uk/competition/1521/overview/44c03277-b4c6-4ee4-90fc-b2ea23a46294

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Funding through CLIMATES

Funding competition

Critical materials for magnets: Strand 1, feasibility studies

UK registered businesses can apply for a share of up to £5 million for innovative projects that stimulate growth in the rare earth elements (REE) critical materials supply chain. This funding is from Innovate UKs CLIMATES programme.

Competition opens: Tuesday 11 April 2023

Competition closes: Wednesday 21 June 2023 11:00am

https://apply-for-innovation-funding.service.gov.uk/competition/1510/overview/7f04405e-296b-40ff-aaf5-aa5c95a6e9c1#summary

New and alternative materials

- development of novel materials for high-performance magnets
- substitution of materials for high-performance magnets
- cross-disciplinary mine to magnet approaches for materials identification

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Funding through AI solutions

These will be to develop Artificial Intelligence (AI) and Machine Learning (ML) driven solutions that address a business challenge or opportunity in target industry sectors:

- construction
- transport, including logistics and warehousing
- creative industries
- agriculture and food processing

The aim of this competition is to support innovative projects prompted by a challenge to business in an area of operations that can drive improvements in business productivity.

This competition supports the Government's goals in the National AI Strategy in the transition to an AI-enabled economy through wider AI adoption across sectors.

Your proposal must:

- address a business challenge in construction, transport including logistics and warehousing, creative industries or agriculture and food processing
- demonstrate an increase in business productivity

Funding competition

Feasibility studies for Artificial Intelligence solutions

UK registered businesses can apply for a share of up to £5 million in grant funding to deliver feasibility studies. These studies will be to develop innovative solutions using Artificial Intelligence (AI) to address business challenges and opportunities.

Competition opens: Tuesday 28 March 2023

Competition closes: Wednesday 24 May 2023 11:00am

https://apply-for-innovation-funding.service.gov.uk/competition/1533/overview/b50c223e-8aea-4f62-a1ef-4c84d69050e6

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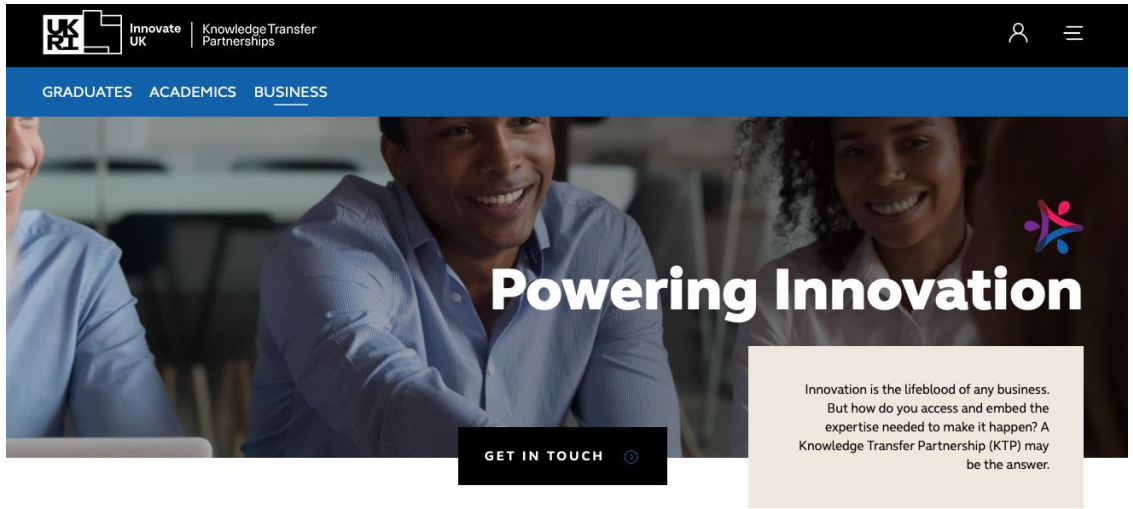
Funding through the KTP scheme



Knowledge Transfer Partnerships can help your business:

- Embed expertise, generate new knowledge, expand capability and foster a culture of innovation
- Drive competitive advantage through accelerated innovation and the possibility of creating Intellectual Property
- Gain privileged and cost-effective access to the UK's world-class knowledge base and resources
- Increase revenue/profits through access to new markets, new product development, increased productivity and better processes
- Benefit from the strategic input of a highly experienced Knowledge Transfer Adviser

https://www.ktp-uk.org

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Funding through Smart Grants

Funding competition

Innovate UK Smart grants: January 2023

UK registered organisations can apply for a share of up to £25 million for game-changing and commercially viable R&D innovations that can significantly impact the UK economy. This funding is from Innovate UK, part of UK Research and Innovation.

Competition opens: Thursday 19 January 2023

Competition closes: Wednesday 14 June 2023 11:00am

https://apply-for-innovation-funding.service.gov.uk/competition/1448/overview/304e6f31-0117-44d1-8c2c-4852876a7928

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Next steps

- Please get in touch to discuss any aspect of the presentation!
- Particularly if you are interested in the funding competitions closing in May/June
- Contact – matthew.reeves@iuk.ktn-uk.org

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