Science and Technology Facilities Council

Hartree Centre

Transforming product development through AI prediction of surfactant phase

STFC Hartree® Centre worked with IBM through the Hartree National Centre for Digital Innovation (HNCDI) to accelerate sustainable surfactant innovation and reduce formulation development time with AI.

Challenge

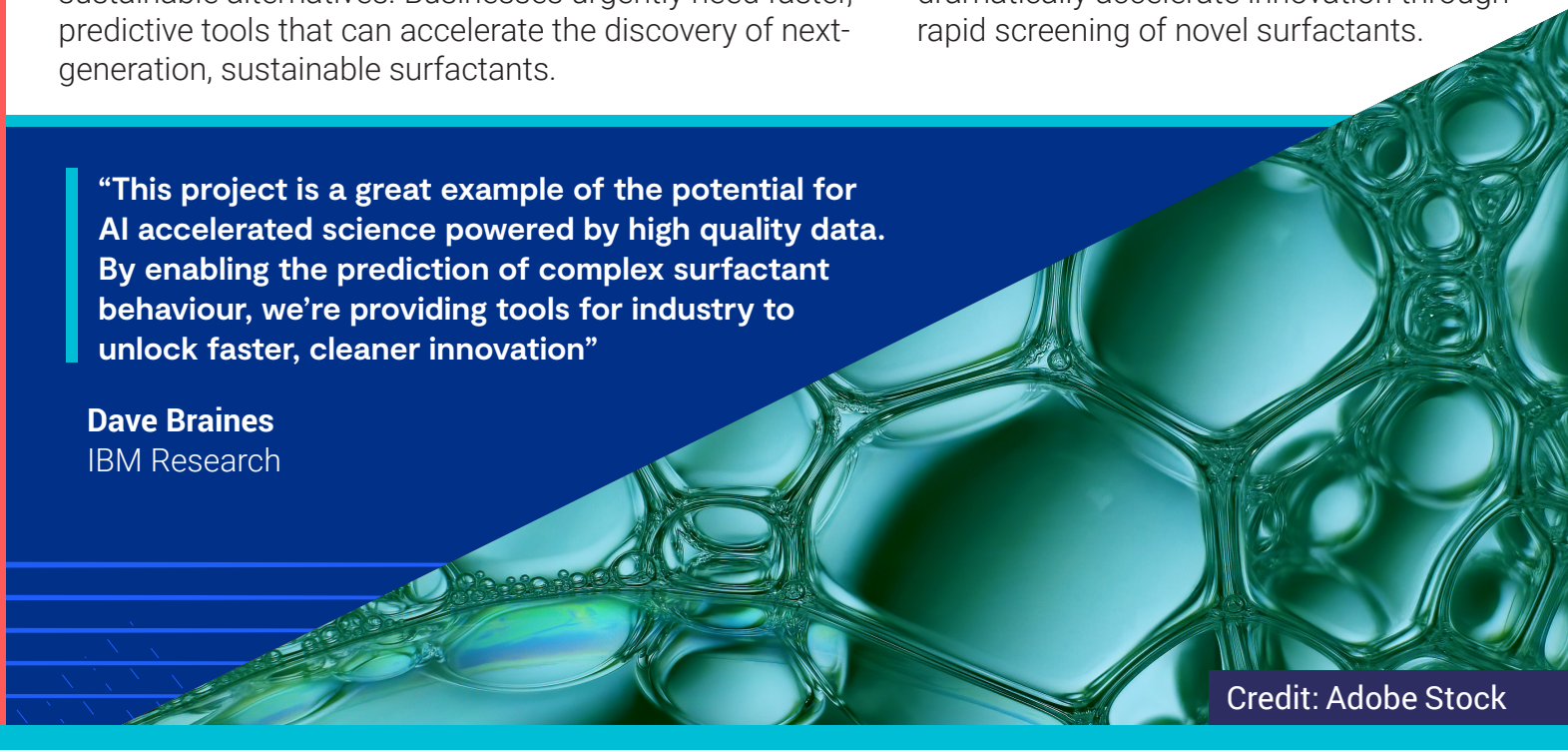
Surfactants play a critical role in everything from everyday essentials such as shampoos and laundry detergents to industrial coatings and crop-protection chemicals. Their behaviour shifts dramatically with temperature, concentration, impurities, and additives, causing them to form different consistencies, or liquid phases that can either support efficient processing or create manufacturing bottlenecks. Traditionally, these phase behaviours are mapped by constructing experimental phase diagrams. While reliable, experimental methods to evaluate surfactant phase behaviour takes significant time and are heavily dependent on skilled labour, limiting how quickly new ideas can be explored. Across the chemical sector, companies are under increasing pressure to decarbonise the surfactant market by moving away from unsustainable feedstocks toward more sustainable alternatives. Businesses urgently need faster, predictive tools that can accelerate the discovery of next-generation, sustainable surfactants.

Approach

Our HNCDI team tested whether AI could reliably predict surfactant phase behaviour. The first barrier was data. Phase diagrams exist mainly as images, not in formats suitable for AI. To solve this the team created CurveClaw, a Python tool that extracts data directly from phase-diagram images. The team also built PhDat, the largest curated database of surfactant phase behaviour to address the challenge. By combining these datasets with calculated molecular descriptors and training an AI model, the team achieved around 80% accuracy in predicting complete phase diagrams. This approach provides potential to dramatically accelerate innovation through rapid screening of novel surfactants.

> **"This project is a great example of the potential for AI accelerated science powered by high quality data. By enabling the prediction of complex surfactant behaviour, we're providing tools for industry to unlock faster, cleaner innovation"**

Dave Braines
IBM Research



Credit: Adobe Stock

Benefits

This work demonstrated how AI can shorten product-development cycles by steering experimental work toward the most promising formulation conditions. This helps direct laboratory effort toward the most impactful areas, reducing waste and supporting sustainability while enabling faster screening of novel surfactant candidates. The openly available CurveClaw tool and the published PhDat database provide a foundation for continued innovation across the sector. By integrating these AI-driven insights into their R&D workflows, industry formulators can explore a far wider design space in a fraction of the time, enabling them to bring next-generation sustainable surfactants to market faster than ever before.

At a glance

- Used AI to shorten product-development cycles in surfactant manufacturing
- Openly available resources created to provide a foundation for continued innovation across the sector
- Solution saves time, reduces laboratory waste, and increases capacity for discovery
- Supports the development of sustainable solutions over a wide range of sectors

The programme

The Hartree National Centre for Digital Innovation is a collaboration between the Hartree Centre and IBM which offers a safe and supportive environment for UK organisations to explore the latest digital technologies and skills, develop proofs-of-concept and apply them to industry and public sector challenges.

Who we are

The Hartree Centre was created by UK Government to help businesses and public sector organisations accelerate the adoption of high performance computing (HPC), big data analytics, artificial intelligence (AI) and quantum technologies. We play a key role in realising UK Government's Industrial Strategy by stimulating applied digital research and innovation, creating value for the organisations we work with and generating economic and societal impact for the UK. We are proud to be part of UK Research and Innovation.

What we do

- Boost productivity and innovation for industry
- Offer training and skills development
- Provide insights into future technologies
- Give tailored business development support