New technology to aid crystallization prediction

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Software designed to assist companies in overcoming common issues associated with crystal formation may be on the market within a year.

The software, which has been developed at the University of Leeds, in collaboration with the Cambridge Crystallographic Data Centre (CCDC) is called Visual HABIT. It offers a significant improvement on existing predictive resources and will enable companies to adopt a more 'bottom up' approach to the design of products or formulated products in the pharmaceutical, agrochemical and fuel sectors.

The software helps companies predict crystal properties in different chemical environments, something which will reduce extensive early-stage laboratory research, bringing down development costs and helping to bring new products to market more efficiently. It also has the ability to show what happens to crystalline particles under different processing conditions.

"Being able to see how crystal properties change within different processing environments is really important, because often companies have put in years of work before they even get to this stage," says Professor Kevin Roberts who is leading the research. "As chemical engineers, we have to make sure that the quality of a product remains the same in a manufacturing environment as in the laboratory. It's a bit like ensuring a meal cooked for 1000 guests is exactly the same quality as the same meal cooked for just four people. Our aim is to ensure that in scaling up different processes, none of the quality is lost. Our technology

will help overcome some of the obstacles that slow down the research and development processes in these sectors."

Visual HABIT will also be a valuable resource for the nuclear sector, where crystallisation during long term storage can create difficulties in the effective processing of waste.

"We're excited about our software because we can see enormous benefits to all the sectors we're working with," says Professor Roberts. "If companies already know – at the beginning of the development process - how different chemical formulations are going to behave under a range of conditions, it'll speed up development times, cut costs and may result in superior products."

The Leeds research group, called Synthonic Engineering, is working with CCDC and five industry partners from across the pharmaceutical, agrochemical, fuel, nuclear and instrumentation sectors to ensure effective translation of the new technology. It aims to commercialise the technology within 12 months.

"We are delighted to be part of this collaborative venture" says Colin Groom, Executive Director of the CCDC. "In the past we have focussed on how knowledge and understanding derived from Cambridge Structural Database can be used in the discovery and development of drugs. This partnership allows us to explore the application of crystallographic and structural information to particle engineering. Our experience in software development will ensure practical and useful software tools are delivered in an exciting area that is new to us."

Provided by University of Leeds