Press release

IMMEDIATE RELEASE
20 March 2014

PSE releases major update of gCRYSTAL process modelling software

Full polymorph handling brings a step change to crystallization process design

LONDON, 20 March 2014 --- Process Systems Enterprise (PSE), the Advanced Process Modelling company, today announced the release of gCRYSTAL 4.0, its industry-leading software tool for increasing R&D efficiency, scaling up with reduced risk and optimising crystallization process design and operation.

With its ability to rigorously predict particle size distributions, gCRYSTAL provides an integrated, easy-to-use, drag & drop graphical environment for R&D personnel, process engineers and scientists engaged in characterisation, design, scale-up and operation of crystallization processes.

A major addition in gCRYSTAL 4.0 is support for multiple crystal phases. This allows accurate modelling of crystallization and transformation of compounds exhibiting polymorphism, providing the ability to maximise yield with respect to the desired polymorph. In addition, the new version contains significantly enhanced parameter estimation and optimisation workflows; the ability to estimate scale-independent kinetic parameters simultaneously using experiments from different scales; various enhancements to kinetic models; new models, including a seed pot model that allows seeding at any (including multiple) points in time; and improved access to model help documentation.

gCRYSTAL 4.0 builds on gCRYSTAL's powerful existing capabilities for batch, semi-batch and continuous crystallization process design and operational analysis, which include capabilities for estimating growth and other kinetic parameters from experimental data; multizonal modelling – utilising links with computational fluid dynamics (CFD) software – for reliable scale-up; and industry-leading optimisation facilities.

The software has been developed in conjunction with several leading companies from industries where crystallization processes – including precipitation – play an integral part, such as pharmaceuticals, fine and bulk chemicals, agrochemicals, food processing, consumer goods and minerals and mining.

Dr Sean Bermingham, VP of PSE's Life Sciences, Consumer Products and Specialty Chemicals businesses, says "The inclusion of full polymorph handling in gCRYSTAL 4.0 brings a significant enhancement to the toolset available to engineers and scientists designing and operating crystallization processes. In addition, the significant improvements in usability of the parameter estimation capabilities streamline the all-important step of validating kinetic models with experimental data in order to provide accurate predictive models that can be used with confidence in scale-up and other critical design activities."

Further information:

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About gCRYSTAL

gCRYSTAL is advanced process modelling software for increasing R&D efficiency and optimising crystallization process design and operations for batch, semi-batch and continuous processes.

A component of PSE's Solids process modelling suite, gCRYSTAL combines ease of use and modelling power. Detailed population balance-based models incorporating first-principles representations of the complex crystallization physics and chemistry provide unprecedented accuracy for activities such as scale-up and product quality improvement, within a user-friendly environment aimed at process engineers, R&D personnel and scientists. gCRYSTAL can also handle multiple solid phases, each with its own particle size distribution and crystallization kinetics for systems with polymorphs and co-crystallization.

gCRYSTAL was developed in conjunction with several leading companies from industries where crystallization processes – including precipitation – play an integral part, such as pharmaceuticals, bulk and fine chemicals, agrochemicals, food processing, consumer goods sectors and minerals and mining.

gCRYSTAL's high-fidelity predictive models are used to optimise crystallization process design and operation, determine the optimal process economics subject to product quality constraints and quantify and manage the risks associated with engineering decisions. The package also provides facilities for validating models against multiple sets of data from steady-state and dynamic experiments. Typical applications are scale-up from laboratory to industrial scale, optimising product particle size distribution (PSD), minimising batch times subject to product quality constraints and determining optimal seeding policy.

A key advantage of gCRYSTAL is that it is built on PSE's gPROMS advanced process modelling platform, which provides the ability to perform full steady-state and dynamic modelling, handle numerous recycles robustly, model and optimise complex operating procedures.

Typical benefits include increased R&D efficiency, improved product quality, higher asset utilisation from optimised recipes, reduced scale-up risk, faster time-to-market with new products, reduced risk and faster development of continuous operations, and importantly, greater understanding of complex crystallization processes.

In addition to its industrial user base of leading companies across the various sectors, PSE works closely with leading research consortia such as the Solid State Pharmaceutical Cluster (SSPC) in Ireland, to maintain the technology at the forefront of innovation and enable knowledge transfer between academia and industry.

About Process Systems Enterprise Ltd (PSE)

PSE (www.psenterprise.com) is the world's foremost provider of Advanced Process Modelling software and services to the process industries. Process companies apply advanced process models to explore the process decision space rapidly and effectively, in order to make better, faster and safer design and operating decisions.

Use of PSE's technology and services results in faster innovation, improved designs of processes and products, enhancement of existing operations and more effective R&D and experimental campaigns. Results are achieved with relatively low investment compared to hardware-based approaches, with rapid return on investment.

PSE's global customer base of process manufacturing companies is served by operations in the UK, USA, Japan and Korea, and agencies in Abu Dhabi, China, Thailand, Malaysia and Taiwan. PSE is a spin-out of Imperial College London, and its software is used in over 200 universities around the world. The company's own ability to innovate was recognised with the award of the prestigious Royal Academy of Engineering MacRobert Award for Engineering Innovation, the UK's highest engineering prize.