Press release

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PSE releases major update of gCRYSTAL process modelling software

Leading batch operation tool now guides batch-to-continuous R&D and Engineering efforts

LONDON, 20 June 2012 --- Process Systems Enterprise (PSE), the Advanced Process Modelling company, today at the ACHEMA exhibition in Frankfurt announced the release of gCRYSTAL 2.0 for increased R&D efficiency and optimisation of crystallisation process design and operation.

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

Building on gCRYSTAL 1.0's capabilities for batch crystallisation, including capabilities for estimating growth and other kinetic parameters from experimental data, gCRYSTAL 2.0 adds a number of features important for modelling industrial-scale crystallisers. Examples are multizonal modelling, with integration to Computational Fluid Dynamics (CFD) models for full hydrodynamic modelling, and new unit operations such as classifier, dissolver, mixer and splitter for modelling crystallisation processes that include recycles.

gCRYSTAL 2.0 brings a step change to the capabilities available to industry for continuous crystallisation processes, allowing for fewer and more-targeted experiments, more reliable scale-up, better operations and improved quality. This is particularly important for the pharmaceuticals industry, where the potential benefits of utilising continuous crystallisation technology in a traditionally batch processing industry are a major current driver. It also takes a step towards integration with downstream handling processes, and provides an unprecedented ability to combine modelling and experimental approaches.

Dr Sean Bermingham, VP of PSE's Solids business, says "Our Advisory Board and close collaboration with leading research consortia such as the Solid State Pharmaceutical Cluster (SSPC) in Ireland enable us to incorporate the latest developments rapidly and facilitate knowledge transfer between academia and industry. The advances in usability brought by gCRYSTAL 2.0 now make these transformational benefits accessible to a growing community of engineers and scientists."

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About gCRYSTAL

gCRYSTAL is advanced process modelling software for increasing R&D efficiency and optimising crystallisation process design and operations. It uniquely combines ease of use and modelling power, with detailed population balance-based models incorporating first-principles representations of the complex crystallisation physics and chemistry providing unprecedented accuracy for activities such as scale-up and product quality improvement.

Aimed at process engineers, R&D personnel and scientists, gCRYSTAL has been developed in conjunction with several leading companies from industries where crystallisation 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 crystallisation process design and operation, determine the optimal process economics subject to product quality constraints and quantify and manage the risks associated with engineering decisions, for both batch and continuous processes. 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 for batch and semi-continuous processes. gCRYSTAL can also handle multiple solid phases, each with its own particle size distribution and crystallisation kinetics for systems with polymorphs and co-crystallisation.

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 crystallisation 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 (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 make better, faster and safer design and operating decisions by reducing uncertainty.

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 alternative approaches, with rapid return on investment.

PSE's global customer base of process manufacturing companies is served by operations in the UK, USA, Germany, Japan and Korea, and agencies in Saudi Arabia, China, Thailand, Malaysia and Abu Dhabi. 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 highest UK engineering prize.