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PSE releases gPROMS Advanced Model Library for crystallization

New techniques for crystallization scale-up and optimization of operations

Process Systems Enterprise (PSE), providers of the gPROMS advanced simulation and modeling environment, will officially release the gPROMS Advanced Model Library for Solution Crystallization (AML:SC) at INTERPHEX. The AML:SC is a set of high-fidelity predictive models for design, scale-up and operational optimization of crystallization processes.

The library – believed to be the most sophisticated crystallization modeling tool available on the market – combines a population balance approach with kinetic models of primary and secondary nucleation, crystal growth, attrition and agglomeration. It represents several years' development and successful prototyping on projects for companies such as BP Chemicals, Friesland Foods, PURAC and pharmaceutical companies.

Typical applications are aimed at improving crystal size distribution, increasing the median size of crystals, limiting growth rates to minimize the number of entrained impurities, reducing batch-to-batch variability and reducing batch times. The result is better quality product, resulting in higher achievable prices; higher throughput; better downstream processing operations; lower design risk and accelerate implementation.

The library has been applied successfully to a range of crystallization processes, from sugars and artificial sweeteners to terephthalic acid production and the manufacture of pharmaceutical-grade lactose.

In particular the library brings a new level of technology for validation of models – the determining of accurate parameters such as growth kinetic constants – against experimental data using the fundamental physics information inherent in the models. Model-based data analysis also provides confidence information that helps pinpoint any additional experimentation required or areas of design risk. Models are typically validated against customers' own laboratory and pilot plant data, providing users with a means to incorporate and enhance their own corporate knowledge within their design tools.

An optional hybrid gPROMS-CFD multizonal interface makes it possible to couple gPROMS and Computational Fluid Dynamics (CFD) model to achieve an unprecedented level of predictive accuracy in cases where fluid dynamics have a significant effect on crystallization.

PSE offers a range of software, models and services to companies wishing to optimize crystallization process design and operation, for batch, semi-batch and continuous processes for a wide variety of products. Services include a well-proven and cost-effective project methodology for addressing crystallization-related engineering and business challenges.

Sean Bermingham, PSE's Crystallization Technology Leader, says "these tools have simply not existed for the designers and operators of crystallization processes in the past. Companies that adopt model-based techniques that couple first-principles models with validation against experimental data are gaining significant competitive advantage".

About Process Systems Enterprise Ltd

PSE (www.psenderprise.com) is one of the world's foremost providers of Advanced Process Modeling software and Model-Based Innovation services to the process manufacturing industries. These apply high-accuracy mathematical models of process equipment and phenomena to provide high-quality information for decision support in process innovation, design and operation.

Use of PSE's technology and services results in faster innovation, improved designs of processes and products, enhancement of existing operations, better economic planning of complex operations and more effective R&D and experimental programmes. Results are achieved with relatively low investment compared to alternative approaches – where these exist – with rapid return on investment and transfer of modeling know-how to industry.

PSE's global customer base of process manufacturing companies and their technology suppliers is served by offices in the UK, USA, Germany and Japan, and agencies in China, India and Korea.

About gPROMS

gPROMS[®] is the world's leading Advanced Process Modeling (APM) environment. It is used to provide high-quality information for decision support in innovation, design and operation across all sectors of the process industries, with particular focus on modeling of complex operations such as reaction, crystallization and polymerisation.

Companies apply gPROMS to reduce time-to-market for new processes or products, improve designs, enhance production, reduce capital and operating expenditure and comply more effectively with safety, health and environmental requirements.

gPROMS is applied across the 'process lifecycle', from laboratory experimentation, through process and detailed design, to online operation, and is central to the emerging technology of Model-Based Innovation. PSE is committed to maintaining gPROMS at the leading edge of modeling technology.

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