PSE is a leading worldwide provider of Advanced Process Modelling tools and expertise for model-based engineering.

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The Advanced Process Modelling company

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gCRYSTAL

ADVANCED PROCESS MODELLING FOR CRYSTALLISATION PROCESSES

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ADVANCED PROCESS MODELLING FOR CRYSTALLISATION PROCESSES

Crystallisation processes are often poorly understood and, as a consequence, design, scale-up and process optimisation are often time and cost intensive.

Businesses use gCRYSTAL® advanced process models, validated against lab or plant data, to enhance design, scale-up and operations and to facilitate breakthrough innovation for their crystallisation processes.

gCRYSTAL is developed in close co-operation with lead users in the pharma, chemicals and food industries to combine the power of advanced process modelling with a user-friendly interface for scientists and engineers.

gCRYSTAL is built on PSE's powerful gPROMS® platform.

Options include:

- gSOLIDS for solids handling
- Hybrid Multizonal CFD interface for equipment scale-up studies
- gO:RUN for execution via MS Excel, web or other custom interface
- gO:CAPE-OPEN for execution within CAPE-OPEN compliant flowsheeting environments

Advanced process optimisation

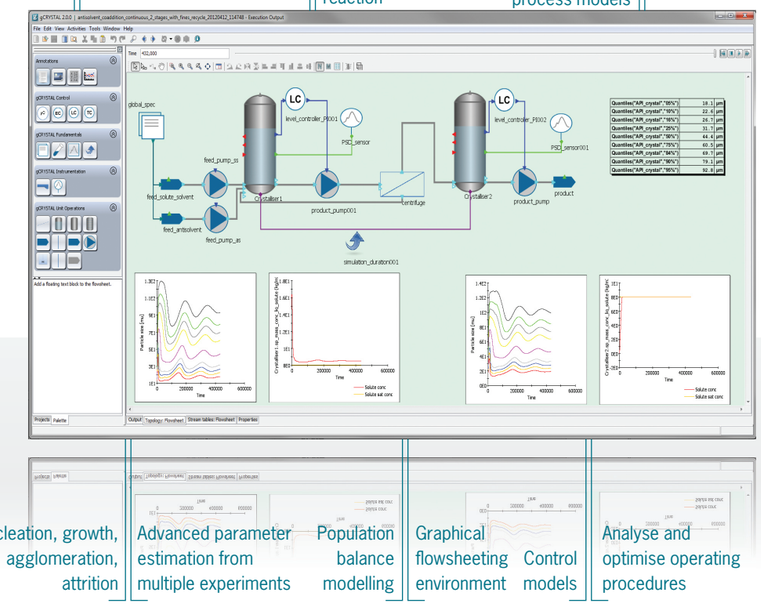
Batch, semi-batch and continuous

Advanced unit operations library

Antisolvent, cooling, evaporative, reaction

Integration with downstream gSOLIDS or upstream gas-liquid process models

Classified outlet streams



Nucleation, growth, agglomeration, attrition

Advanced parameter estimation from multiple experiments

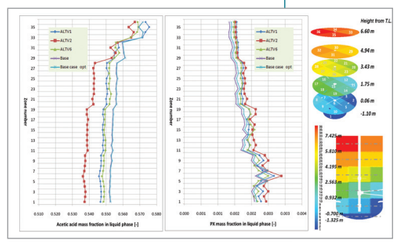
Population balance modelling

Graphical flowsheeting environment

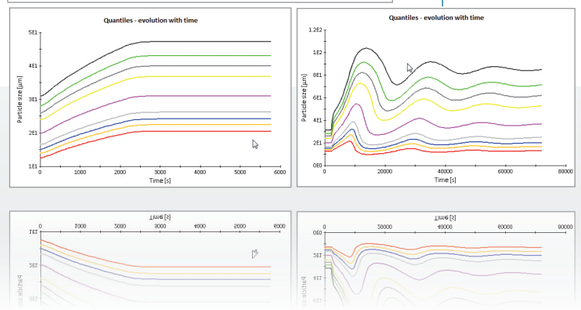
Control models

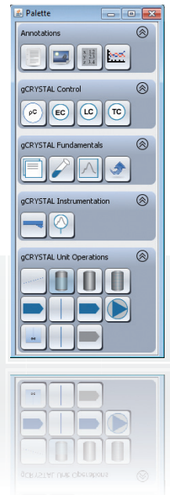
Analyse and optimise operating procedures

Hybrid Multizonal CFD interface



PSD evolution over time





Unit operations

Control

- Density controller
- Evaporation rate controller
- Level controller
- Temperature controller

Fundamentals

- Global specifications
- Properties tester
- PSD input tester
- Simulation duration

Instrumentation

- Sample line
- PSD sensor

Unit Operations

- Classifier
- Crystalliser MSMPR
- Crystalliser MSMPR (fixed volume)
- Crystalliser multizonal
- Feed source
- Mixer
- Product sink
- Pump
- Shortcut dissolver
- Splitter
- Vapour sink

APPLICATIONS & BENEFITS

Extract better kinetic information from fewer experiments

Use gCRYSTAL's integrated model validation capabilities to estimate kinetic parameters and their accuracy (confidence intervals) from steady-state or dynamic experiments. If the uncertainty and associated business risk is too high, use gCRYSTAL to design the minimum number of experiments required to obtain sufficient parameter accuracy.

Quantify the risk associated with imperfect knowledge of your process

In practice you will never have full knowledge of a process as neither models nor measurements are perfect. gCRYSTAL allows you to understand how imperfect process knowledge, captured by the parameters' confidence intervals, translates to uncertainty in model predictions for process optimisation and scale-up.

Robust and efficient batch processes

Reduce batch-to-batch variability by designing robust recipes that ensure high asset utilisation and on-spec product quality (PSD and purity). gCRYSTAL can simultaneously consider decisions such as seed amount, seed PSD, initial loading, temperature profile, anti-solvent addition profile, etc.

Batch to continuous

Transfer your manufacturing process from batch to continuous operation without having to change your R&D set-up and techniques. Use gCRYSTAL to capture knowledge from lab-scale batch experiments and apply that knowledge to the optimal design and operation of a continuous, manufacturing scale process.

Flexible and reliable continuous processes

Use gCRYSTAL's steady-state and dynamic optimisation capabilities to determine the optimal number of crystallisation stages, recycle structure, operating conditions as well as start-up and shutdown procedures. This approach results in an economically optimal process subject to product quality (PSD and purity), operability and safety constraints.

Scale-up & design: crystalliser geometry and mixing

The risk of a scaled up process not yielding the desired product quality, process and economic performance can be significantly reduced by combining hydrodynamic models (CFD) with gCRYSTAL's crystallisation models using PSE's Hybrid Multizonal capability.

SCOPE

gCRYSTAL caters for:

- solution crystallisation and precipitation
- single and multiple-stage crystallisers
- continuous, batch and semi-batch operation
- multiple liquid phase species and multiple solid phases (e.g. different polymorphs)
- supersaturation generated by cooling, flash-cooling, evaporation, reaction and anti-solvent addition
- primary and secondary nucleation, growth and dissolution, attrition and agglomeration
- preconfigured templates for custom kinetic and/or physical property models
- hydrodynamics: well-mixed (MSMPR) or hybrid gCRYSTAL/CFD (Hybrid Multizonal)
- characterisation of PSD: number / volume densities, volume fractions and quantiles.