# **Crystallization Process Development**

ClearWaterBay Technology The Process Development Company

### From Data to Knowledge: Minimize Experiments and Maximize IP Position

















Solid-Liquid Equilibrium Engineering Kit





"Anyone looking to design crystallization unit operations should look seriously at the abilities of SLEEK<sup>™</sup> to optimize overall plant design." Dr. Timothy Nordahl President Swenson Tecnology, USA "SLEEK<sup>™</sup> provides cutting-edge technology for the design of crystallization process. We are confident that SLEEK<sup>™</sup> will give us the boost we need to make our process development effort more efficient." Dr. Masashi Inaba Vice President Mitsubishi Chemical Group Science and Technology Research Center, Inc., Japan

Correct thermodynamic model with parameters regressed from minimal data

Focussed experiments to minimize number of experiments

Objective-oriented engineering solution

Total Solution: From Experiment to Design

#### Introducing $SLEEK^{m}$

SLEEK<sup>™</sup> is CWB Tech's state-of-the-art software solution for crystallization process development. It shortens total development time, builds rapid understanding of the system, facilitates logical selection of solvents/experiments and reduces overall project cost. It is targeted to assist chemical engineers and chemists in understanding and effectively designing crystallization-based separation processes.

 $\mathsf{SLEEK}^{\scriptscriptstyle\mathsf{M}}$  achieves this target though a combination of the following technology features:

- Thermodynamic database access and management for diverse systems: highly non-ideal systems,
- polymorphs, electrolytes, solid-complexes, systems with reactions in liquid phase, etc.
- Organization and regression of solid-liquid experimental data
- Selection of suitable solvents
- Understanding solid-liquid equilibrium phase diagrams
- Design and sensitivity analysis for continuous crystallizers
- Operating policies, design and PSD calculations for batch crystallizers

## $S {\it LEEK}^{ imes}$ - For Thermodynamic Analysis

SLEEK<sup>™</sup> has several features that will help you build comprehensive understanding of the solid-liquid system on hand. These features will help you to:

- Select property methods and thermodynamic models that best describe the system.
- Plot solubility curves, polythermal phase diagrams, and isothermal phase diagrams.
- Examine the overall composition space, visualize crystallization regions, and identify separation barriers.
- Understand how liquid phase reactions affect solubilities and phase behavior.
- $\bullet$  Understand how and when solid-complexes/co-crystal may be formed.  $\bigcirc \times$
- Understand polymorphic crossovers (components may have any number of polymorphic forms in SLEEK<sup>™</sup>) and identify regions in which different polymorphic forms may be obtained via crystallization.
- Understand the phase behavior of electrolytic systems.
- Calculate mixture properties.

## $S \mathcal{L} \mathcal{E} \mathcal{F} \mathcal{K}^{{}^{\scriptscriptstyle \mathcal{M}}}$ - For Solvent Selection

Solvent and/or anti-solvent selection is very crucial for solid-liquid separation. SLEEK<sup>™</sup> recognizes this importance and offers the following two tools to help you accomplish this task:

The solvent screening tool enables you to filter and screen solvents based on a solute's solubility in a specified temperature and composition range.
The solubility study tool enables you to estimate the solubility of a solute in mixtures that include co-solvents, anti-solvents, other components, and impurities.

#### Introducing SLEEK-EX

One of the most common setbacks in using SLE to design a crystallizationbased separation system is the lack of data. SLE measurement is also important to gather information for process design and to develop an accurate model for the crystallizer. We combine the strength of modeling of SLEEK<sup>™</sup> and the strength of experiments of SLEEK-EX in solving the above critical design issue. For example, using the SLE modeling, synthesis and simulation abilities in SLEEK<sup>™</sup>, optimum operability conditions for the crystallizer can be identified with minimum thermodynamic information of the system. SLEEK<sup>™</sup> helps the user identify operating conditions that give maximum recovery of a desired compound with a certain solvent or solvent mixture. Focused experiments can then be performed in parallel using SLEEK-EX to validate the SLE model and improve its accuracy.

## $S \mathcal{L} \mathcal{T} \mathcal{T} \mathcal{K}$ - $\mathcal{T} \mathcal{X}$ - For SLE Data Measurement

The ability to perform experiments in parallel, i.e. multiple data points in one measurement, and have the output relayed digitally to the computer (to SLEEK™)
The accuracy of measurement using "turbidity analysis" with an electronic output rather than visual observation



### $SLEEK^{ imes}$ - For Regression of Data

One of the most challenging development tasks is organizing experimental data and converting it into more meaningful and more useful form. With the help of binary and ternary (pseudo-binary) regression tools in SLEEK<sup>™</sup>, you can:

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- Regress experimental solubility data to obtain thermodynamic model parameters.
- Handle data in mixed solvent or in presence of fixed impurity levels.
- Determine the conditions for additional experiments.
- Save and re-use the thermodynamic model parameters

#### $SLEEK^{TM}$ - For Crystallizer Design

#### **Continuous Crystallizer**

With the help of the SLEEK<sup>™</sup> continuous crystallizer design tool, you can calculate the percent recoveries, total heat requirement, and crystallizer performance under specified operating conditions. This design tool has models that allow you to calculate the particle size distributions by taking into account the effects of crystallizer size, nucleation and growth, agitator speed, fines dissolution, and product classification.

SLEEK<sup>™</sup> also has a powerful sensitivity analysis tool that lets you study the effects of design variables on the performance of your crystallizer by being able to:

- Find the most suitable operating conditions for the optimal recovery of your product. • Find the most suitable operating conditions that will produce the desired polymorphic form of your product.
- Determine ways to optimize the product recovery and other performance parameters.
  Study the effects of crystallizer operation on the particle size distribution.

#### **Batch Crystallizer**

SLEEK<sup>™</sup> batch crystallizer model allows you to create your own batch operating policies and then study the effect of these policies on crystallizer performance. The batch crystallizer model also lets you calculate the particle size distribution properties dynamically. With these capabilities you can do the following:

- Create operating policies by various combinations of "Cooling/Heating", "Solvent/Anti-Solvent Addition", and "Evaporation" steps.
- Determine how recoveries, crystallizer variables, and component attributes change with time.
- Determine how mean particle size and variance change with time.
- Specify seeding and study its effect on mean particle size and variance.

#### The Benefits with $\textit{SLEEK}^{\mbox{\tiny TM}}$

SLEEK<sup>™</sup> comes with an intuitive and user-friendly architecture and interface. At its core is a powerful engine that is based on proven technologies. It has a built-in pure component database with over 1500 components and a built-in aqueous component database with over 1000 components. It also provides a local database, to store new physical properties and thermodynamic model parameters and share them with other users. Whether to try a quick simulation to get an idea of what experiments to perform, or to go to the lab to measure the phase diagram before doing the design calculations, SLEEK<sup>™</sup> can handle the right amount of data at the right time. On the other hand, SLEEK-EX is the right tool for the SLE measurement.

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