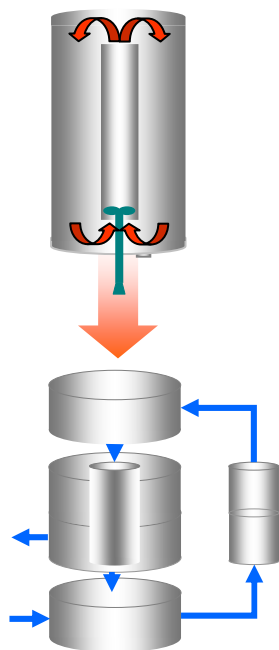


# Advanced Model Library for Solution Crystallisation

## AML:SC at-a-glance ...

- Support for batch, semi-batch and continuous crystallisation
- Multi-zone (compartment) models for enhanced accuracy
- Multiple rigorous crystal population balances
- Built-in or user-defined kinetics
- Multiple components in the liquid and vapour phase
- Unprecedented accuracy for design scale-up
- Access to all standard gPROMS facilities for parameter estimation, optimisation, experiment design and batch optimisation



Draft tube crystalliser represented as a multi-zone model

The gPROMS **Advanced Model Library** for **Solution Crystallisation** (AML:SC) is a library of high-fidelity modelling components for solution crystallisation.

The AML:SC covers a wide range of geometries and types of operation – for example batch, semi-batch and continuous – and includes default options for kinetics and thermophysical calculations as well as all the mathematical techniques for handling multiple complex population balance calculations.

The library is highly modular. Hydrodynamics and kinetic calculations are separated, which is important for key operations such as scale-up. Generic and case-specific information is also separated, which significantly reduces the effort required to build and maintain a validated predictive model of a particular process.

When using the AML:SC, modellers can take advantage of all the standard facilities of gPROMS, such as the powerful built-in parameter estimation and experiment design techniques and the support for batch process design and optimisation.

## How do you use AML:SC models?

The AML:SC models contain relationships describing the fundamental physical and chemical relationships governing crystallisation processes, and the complex population balance calculations.

Built-in kinetic models provide the expressions used for primary and secondary nucleation, growth, dissolution and attrition. However as with other gPROMS libraries, the AML:SC is open-source, meaning that you can supply your own kinetic models if preferred, as well as customise models to your own requirements.

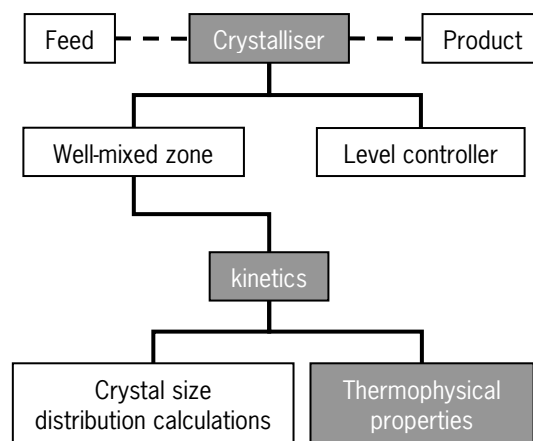
A typical approach when using the AML:SC is as follows:

- Specify the **zone configuration**, if multiple zones are required, and geometry.
- Provide **kinetic information** for one of the built-in models, or, if preferred, provide your own kinetic models.
- Optionally, use gPROMS' parameter estimation capabilities to **fit parameters** to experimental data. gPROMS can also be used to **design experiments** that provide the maximum amount of information from the fewest experiments.
- Provide **thermophysical constant** data or your own thermo calculations.
- Specify the **operating procedure**, especially for batch or semi-batch operations.
- **Execute the model** in simulation or optimisation mode.

The AML:SC has been used to model crystallisation of materials as diverse as sucrose, terephthalic acid, artificial sweeteners such as lactitol monohydrate and ammonium sulphate.

## AML:SC components

The AML:SC comprises a number of element models, each of them implemented as a separate gPROMS MODEL entity, and covering the hierarchy of calculations show in the diagram (right). Elements coloured grey in the diagram are user-configurable from supplied templates.



## Topology models

### Multi-zone (multi-compartment) models

These top-level models provide you with complete freedom to specify crystalliser zone configuration – from a single zone to a multi-zone vessel containing one or more propeller zones. Multi-zone configurations are used where there is a wide variation in process conditions or crystal concentrations within the vessel.

PSE's Hybrid Multizonal gPROMS-CFD tool (see separate brochure) can be used to incorporate inter-zone flowrates and other relevant information from Computational Fluid Dynamics (CFD) calculations.

### Zone models

These are models of a well-mixed single zone, with or without propeller, used as the building blocks for the multi-zone models above. The well-mixed zone model allows for multiple inlets, multiple outlets, multiple liquid phase components, multiple crystal populations and has submodels for kinetics and thermophysical properties.

## Submodels

### Kinetic models

These provide kinetic expressions for all rate terms in the population balance equation:

- birth rate at the lower bound of the crystal size domain.
- birth and death rates distributed over the crystal size domain, used for attrition, agglomeration and breakage.
- growth rate, which may be size dependent and also covers dissolution.

Power Law, O' Meadhra and Gahn kinetics are provided as standard. If you wish, you can create your own kinetic model using the template provided.

### Crystal size distribution calculations

These handle the complex mathematical techniques required to compute crystallisation phenomena by population balance – i.e. the size-distributed mass balance for the solid phase(s) – according to the selected different distribution options.

### Thermophysical properties

The zone models support the use existence of multiple components in the liquid or vapour phases. Data for solubility, enthalpies, densities, viscosities is obtained by calls to one of the physical property packages supported by gPROMS (these include the OLI Electrolytes and SAFT packages), or supplied by the user.

## Licensing, supported platforms and pre-requisites

The open-source AML:SC is available to existing licensees of gPROMS as a corporate-wide perpetual licence for a one-off advance payment plus annual maintenance. The Hybrid Multizonal gPROMS-CFD interface is available on annual lease.



Available

