

Research topics

Design and Optimisation of Crystallisation Operations

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Abstract

Many of the products from the chemical process industries are in the form of crystals. Processes for the manufacture of fine and speciality chemicals usually involve a crystallisation step. In such operations, the quality of the crystal size and size distribution are usually of paramount importance. Few design tools are allowable to direct the process design parameters to an optimal product in a systematic way. This project has developed systematic methods for the design and optimisation of crystallisation operations.

Project description

Crystallisation involves formation of a solid product from a liquid solution. The design of crystalliser for a given separation depends on the method used to bring about supersaturation. The methods used to bring about supersaturation are through cooling the solution using indirect heat exchange, evaporation of the solvent, vacuum to assist evaporation of the solvent, salting (or knock-out) by adding an extraneous substance to induce crystallization or reaction to create metastable conditions directly. Batch, semi-batch and continuous crystallisers can be used.

Modeling crystallization must account for nucleus formation through primary and secondary mechanisms and crystal growth around the nucleus. Secondary mechanisms depend on agitation and mixing and seeding through the addition of crystals. The size of the crystals and the size distribution of the final crystals are both important in determining the quality of the product.

When optimizing crystallization there are many important degrees of freedom to be optimized to obtain the best design. The temperature, pressure, mechanism of supersaturating, mechanism of nucleation (e.g. seed addition policy), feed addition policy in semi-batch operation and cycle time in batch and semi batch operation must all be optimized. This project has developed methods by which these degrees of freedom can be optimized simultaneously for crystal quality. The project has also explored combined methods of creating supersaturation that has led to novel crystallization processes.

The application of the technology leads to the development of novel reactor schemes that would be virtually impossible to derive using an approach based on trial and error. The technology has either led to designs with very significant improvements in the yield of the process when compared with those based on conventional reactor designs, or significantly reduced capital investment.