## Design, Analysis and Optimization of Batch Distillation Processes

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Batch distillation is an important unit operation in the batch processing industry and is used in a wide range of applications: fine chemical industries, pharmaceuticals, specialty chemicals, biochemical, essential oils, alcohols... The great flexibility of batch distillation allows engineers and scientist to separate complex mixtures with a single column. However, this very same flexibility, combined with the inherent unsteady state nature of the process, poses challenging design and operation problems [1]. There is no 'rule of thumb' to achieve the optimal solution (reduced operating time, good product separation, minimum energy consumption...) and dedicated tools are required.

A prerequisite for a good process model is its ability to well represent the thermodynamic behavior of the mixture of components involved in the process in its operating conditions. Thus, it should be linked with a thermodynamic library which includes well-established models (e.g. cubic equation of state like PR, RSK or Gibbs excess models like NRTL or UNIQUAC) but also state of the art models (like SAFT equations of state or COSMO based models). Moreover, in order to design, analyze and optimize batch distillation columns, a dedicated dynamic model should include a detailed representation of almost any type of distillation column, e.g. azeotropic and close boiling separation using heterogeneous or homogeneous entrainers [2, 3, 4], batch distillation with a middle vessel column [5]... The model has also to take into account the detailed geometric characteristics of associated equipment technology (boiler, condenser...) and column hydrodynamics. At the end, chemical engineers, in order to investigate batch distillation processes development, need to be provided with the evolution through time of all parameters of interest such as compositions, temperature, pressure, reflux ratio... Through the creation and analysis of operating scenarios, process engineers should then be able to identify the best resource management policies, recipes for product quality optimization and cost reduction.

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