

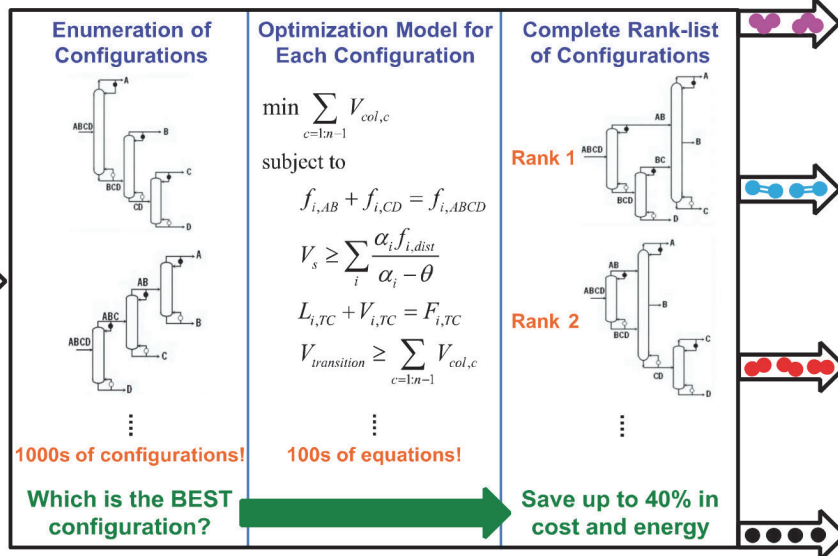
New Design Methods and Algorithms for Energy Efficient Multicomponent Distillation Column Trains

Enabling optimal configurations for
high volume chemical separations

Distillation is a ubiquitous method in the chemical and petrochemical industries to separate mixtures into their individual components and accounts for a large percentage of all separations in chemical and petrochemical plants. A large fraction of the separations are mixtures containing four or more components requiring multiple distillation columns that may not be optimized for energy efficiency. As a result, there are tens of thousands of sub-optimal distillation columns in operation in the U.S. consuming approximately 2-3 Quads of energy per year. In addition, the equipment dedicated to separations contributes 40 – 70% of the capital and operating costs in a typical processing plant.

Currently, an industrial multicomponent distillation train is designed based on heuristics, experience, and creativity of the process designers. But as the number of components in a mixture increases beyond three (see table below), the opportunity space for

Number of Components in Feed	Number of Possible Configurations
3	8
4	152
5	6,128
6	506,912
7	85,216,192
8	2.9 E +10



This graphic summarizes the process in which the algorithm provides globally optimal solutions for multi-component mixtures based on heat duty and total cost. *Image courtesy of Purdue University*

potential configurations contains hundreds to thousands of configurations. Consequently, industrial distillation trains often consume much more energy compared to some of the unexplored configurations. Furthermore, when near optimal configurations are designed it often takes multiple iterations and consequently a substantial investment of time and money before a successful configuration is identified.

The ability to generate and design low-energy distillation configurations would allow the chemical and petrochemical industries to reduce energy consumption of both existing plants as well as new plants. Under a previous DOE award, Purdue researchers developed multicomponent algorithms that systematically generated the universe of useful distillation configurations from the large opportunity space of all possible configurations and ranked them according to their heat duty requirements. The goal of this research is to develop the tools needed to optimize and rank the entire configuration set based on one or multiple criteria to provide the top candidates of energy-efficient, low-cost distillation configurations. The updated

algorithm will also include optional methods for thermally-coupled dividing wall distillation columns and options for retrofitting distillation columns currently in use. The algorithm will be tested throughout the project on high-volume, high-impact industrial distillation processes at several chemical companies in order to ensure delivery of a user-friendly software tool into the hands of practicing process designers.

Benefits for Our Industry and Our Nation

The ability to determine the optimal distillation configuration for a particular application can potentially reduce energy consumption up to 40% and capital/operating costs by 10% – 40% when compared to conventional configurations. The software will enable energy-efficient, low-cost distillation configurations that have never been built before as well as energy-efficient retrofit options for existing plants. Additional benefits include reduction in CO₂ emissions while increasing the U.S. competitiveness in these industries.

Applications in Our Nation's Industry

Distillation is the dominant separation process in the chemical and petrochemical industries, however, this method is broadly applicable across the manufacturing sector where distillation-based separations are needed, such as the food processing industry. Also, as the renewable biomass resource industry matures, distillation will likely be needed to produce chemicals and fuels from these non-traditional sources.

Project Description

The major objectives of this research project are to develop methods, tools, and user-friendly software that will readily generate low-energy solutions for a large class of multicomponent distillation applications found in typical chemical and petrochemical plants. Having such software at the disposal of process engineers will allow chemical manufacturers of all sizes to reduce energy consumption in new as well as existing plants.

Barriers

- Ease of use of final software by process designers.
- Successfully interfacing with a commercial process simulator and other software commonly used by the industry.

Pathways

Researchers will first focus on improving the current algorithm to increase the convergence speed and robustness for up to six-component feed configurations based on overall heat duty as well as total cost. They will also improve the current algorithm by providing an array of operable configurations for thermally-coupled dividing wall distillation columns, and later a method will be

developed that will provide options for retrofitting distillation columns currently in use. The algorithms and software will be tested throughout the project on relevant applications at three companies. The feedback and additional features suggested by industry partners will be incorporated into the software to improve user friendliness and usability.

Milestones

This 3 year project began in December 2014.

- Develop an algorithm that provides globally optimal solutions based on heat duty and total cost for five-component and six-component configurations (Completed).
- Develop a method to draw operable dividing wall column configurations from thermally-linked basic multicomponent configurations (Completed).
- Develop a method that will enable users to retrofit existing distillation configurations based on energy savings (2016).
- Deliver final software program to the selected vendor for distribution to users (2017).

Commercialization

During the research and development phase, the algorithm and software will be tested in real manufacturing environments at some of the largest chemical and petrochemical companies in the world. Internships by Purdue graduate students at these companies will provide an opportunity to get industrial feedback on the performance of the software tools and help identify additional features that will further enhance the utility of the software. Larger market needs will be addressed by exploring options that will make it convenient to retrofit currently

existing distillation configurations and providing links to popular commercial process simulation software will enable quick and error-free transfer of distillation configuration designs. In the second year of the project, a postdoctoral fellow will develop and implement a commercialization strategy including identifying and selecting a software vendor and investigating licensing options.

Project Partners

Purdue University West Lafayette, IN
Principal Investigator (PI): Rakesh Agrawal
Email: agrawalr@purdue.edu
Co-PI: Mohit Tawarmalani
Email: mtawarma@purdue.edu

The Dow Chemical Company
Freeport, TX

Eastman Chemical Company
Kingsport, TN

ExxonMobil Research & Engineering Co.
Clinton, NJ

For additional information, please contact

Dickson Ozokwelu
U.S. Department of Energy
Advanced Manufacturing Office
Phone: (202) 586-2561
Email: Dickson.Ozokwelu@ee.doe.gov ■