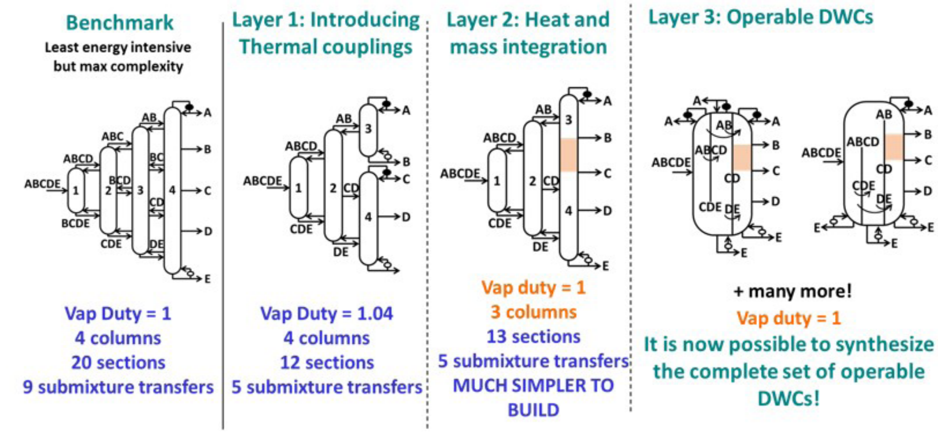
U.S. DEPARTMENT OF
ENERGY

Office of
ENERGY EFFICIENCY &
RENEWABLE ENERGY

Optimizing Multicomponent Distillation Configurations



An example flowchart of the steps (layers) followed to create easy-to-operate divided wall columns (DWCs) for fully thermally coupled configurations.

Graphic courtesy of Purdue University

Distillation is a ubiquitous process 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 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.

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

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 U. S. Department of Energy 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. This research project developed the tools needed to optimize and rank the entire configuration set based on one or multiple criteria such as overall heat duty, cost, or exergy. The updated algorithm also includes optional methods for thermally-coupled dividing wall distillation columns and user defined constraints for retrofitting distillation columns currently in use. The algorithm was 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 enables 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 CO_2 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 Addressed

- Making final software package easy to use for process engineers
- Successfully interfacing with a commercial process simulator and other software commonly used by the industry

Pathways

Researchers first focused on improving the existing 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 improved the algorithm by providing an array of operable configurations for thermally-coupled dividing wall distillation columns, and allowed incorporation of user defined constraints to find retrofittable, efficient distillation configurations that improve existing designs. The algorithms and software were tested throughout the project on relevant applications at three companies. The feedback and additional features suggested by industry partners was incorporated into the software to improve user friendliness and usability.

Milestones Completed

This project began in December 2014 and completed successfully in December 2018.

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

Accomplishments

- Developed **DISTOPT**, an easy-to-use software that takes feed properties as input and displays multicomponent distillation configurations along with optimal operating conditions that minimize total heat duty, total annual cost, and total exergy loss
- Discovered new divided wall column configurations that circumvent operational difficulties without compromising on the overall energy requirement
- Developed a systematic and comprehensive multi-layer approach to conduct process intensification through new and highly intensified design configurations that further enhance operability, improve energy efficiency, and reduce capital and operating costs compared to conventional configurations

Technology Transition

Algorithm and software testing in real manufacturing environments at some of the largest chemical and petrochemical companies in the world was undertaken to ensure the final product would address industrial needs. Internships by Purdue graduate students at these companies provided an opportunity to get industrial feedback on the performance of the software tools and help identify additional features that further enhance the utility of the software.

The academic tool has been converted to commercial software encompassing suggested improvements from industrial process engineers. A licensing agreement with Purdue University through the Purdue Office of Technology Commercialization was completed in the final year of the project. The software, **DISTOPT**, is now available for industrial users.

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The Final Report is available at *www.osti.gov/scitech*: *OSTI Identifier 1543270*

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