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

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Purdue University
12/15/2014 to 12/14/2018

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Washington, D.C.
July 17-19, 2018

Overview

Timeline

- Project award issued in December 2014
- Project end date is December 2018
- More than 95% of the project is complete

Budget

	FY 15 Costs 12/14/2014-9/30/2015	FY 16 Costs 10/1/2015-9/30/2016	FY 17 Costs 10/1/2016-9/30/2017	FY 18 Costs 10/1/2017-12/14/2018
DOE Funded	$83,546.9	$321,484.22	$363,706.27	$131,262.60
Project Cost Share	$38,642.8	$91,146.70	$107,881.87	$14,035.63

Based on 425 figures submitted

Partners

- Collaboration with major chemical industries in the form of student internships
  - Dow Chemical
  - Eastman Chemical Company
- On-going collaboration with ExxonMobil

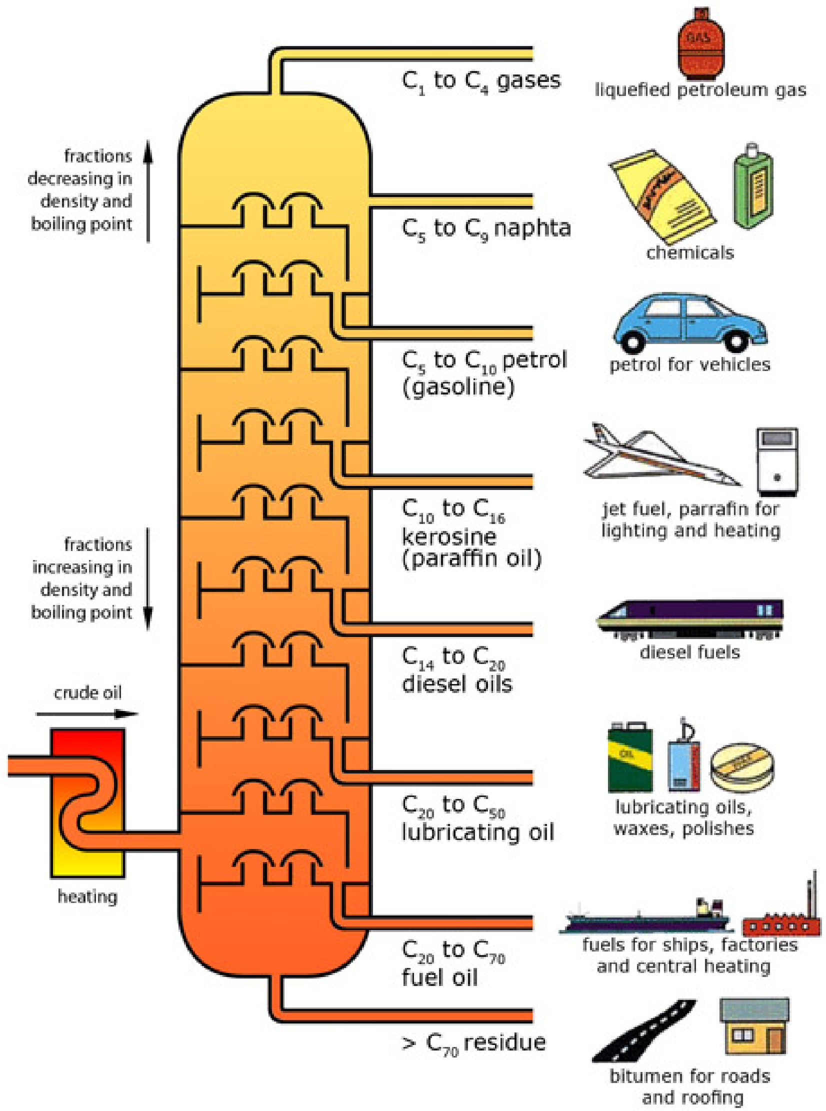
Barriers

- Three major companies used our software, one continues to use it, and the software is awaiting widespread use

Project Objective

- Multicomponent distillation: Ubiquitous in all chemical and biochemical plants
- Accounts for ~3% of World's energy consumption
- US refineries consume ~0.4 million bbl of oil per day for crude oil distillation
- Thousands of configurations exist: current state-of-the-art is heuristic

How to identify the set of configurations with lowest CapEx plus OpEx?



Crude oil Distillation

Courtesy: static.squarespace.com/

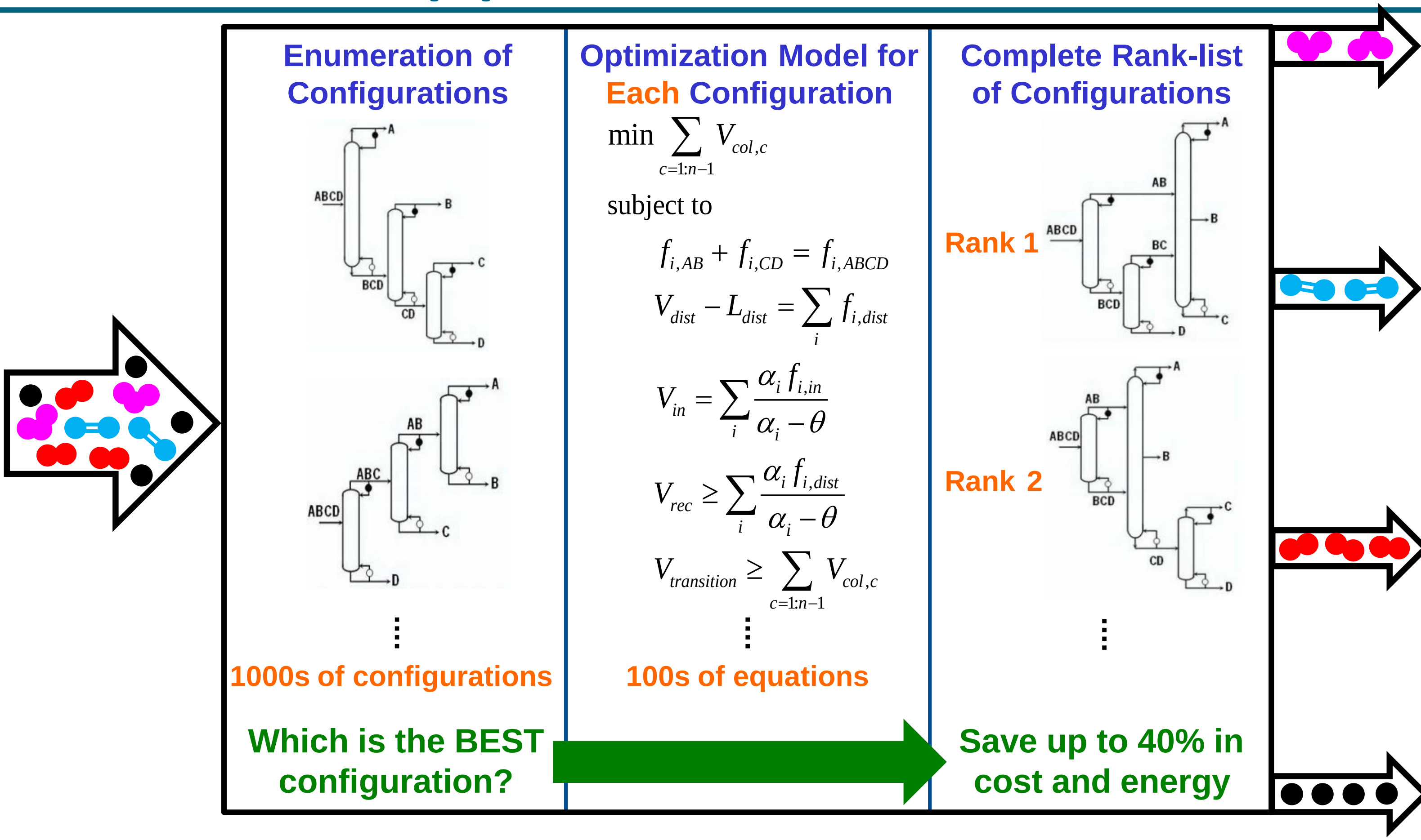
Project Objective

Enable identification of the most energy-efficient and cost-effective multicomponent distillation configurations by industrial practitioners

The objective is achieved through

- Determination of **energy-efficient** and **cost-effective** alternatives for multicomponent distillation
  - Develop rigorous mathematical models and algorithms
- Development of systematic **Process Intensification** (**PI**) strategies
  - A theory for multiple layers of PI to further reduce CapEx and OpEx
- Delivery of a powerful user-friendly software, **DISTOPT**, for industrial practitioners
  - Test the software on industrially relevant applications at participating chemical industries
- Development of methods to quickly and reliably estimate minimum energy requirement of multi-feed multi-product columns

Technical Approach and Innovation

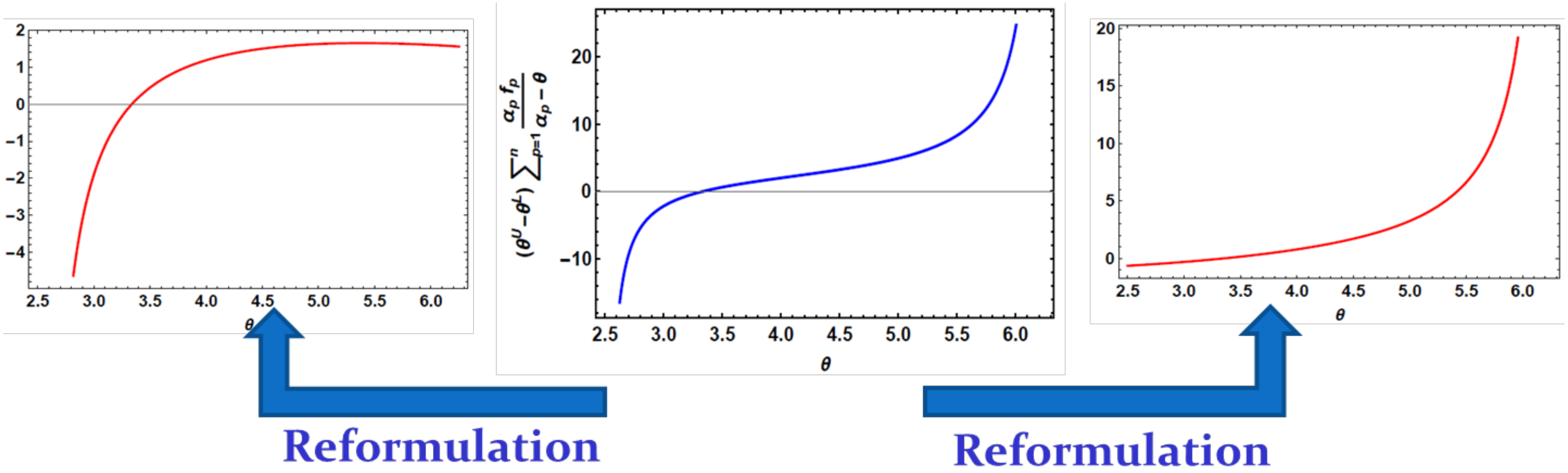


Rely on rigorous mathematical methods, instead of heuristics. Solve challenging optimization problems to determine optimum operating conditions

First group to identify all the configurations, their global optimum and to rank-list all configurations based on heat duty, cost and exergy loss!

Technical Approach and Innovation

Innovations on the Mathematical Front



- Reformulate: Multiply with bound factors of underwood roots
- Partial-fraction-decomposition: Cancels some nonlinear terms enabling us to express the nonconvex left-hand-side in a significantly simpler form
- Linearization: relaxes remaining nonconvexities
- Piecewise estimators are constructed using recently introduced 'Outer-approximation followed by outer-linearization' technique
- **Algorithm outperforms state-of-the-art global solvers!**

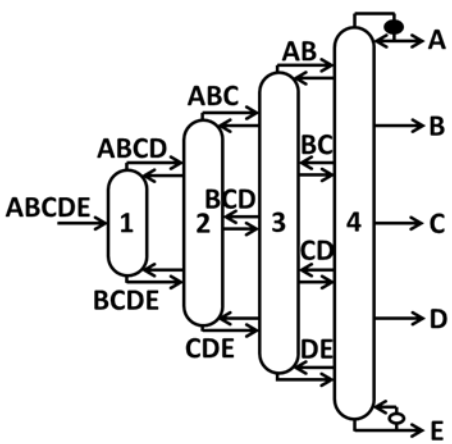
Technical Approach and Innovation

Enumerate basic configurations → Attractive thermal couplings → HMA and DWC

Case study Parameters: $\{\alpha_{AB}, \alpha_{BC}, \alpha_{CD}, \alpha_{DE}\} = \{2.5, 2.5, 1.1, 1.1\}$; $\{f_A, f_B, f_C, f_D, f_E\} = \{5, 80, 5, 5, 5\}$

Benchmark

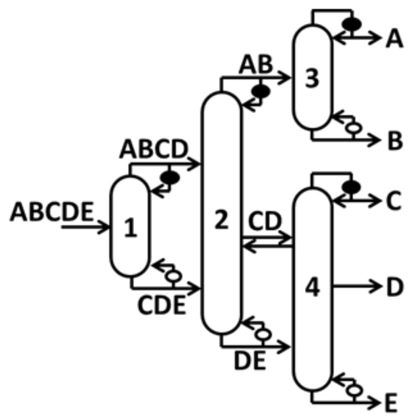
Least energy intensive but max complexity



Vap Duty = 1
4 columns
20 sections
9 submixture transfers

Basic configuration

From GMA



Vap Duty = 1.50
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12 sections
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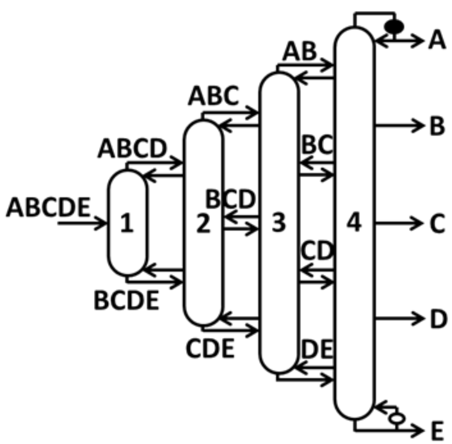

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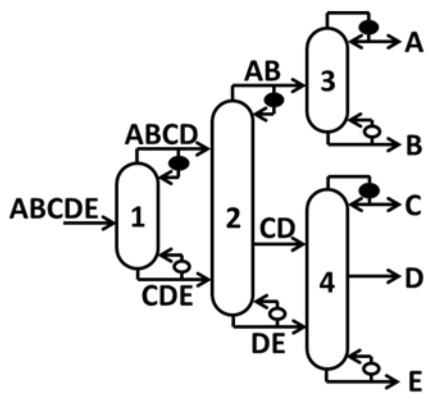

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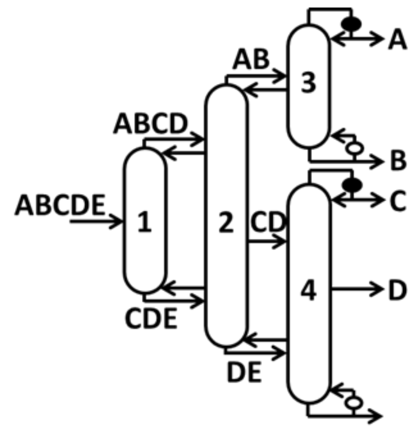
Layer 1: Introducing Thermal couplings



Vap Duty = 1.04

30.7% reduction!

Technical Approach and Innovation

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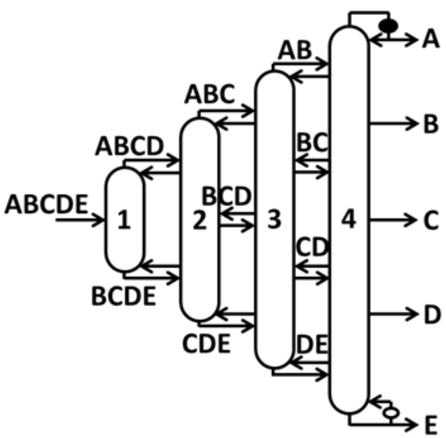

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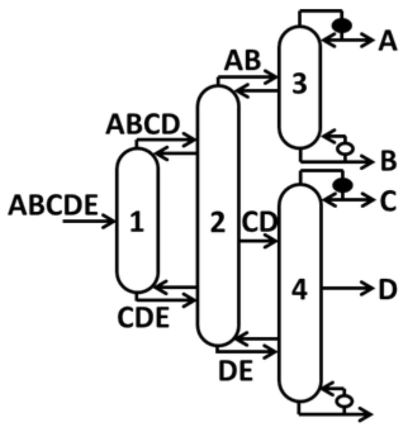

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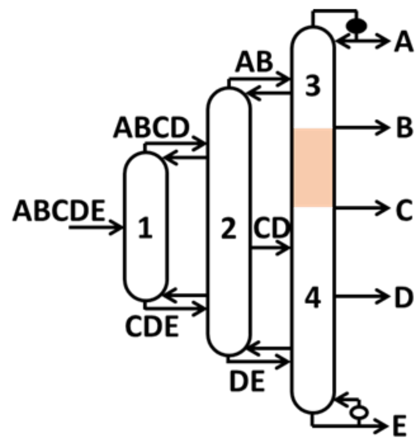
Layer 2: Heat and mass integration



Vap duty = 1
3 columns
13 sections
5 submixture transfers

Through PI, we achieve the same lowest heat duty with less equipment pieces

Energy efficient and cost effective configuration

Technical Approach and Innovation

Enumerate basic configurations → Attractive thermal couplings → HMA and DWC

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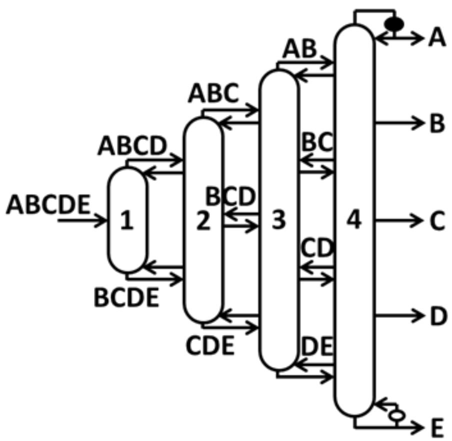

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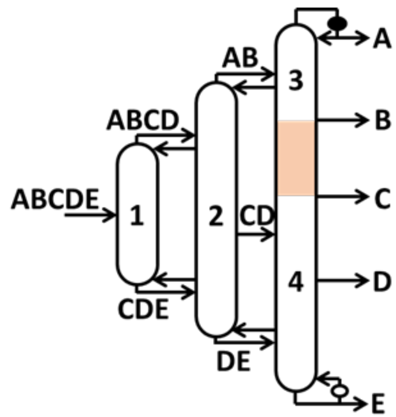
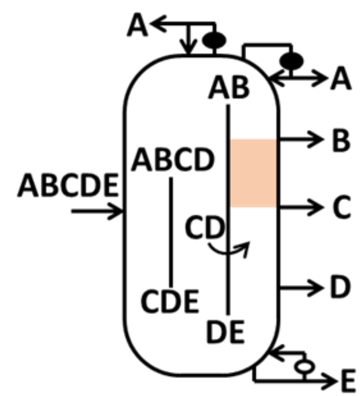


Vap duty = 1
Much simpler to build

Conventional DWC



NOT OPERABLE!
Vapor split is difficult to control

Technical Approach and Innovation

Enumerate basic configurations → Attractive thermal couplings → HMA and DWC

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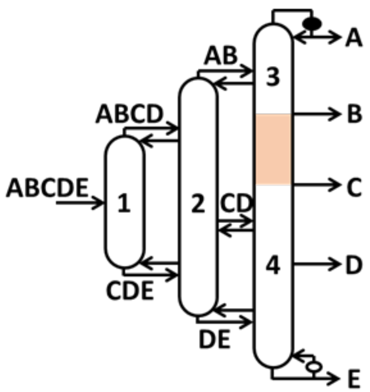

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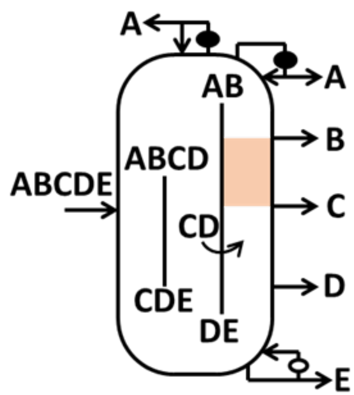
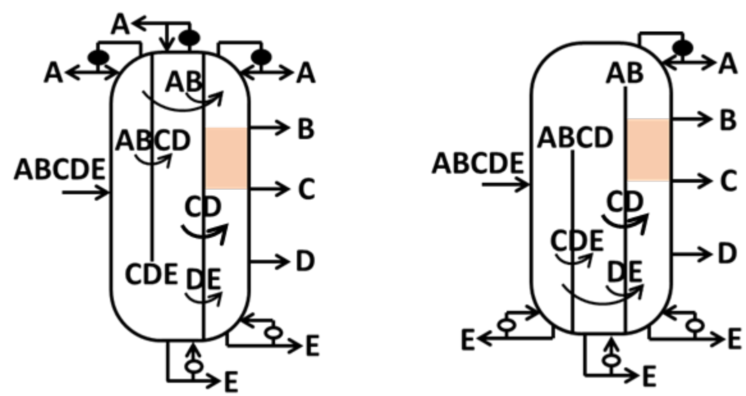


NOT OPERABLE!
Vapor split is difficult to control

Layer 3: Operable DWCs

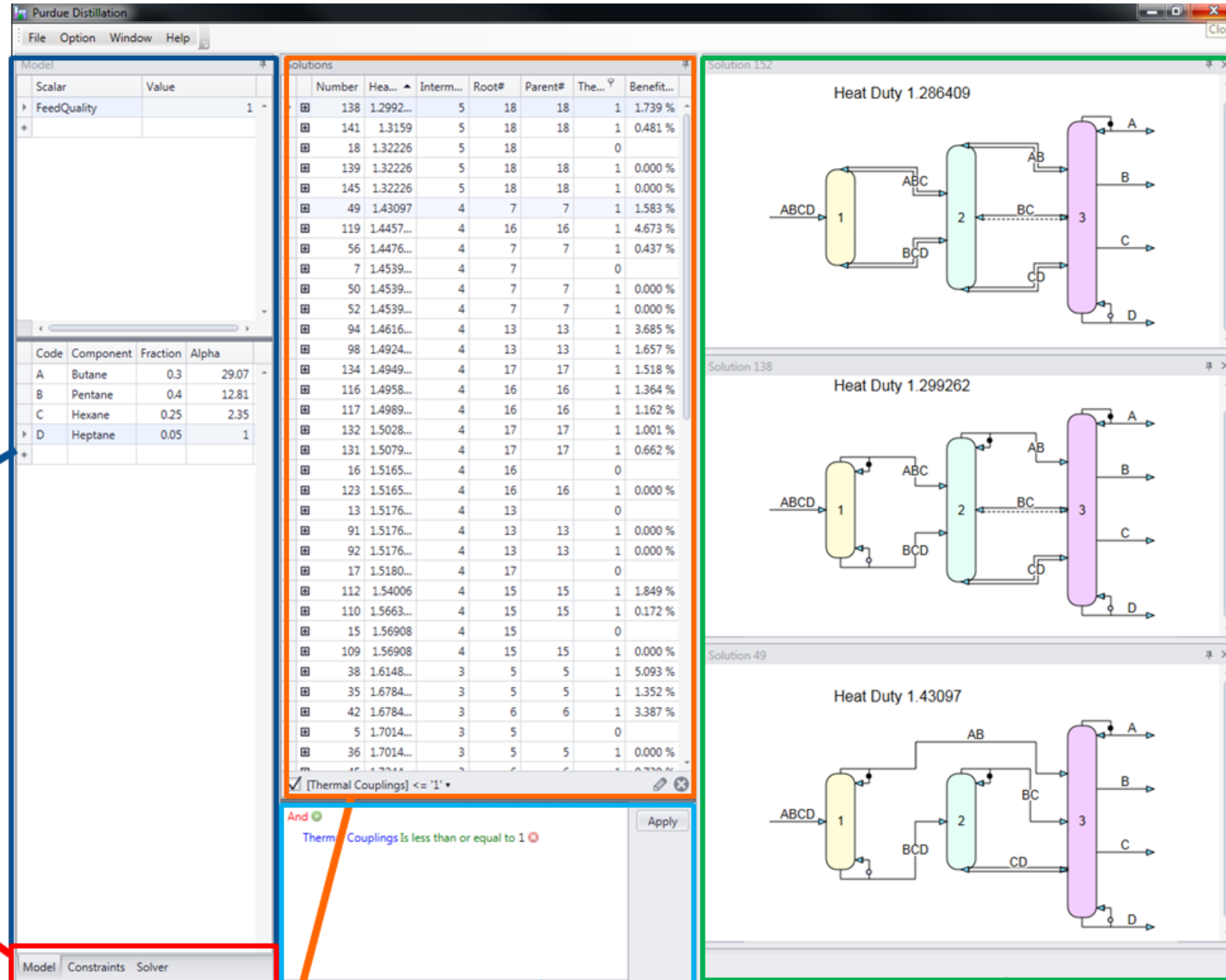


+ many more!

Vap duty = 1

Now, we can synthesize the complete set of operable DWCs!

Interface of DISTOPT



Define model parameters

- Impose constraints
- Solve the model

Ranklist the solutions

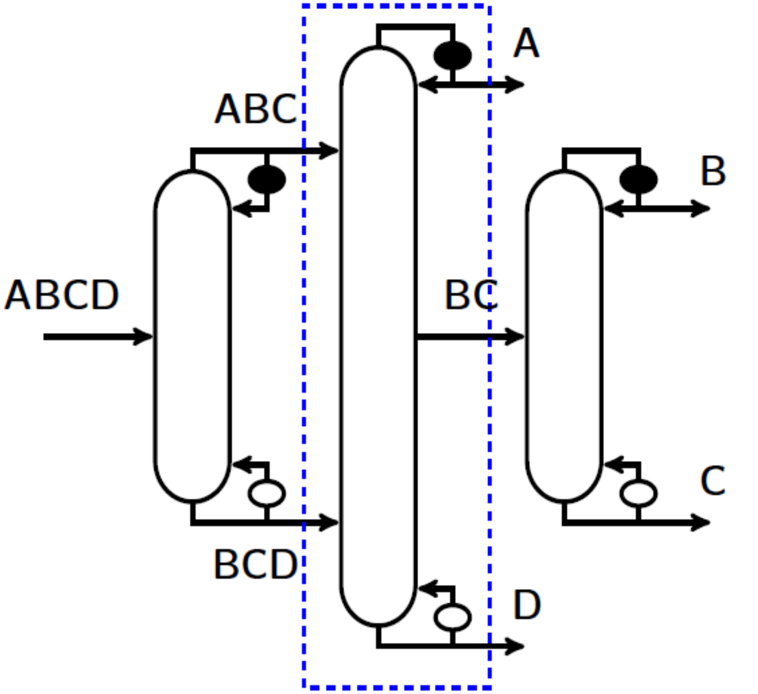
Filter the solutions

Visualize the configurations

Technical Approach and Innovation

Longstanding challenge: How to calculate the minimum energy requirement of a multi-feed, multi-product column

- Multi-feed, multi-product (MFMP) columns are commonly used in industry
- Current approach does not lead to accurate solutions
- **Our group has solved this longstanding challenging problem!**
- Constructed an accurate mathematical model to quickly and reliably calculate the minimum energy requirement
- Key features: Allows for components to flow freely across sections, identifies distillation composition path and thus feasibility constraints on side-draw composition



Results and Accomplishments

- All milestones and Go/No-Go decisions of the first two budget periods have been accomplished

Milestones	Description
5.2.1	Formulated and implemented a Mixed-Integer-Nonlinear Program (MINLP) for overall vapor duty
5.3.1	Formulated and implemented a MINLP for overall cost
5.5.1	Developed a preliminary version of Mixed-Integer-Linear program (MILP) for overall vapor duty. This is a first-of-a-kind formulation in chemical engineering literature.
7.1.2	Incorporated industrial feedback from Dow Chemical (participating partner) in DISTOPT
7.2.3	Successfully completed the licensing agreement with Purdue
10.2.3	The distributable version of DISTOPT is ready for commercialization
11.1.1	Successfully solved a longstanding problem to accurately compute the minimum reflux ratio of a two feed-two products column
11.1.2	Successfully solved a longstanding problem to accurately compute minimum reflux ratio of a three feed-two products column

Transition

- Results are of interest to practitioners in broad industries
  - Chemicals – e.g. purification of alcohols, ketones, etc.
  - Petrochemicals – e.g. NGL (associated with shale gas boom), Crude oil
  - Biochemicals – e.g. pyrolysis, fermentation, gasification
- Process designers in above industries are prime users
  - New plants and facilities
  - Retrofit of current plants and facilities
- Leveraging experience and expertise of 'Purdue Office of Technology Commercialization' to commercialize our software
- Converted academic tool to commercial software by hiring a vendor (Abnaki Light Industry, Inc.)
  - First version of the software is ready for commercialization

Transition

- Various companies showing great interest in our methodology and software
    - Signed an agreement with ExxonMobil to use our software for real industrial applications at their refineries
    - Approached by SABIC regrading purchasing the software
- Technical presentations and talks to introduce our research products and software
    - AIChE Spring and Annual Meetings
    - Process Systems Engineering (PSE) conference (San Diego)
    - Distillation & Absorption conference (Italy)

Questions?