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

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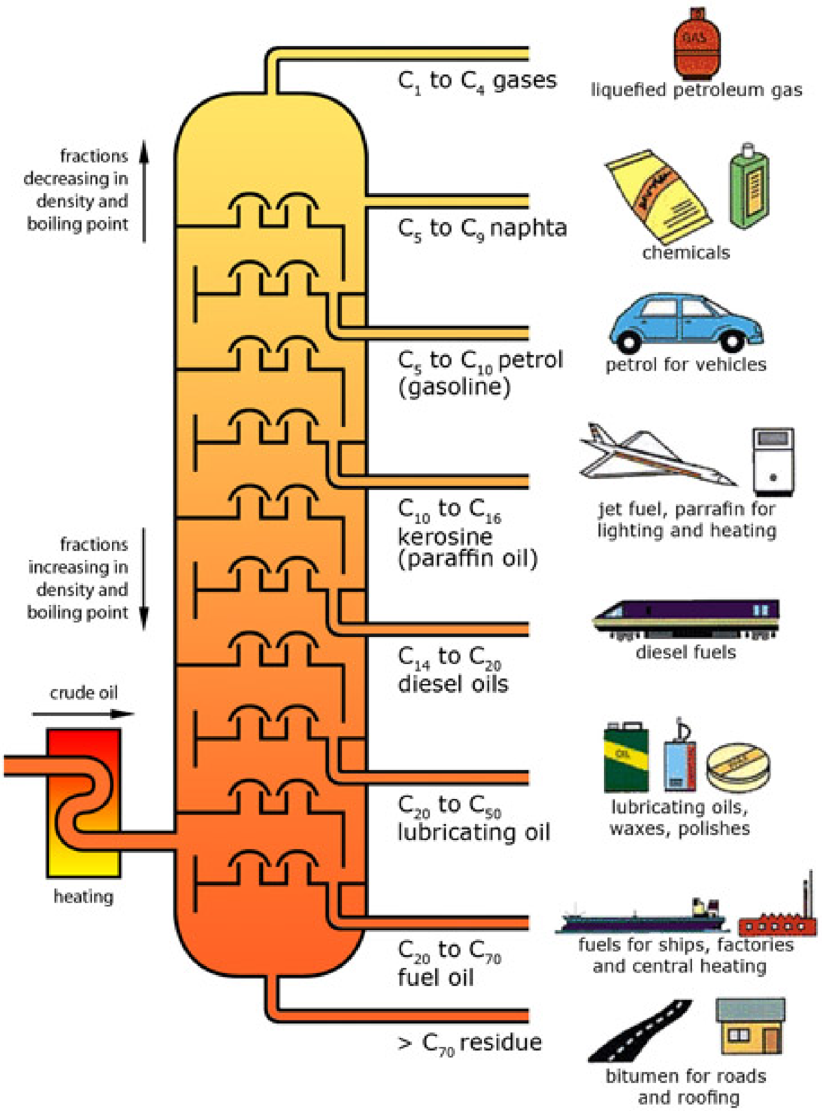
Project Objective

- 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 to carryout the separation

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



Crude oil Distillation

Courtesy: static.squarespace.com/

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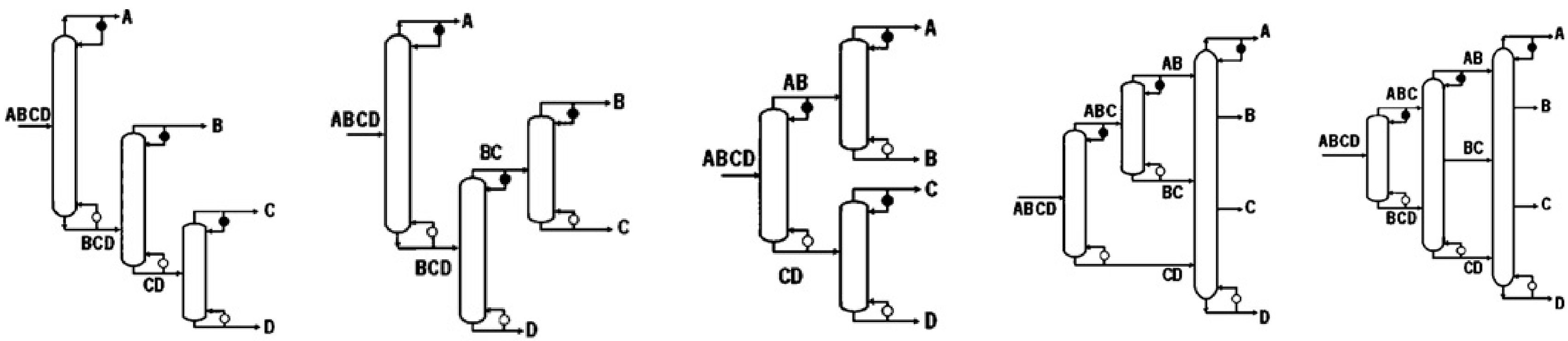
Technical Innovation

- **Identification of the set of lowest CapEx plus OpEx configurations**
- **Current distillation practices:**
  - Unable to generate ALL configurations
  - Use of heuristics, experience, guess, trial-and-error
  - Efficient configurations are lost in the huge search space



A few four component configurations performing the same task of separating ABCD mixture

Often results in energy-inefficient plants!*

*Shah & Agrawal, AIChE J, 2010

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Technical Innovation

- Current distillation practices do not take full advantage of process intensification
- Thermally coupled columns, though energy efficient, are not built due to challenges in operability
- For the same reason, Dividing Wall Columns (DWC) – process intensification at its best – are not used extensively in separation industry
- Existing DWCs have operational difficulty in producing high purity intermediate products

Current practices lead to millions of dollars of penalty due to inefficient plants!

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Technical Innovation

- **Our Approach to identify the set of lowest CapEx plus OpEx configurations**
  - Rely on rigorous mathematical methods, instead of heuristics and trial-error-approach
  - Solve Mathematically challenging optimization problem to determine operating conditions that minimize heat duty
  - Develop innovative methods to help solvers in navigating them to global optimum
  - Build an easy-to-use software that ranklists configurations, and make it available to industrial practitioners
  - Develop hitherto unknown Dividing Wall Columns that minimize the energy consumption, and are operable

Drive the distillation industry in the direction of process intensification, to make plants efficient and cost effective!

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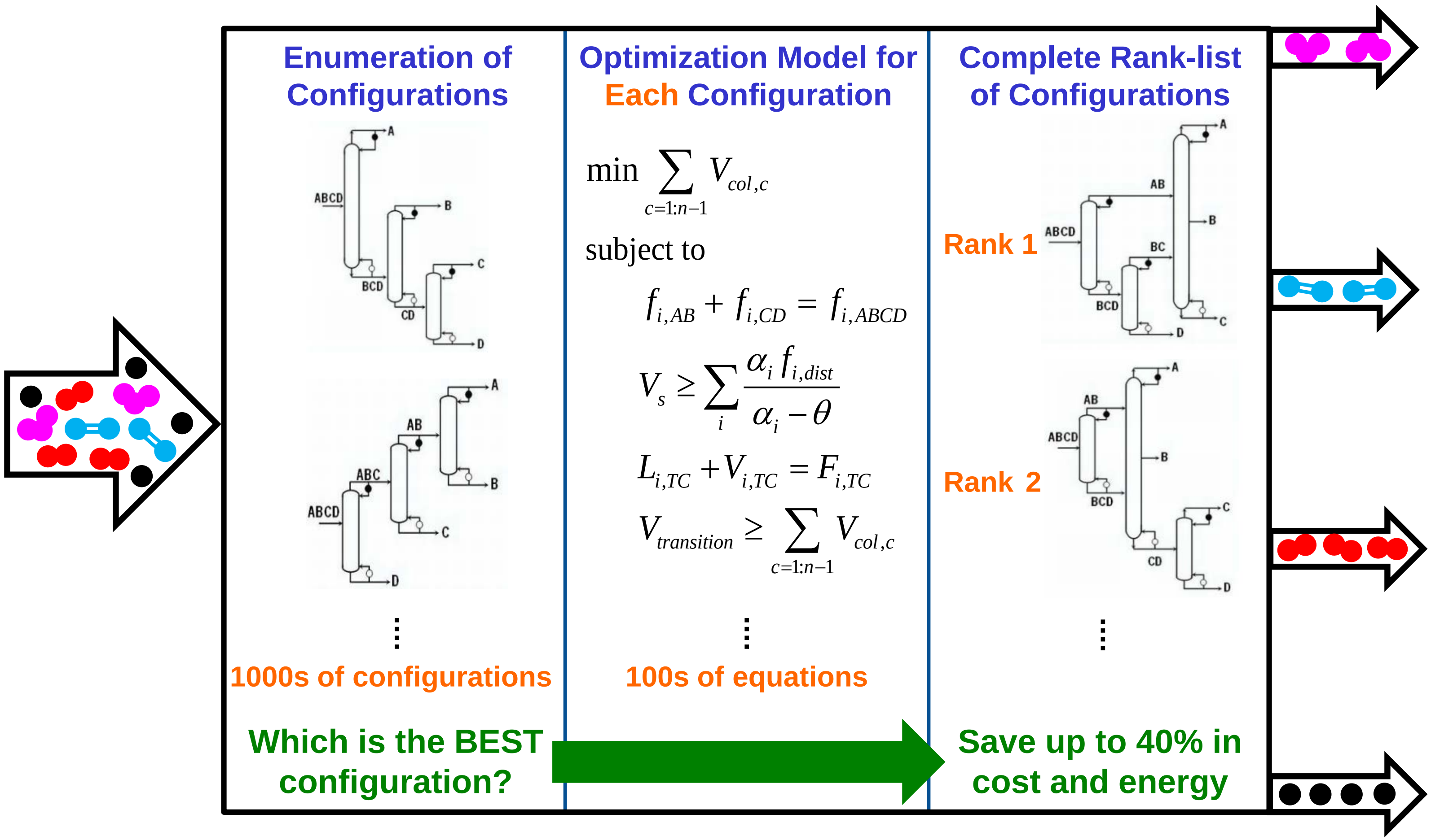
Technical Approach



Simplicity of the enumeration method is receiving attention in both academia and industry

Our approach results in a software which quickly screens through all configurations, and gives a ranklist of configurations

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Technical Approach

We develop an advanced global optimization program to identify energy efficient, cost effective configurations

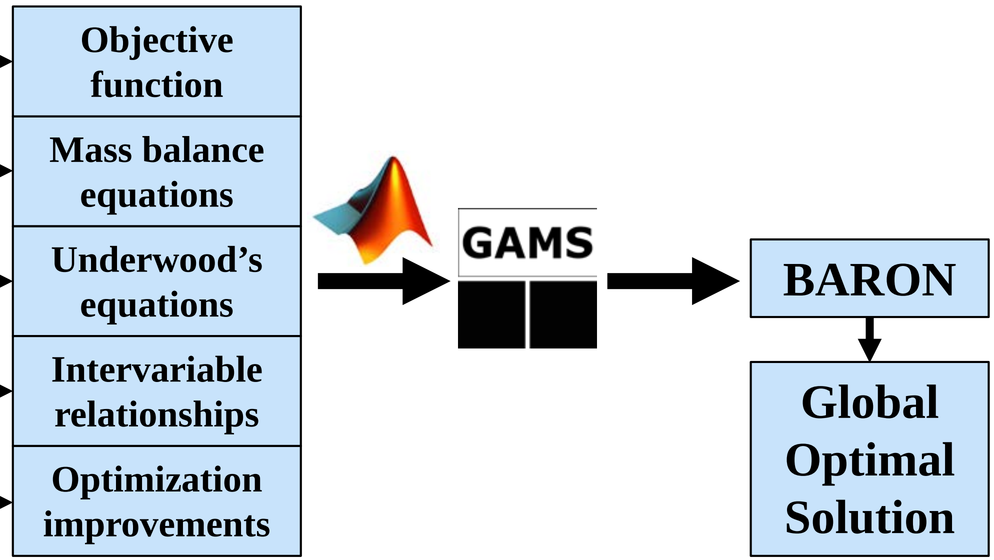
$$\min \sum_{i=1}^{n-1} V_{reb,i}$$

$$F_{i,AB} = B_{i,AB} + D_{i,AB}$$

$$V_s \geq \sum_{i=1}^{n} \frac{\alpha_i D_{i,s}}{\alpha_i - \theta_j}$$

$$F_{TC,i} = L_{TC,i} + V_{TC,i}$$

$$\sum_{i=1}^{n-1} V_{reb,i} \leq V^{UB}$$



- **Thanks to the AMO support:**
  - **Initial version of Mathematical models and computer code for heat duty, total cost (CAPEX+OPEX), and exergy loss have been completed**
  - **First group to identify all the configurations, their global optimum and to rank-list all configurations**

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Technical Innovation

- Developed a tool to identify efficient configurations from the perspective of both heat duty and exergy (‘work’)
- Exergy should be considered in heat pump applications and cryogenic distillations
- Exergy loss is an important parameter in gas and shale gas separation
- Shale gas consists predominantly c1 – c4
- Distillation temperatures range from cryogenic values to above ambient values

Essential to consider energy and exergy simultaneously!

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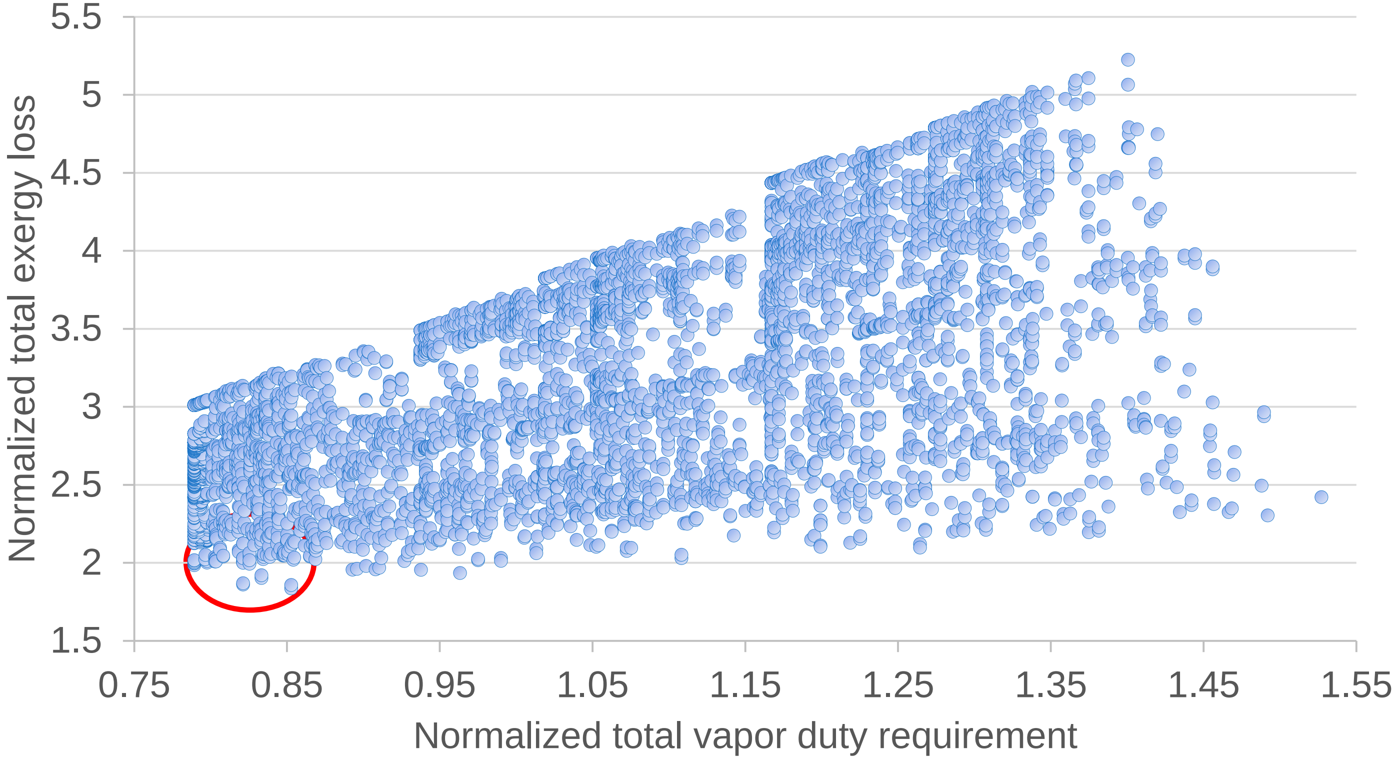
Technical Innovation

A tool which readily tells us the configurations to be considered



Now, we can consider energy and exergy simultaneously!

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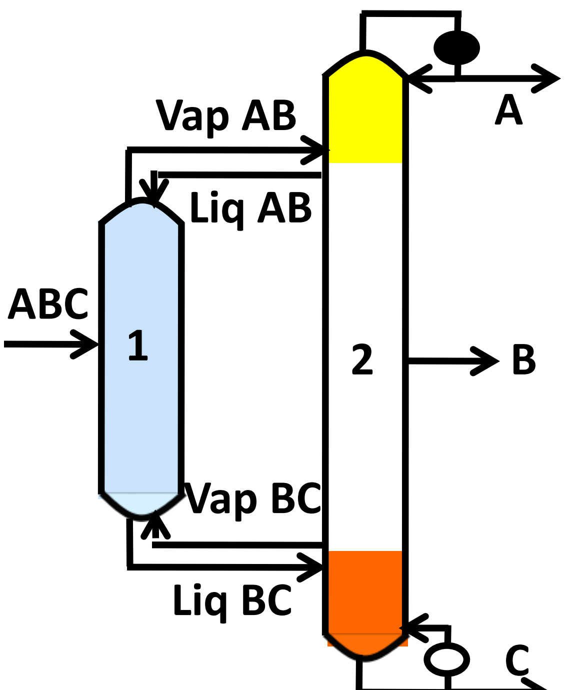
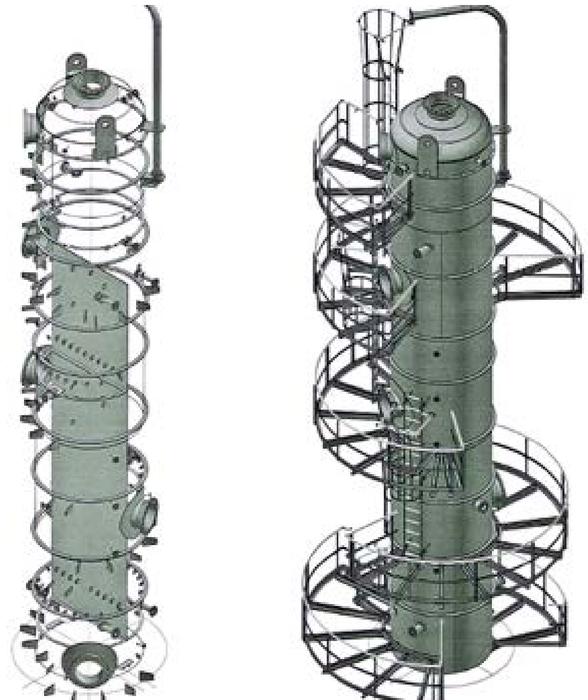
Technical Innovation

What is a Dividing Wall Column (DWC)?

A Three-component Configuration



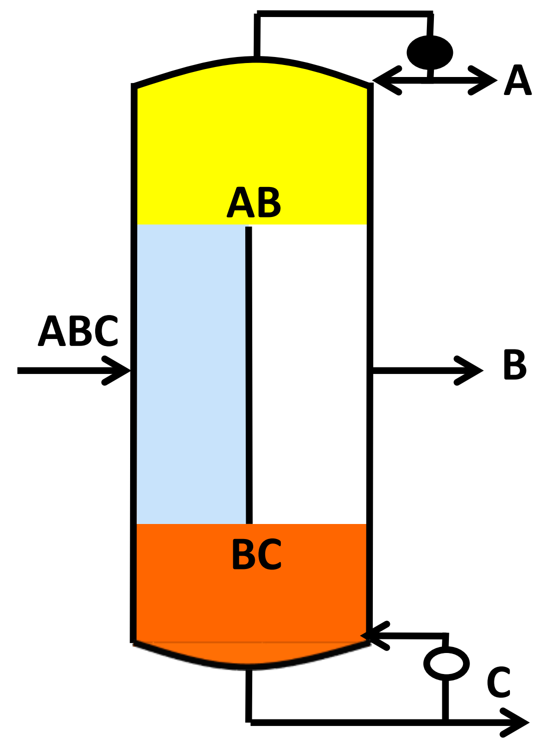
2 Distillation Columns



Courtesy: http://www.hydrocarbonprocessing.com/

Wright 1949

Dividing Wall Column (DWC)



1 Distillation Column

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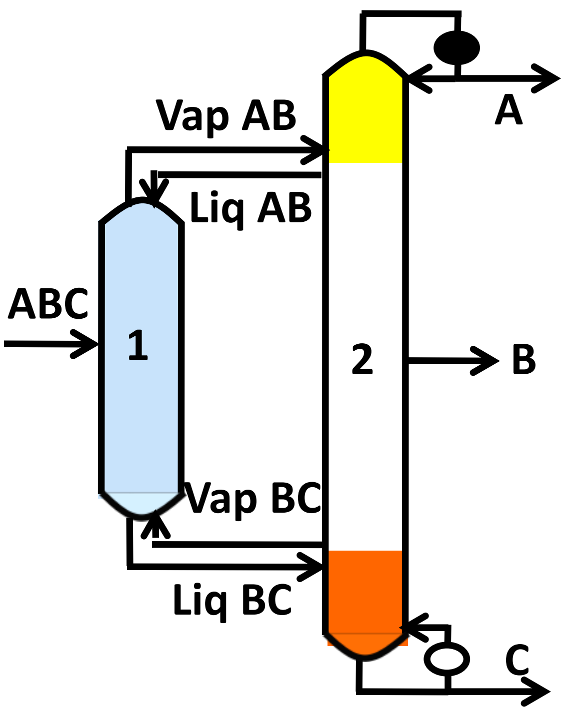
Technical Innovation

What is a Dividing Wall Column (DWC)?

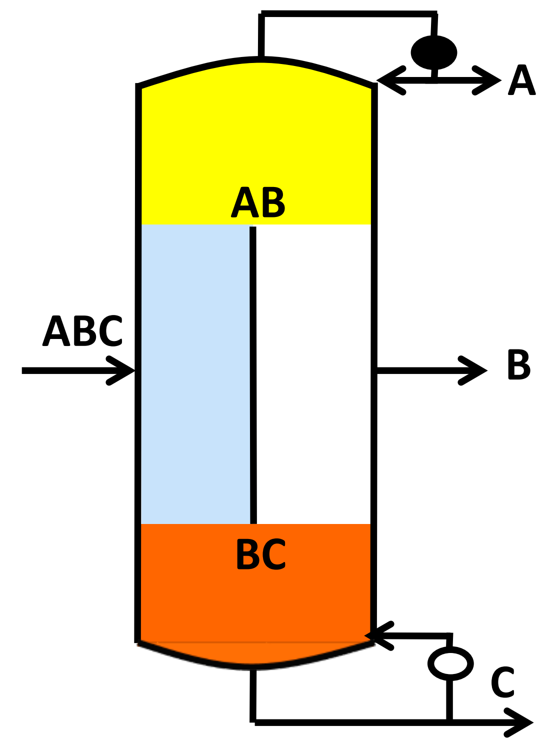
A Three-component Configuration



2 Distillation Columns

~30% capital cost savings

Dividing Wall Column (DWC)



1 Distillation Column

Wright 1949

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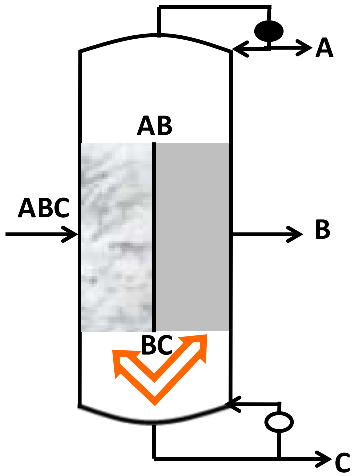
Technical Innovation

However, DWCs are not common in industry due to operational challenge

3-component DWC



Uncontrolled vapor split at bottom

Optimal operation cannot be achieved in practice

Difficulty in withdrawing middle component B purely

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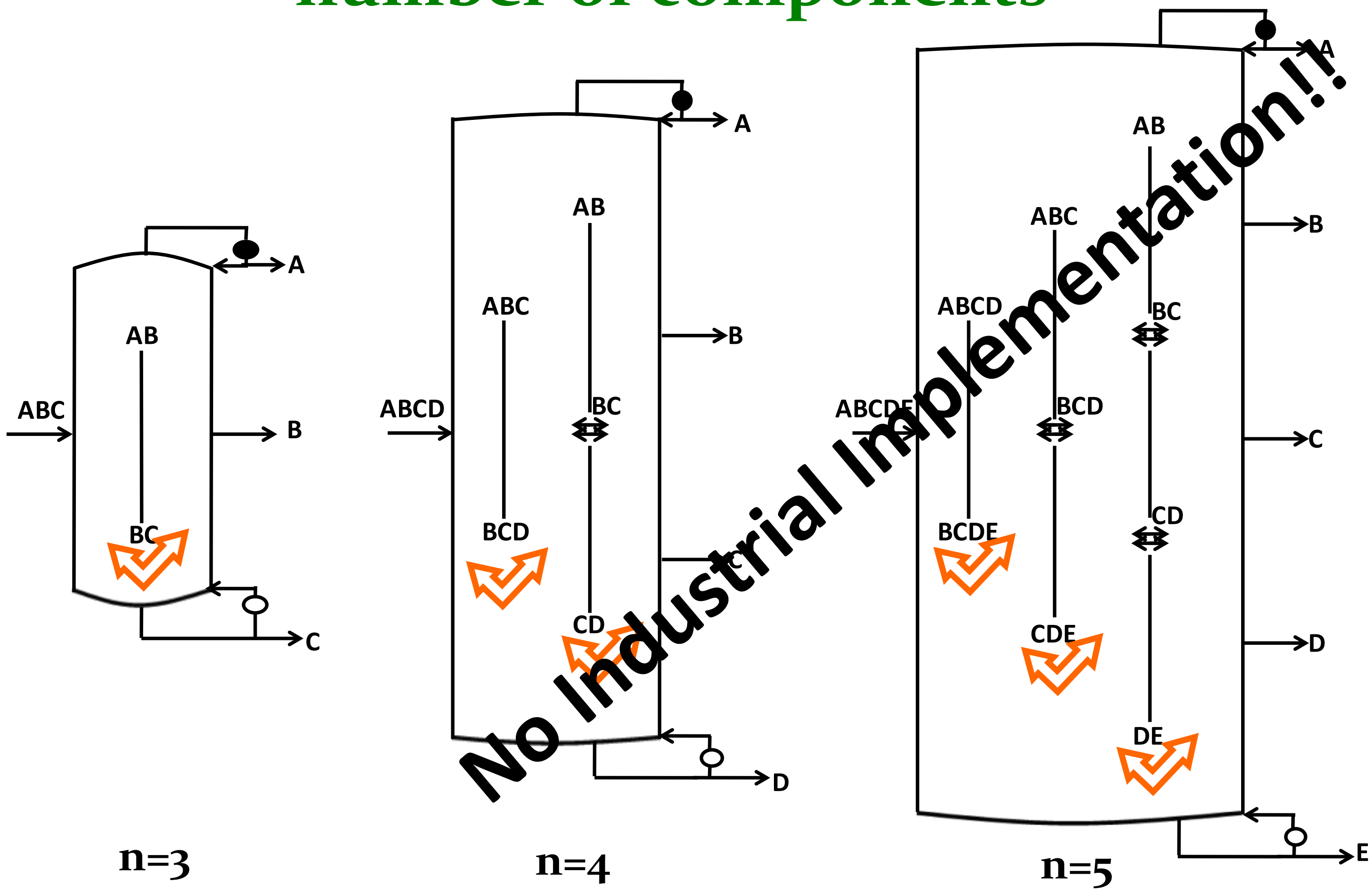
Technical Innovation

Operational issue becomes more severe for higher number of components



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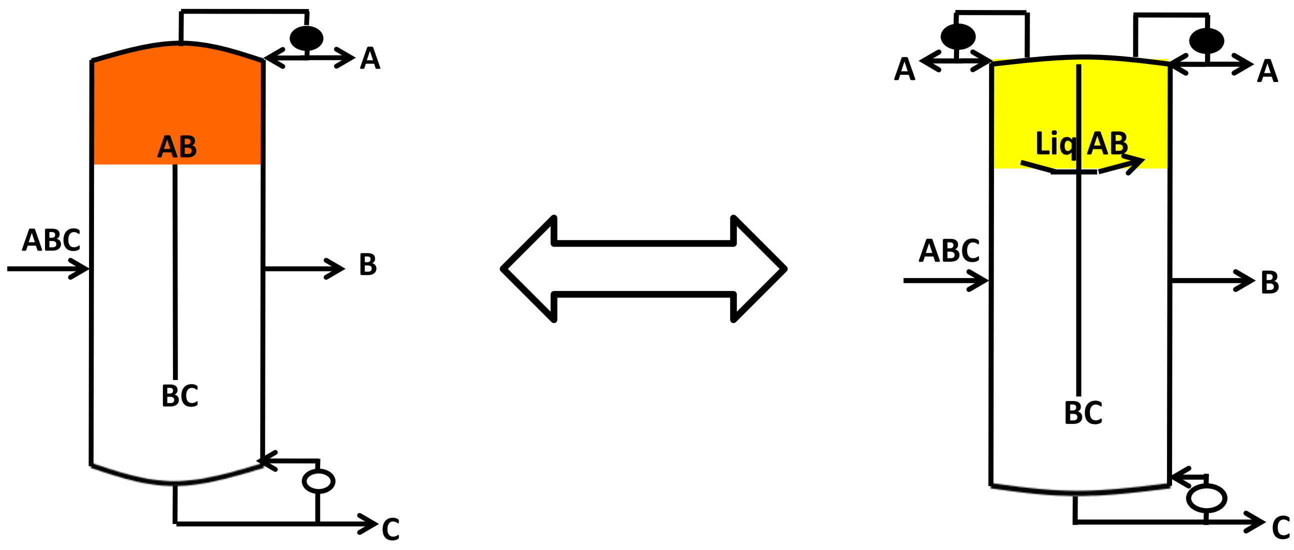
Technical Innovation

We are the first group to overcome the operational challenge



Vapor split can now be easily controlled externally!

Madenoor Ramapriya, Tawarmalani, Agrawal, AIChE Journal, 2014

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Technical Innovation

We are also the first group to synthesize ALL possible operable DWCs

n	DWCs	Vapor Flow Control
3	4	3
4	36	15
5	576	105
6	14,400	945
7	518,400	10,395

Madenoor Ramapriya, Tawarmalani, Agrawal, AIChE Journal, 2016

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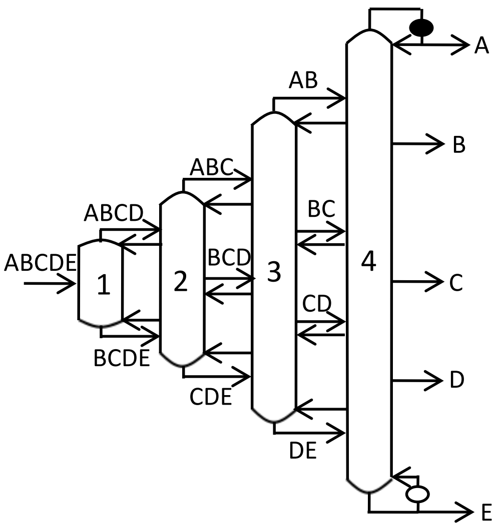
Technical Innovation

We developed a hitherto unknown theory of process intensification

A Case Study -> $\{\alpha_{AB}, \alpha_{BC}, \alpha_{CD}, \alpha_{DE}\} = \{1.1, 1.1, 2.5, 2.5\}$;
$\{f_A, f_B, f_C, f_D, f_E\} = \{0.3, 0.05, 0.05, 0.3, 0.3\}$

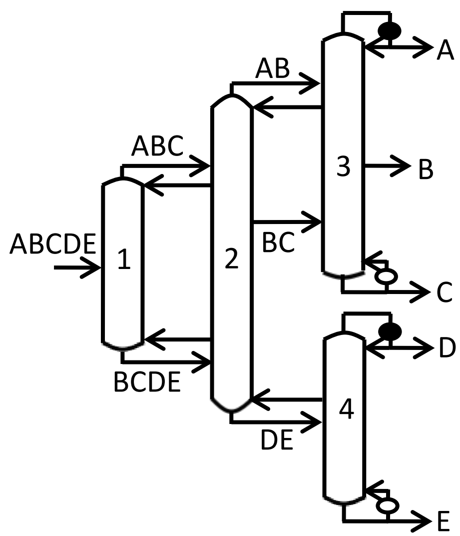
Least Energy Consuming Configuration



Vap Duty = 1

20 sections

From GMA



Vap Duty = 1.14

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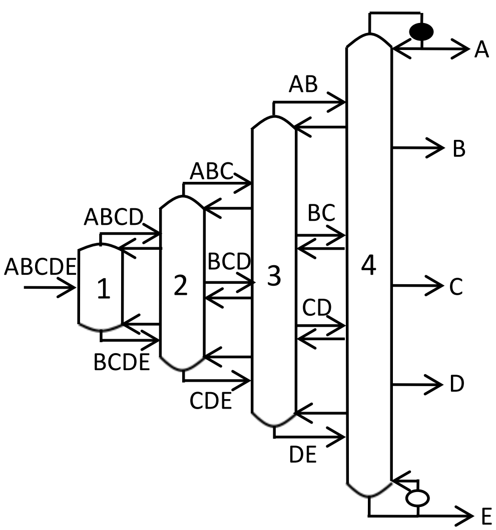
Technical Innovation

Strategy 1: Combining columns to integrate heat and mass transfer

A Case Study -> $\{\alpha_{AB}, \alpha_{BC}, \alpha_{CD}, \alpha_{DE}\} = \{1.1, 1.1, 2.5, 2.5\}$;
$\{f_A, f_B, f_C, f_D, f_E\} = \{0.3, 0.05, 0.05, 0.3, 0.3\}$

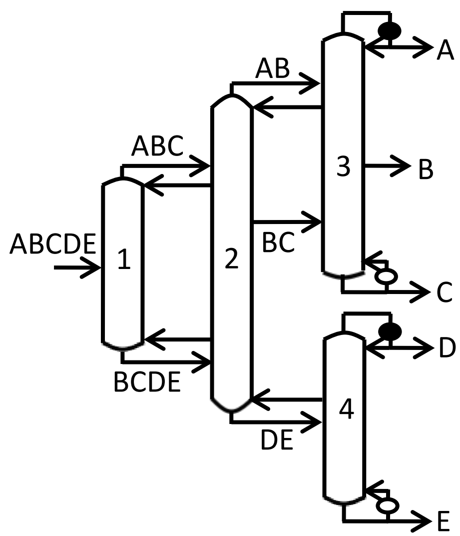
Least Energy Consuming Configuration



Vap Duty = 1

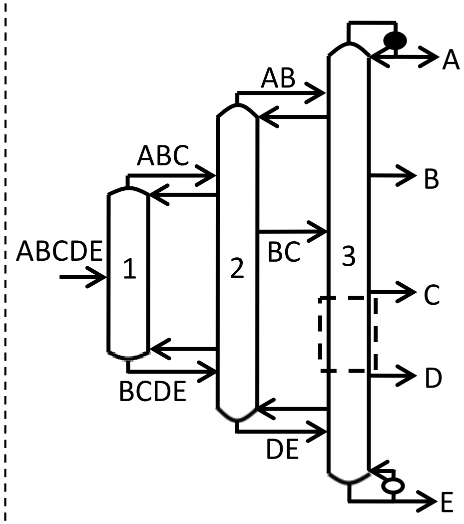
20 sections

From GMA



Vap Duty = 1.14

Process Intensification: Combine Columns



Vap Duty = 1

3 Columns

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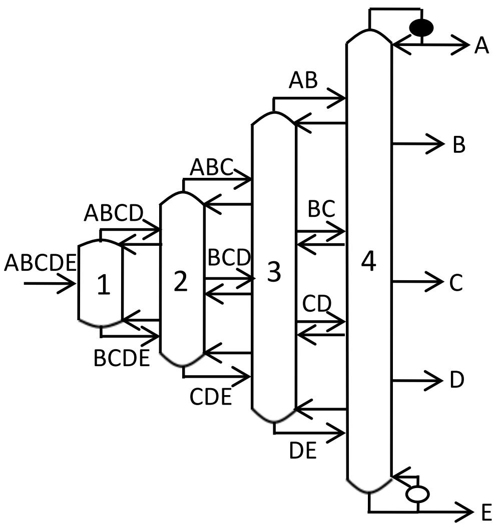
Technical Innovation

Strategy 2: Further reduce the number of columns with DWC

A Case Study -> $\{\alpha_{AB}, \alpha_{BC}, \alpha_{CD}, \alpha_{DE}\} = \{1.1, 1.1, 2.5, 2.5\};$

$\{f_A, f_B, f_C, f_D, f_E\} = \{0.3, 0.05, 0.05, 0.3, 0.3\}$

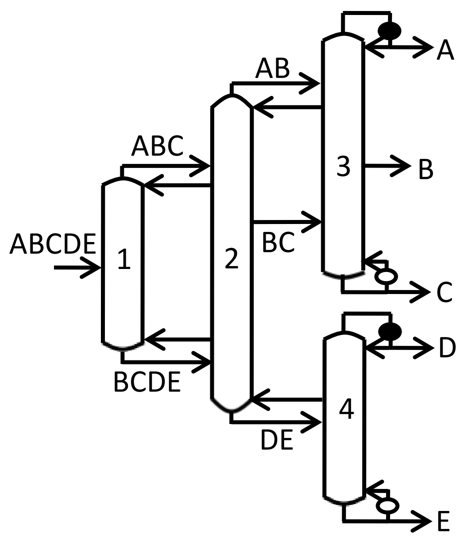
Least Energy Consuming Configuration



Vap Duty = 1

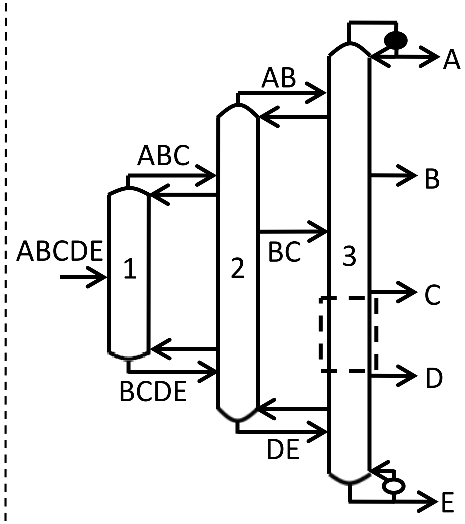
20 sections

From GMA



Vap Duty = 1.14

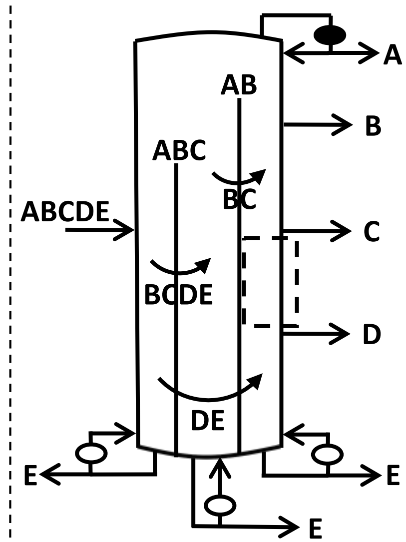
Process Intensification: Combine Columns



Vap Duty = 1

3 Columns

Process Intensification: DWC



Vap Duty = 1

Only 1 Column

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Transition (beyond DOE assistance)

- 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), LNG, petroleum crude
  - Biochemicals – e.g. pyrolysis, fermentation, gasification
- Process designers in above industries are prime users
  - New plants and facilities
  - Retrofit of current plants and facilities

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Transition (beyond DOE assistance)

- Leveraging experience and expertise of Purdue Office of Technology Commercialization to commercialize our software
  - Filed technology disclosures to the latest computer programs
  - Decided the structure of the start-up company
  - Identified an individual who will be in charge of the company
- Industrial internships at the various participating companies
  - Eastman Chemical (Summer 2015), Dow Chemical (Summer 2016)
  - Gathered feedback from process engineers to enhance usability and user-friendliness of the software
- Hired a vendor (Abnaki Light Industry, Inc.) to convert academic tool to commercial software
  - A brand new software has been created and is on its way towards commercialization by December 2017

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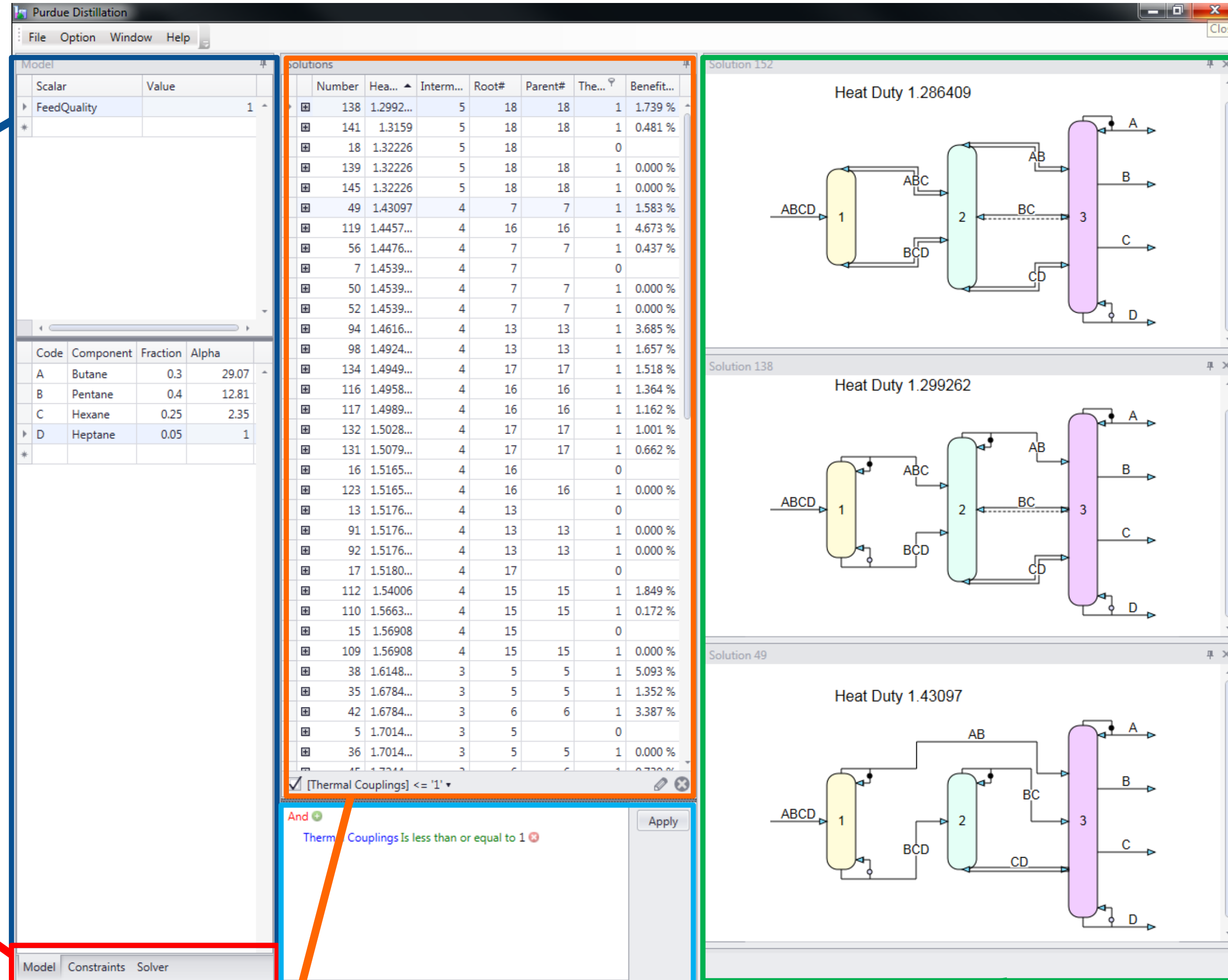
Demo Software



Define model parameters

- Impose constraints
- Solve the model

Ranklist the solutions

Filter the solutions

Visualize the configurations

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Transition (beyond DOE assistance)

- Various companies showing great interests in our methodology and software tool
    - Signed agreement with ExxonMobil to use our algorithms for real industrial applications at their refineries
    - Approached by SABIC regrading purchasing the software as soon as it is ready for commercialization
- Having dialogues with DOE RAPID (Rapid Advancement in Process Intensification Deployment)
    - Communicated with RAPID's CTO – Dr. Jim Bielenberg, and Dr. Tom Edgar from RAPID's Chemical and Commodity Processing sector
    - Will participate in RAPID's weekly roadmapping calls and workshops
- Actively engaging in technical presentations and talks to introduce our research products
    - AIChE Spring Meeting, Annual Meeting, AIChE webinar
    - International conferences (Portugal, Belgium, etc.)

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Measure of Success

- Commercialization of our software
- Applications from ExxonMobil for the next 3 years
    - Demonstration of energy and cost savings of the new configurations at ExxonMobil refineries
- Convincing RAPID to design and build new DWCs
- Ultimate impacts on world's energy and environmental landscapes
    - 30-50% reduction in 3% of total world energy consumption
    - Significant environmental impact in terms of reduction in CO_2 emissions
    - In addition, the CAPEX and OPEX goes down by 30-50%

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Project Management & Budget

- Duration of the project: Three years (2015-2017)

Task	Task name	Duration
5	MINLP formulation for vapor duty and total cost	Q9 – Q12
7	Commercialization of the software	Q9 – Q12
8	Software for operable configurations	Q11 – Q12
9	Retrofit Options	Q12
11	Minimum reflux for complex columns	Q9 – Q12

Total Project Budget	
DOE Investment	900,000
Cost Share	251,708
Project Total	1,151,708

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