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

DE-EE0005768

Purdue University

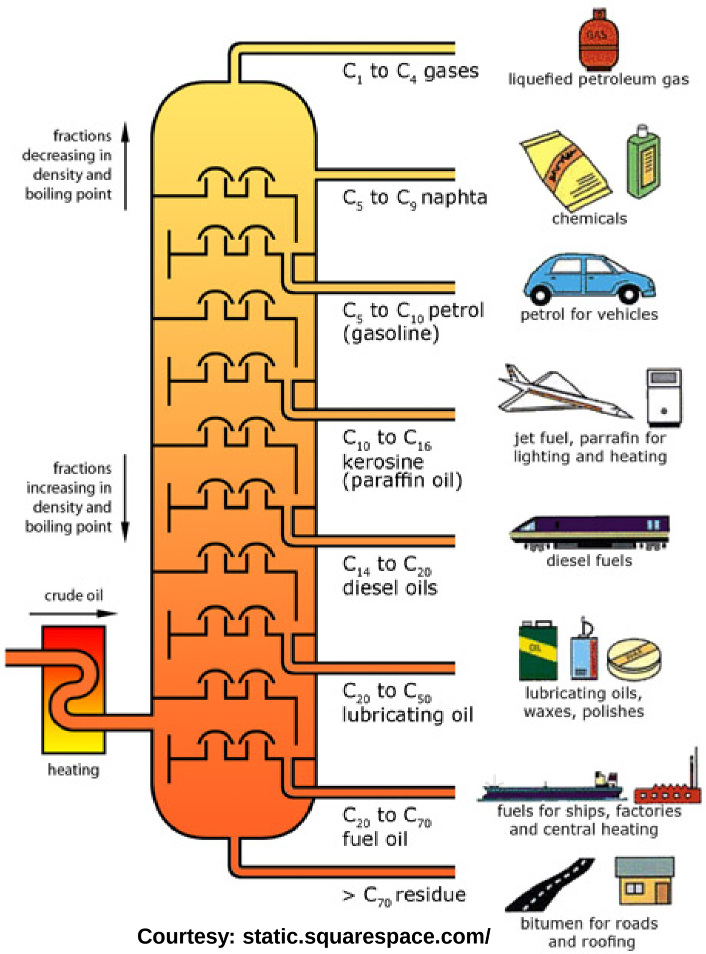
12/15/2014 to 12/14/2017

Rakesh Agrawal,
School of Chemical Engineering,
Purdue University

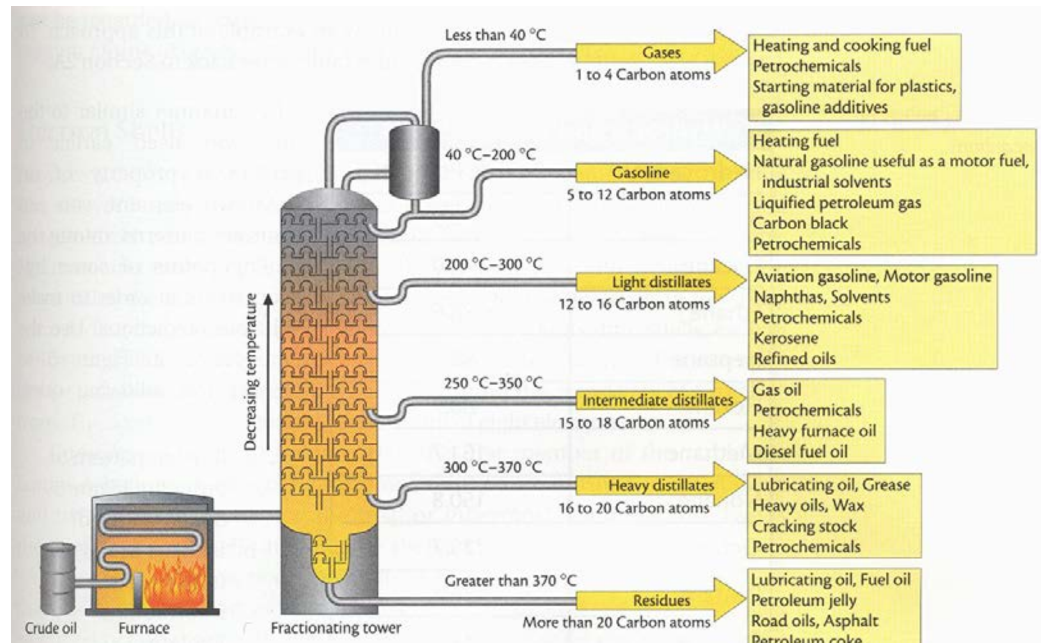
U.S. DOE Advanced Manufacturing Office Program Review Meeting
Washington, D.C.
June 14-15, 2016

Project Objective

Distillation: Essential to Meet Human Needs



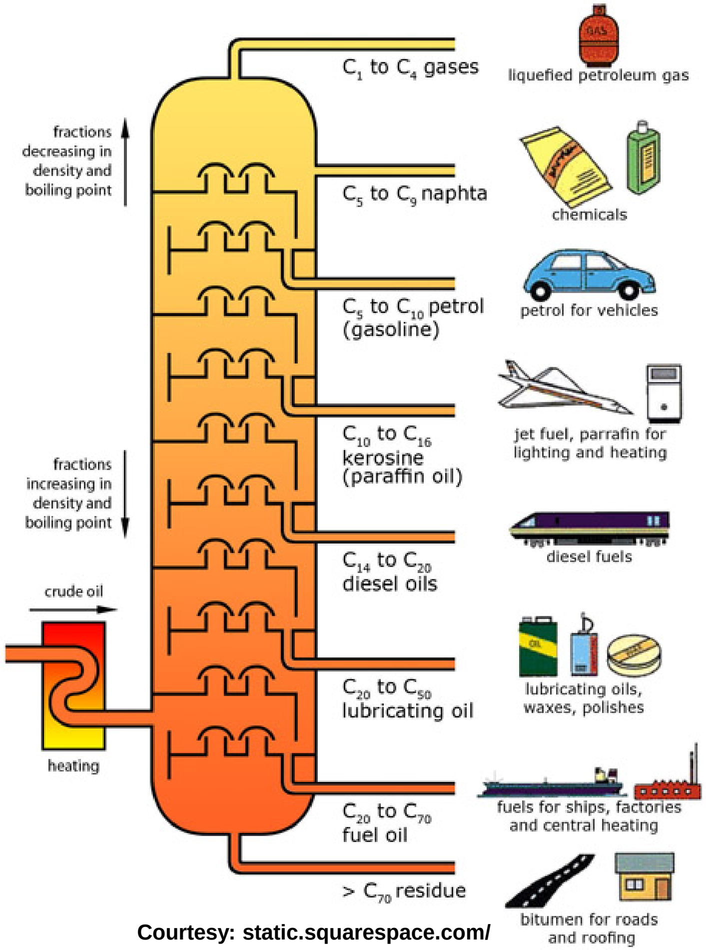
Courtesy: static.squarespace.com/



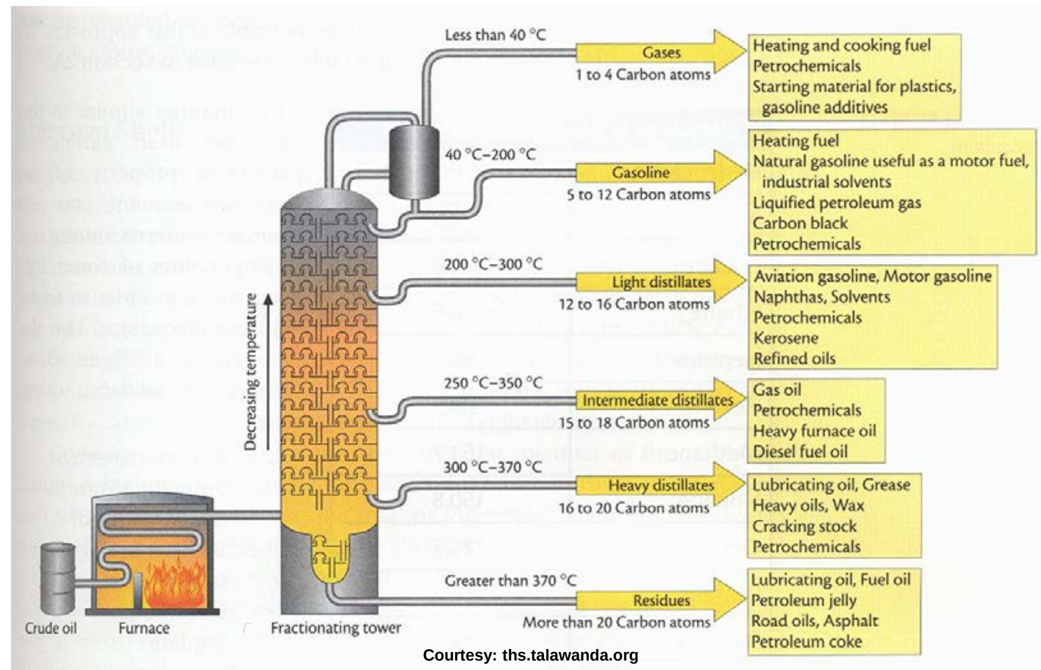
Courtesy: ths.talawanda.org

Project Objective

Distillation: Essential to Meet Human Needs



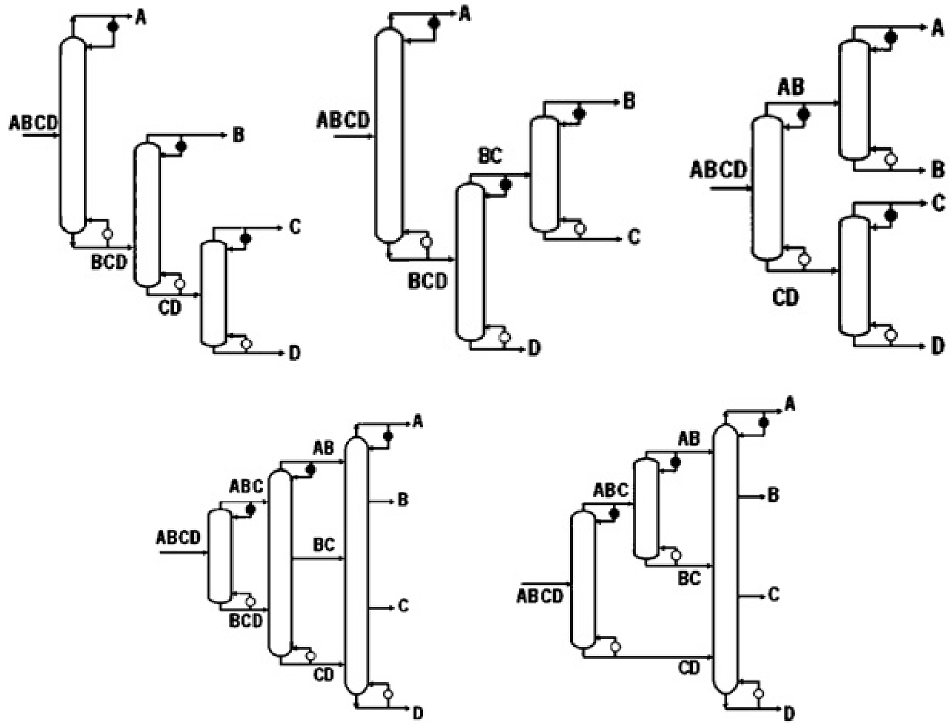
Courtesy: static.squarespace.com/



- Multicomponent distillation: ubiquitous in all chemical and biochemical plants
- Distillation accounts for ~3% of the world’s energy consumption
- US refineries: ~0.4 million bbl of oil per day for crude oil distillation alone

Project Objective

However, Many Multicomponent Configurations Exist

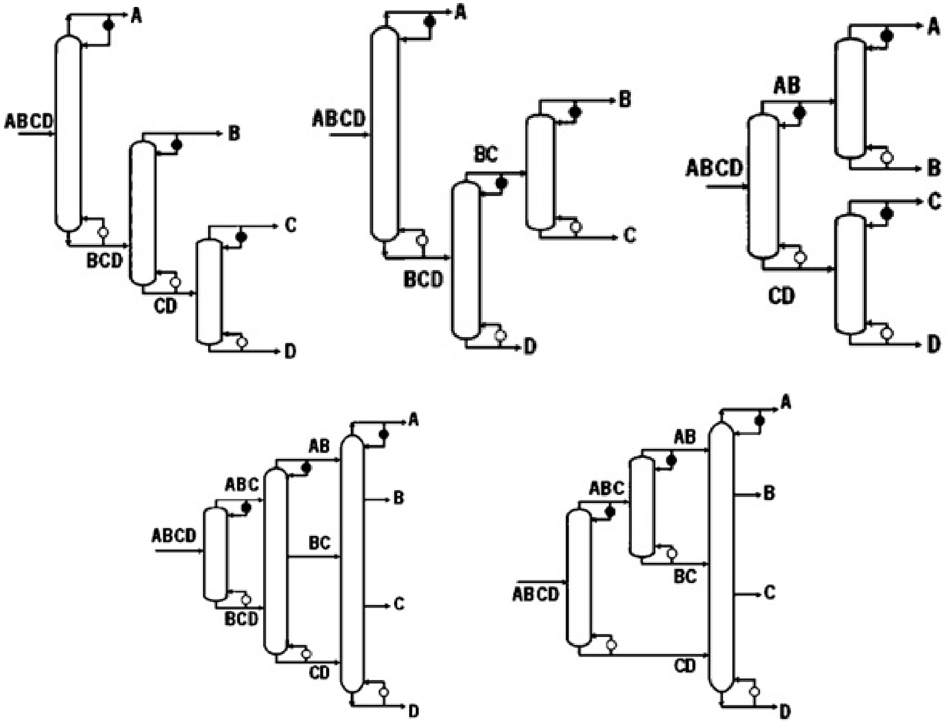


Current Industrial Practice:

- **Unable to generate numerous configurations**
- **Use of heuristics, experience, guess, trial and error**
- **Often results in energy-inefficient plants**

Project Objective

Find the Most Cost Effective Multicomponent Configuration



Our Goal: Provide an easy to use stepwise method to:

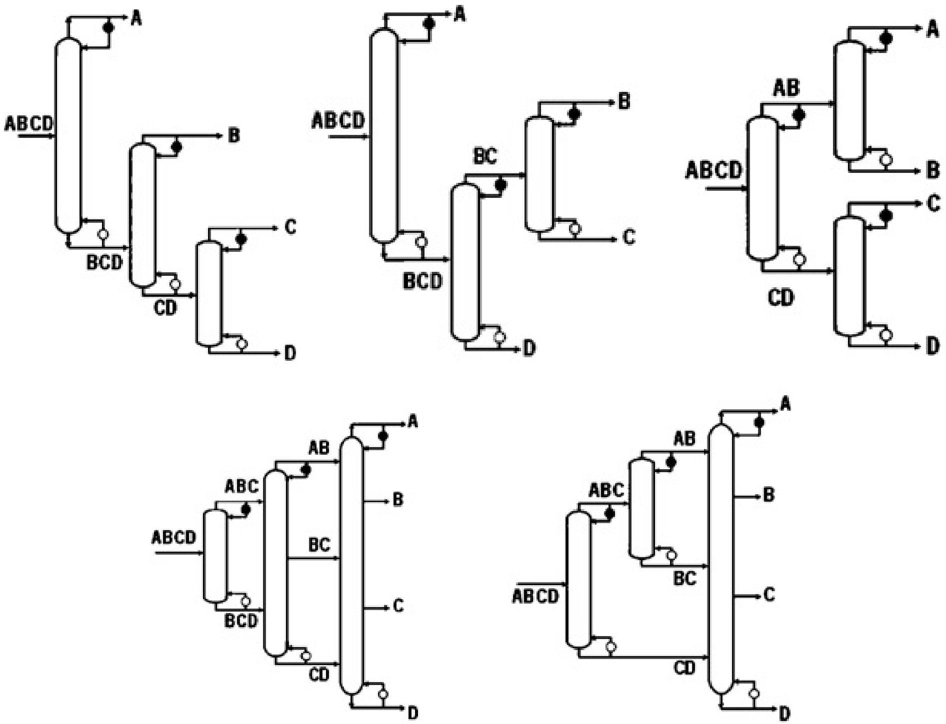
- **create the entire search space of distillation configurations,**
- **perform process intensification,**
- **Identify the lowest cost (optimal) configuration among them.**

Technical Innovation

First Step: Generate All Possible Configurations[1]

- Systematic and easy-to-use method to generate complete set of basic distillation configurations[1]

Number of components in feed	Number of configurations
3	8
4	152
5	6,128
6	506,912
7	85,216,192
8	2.9E+10

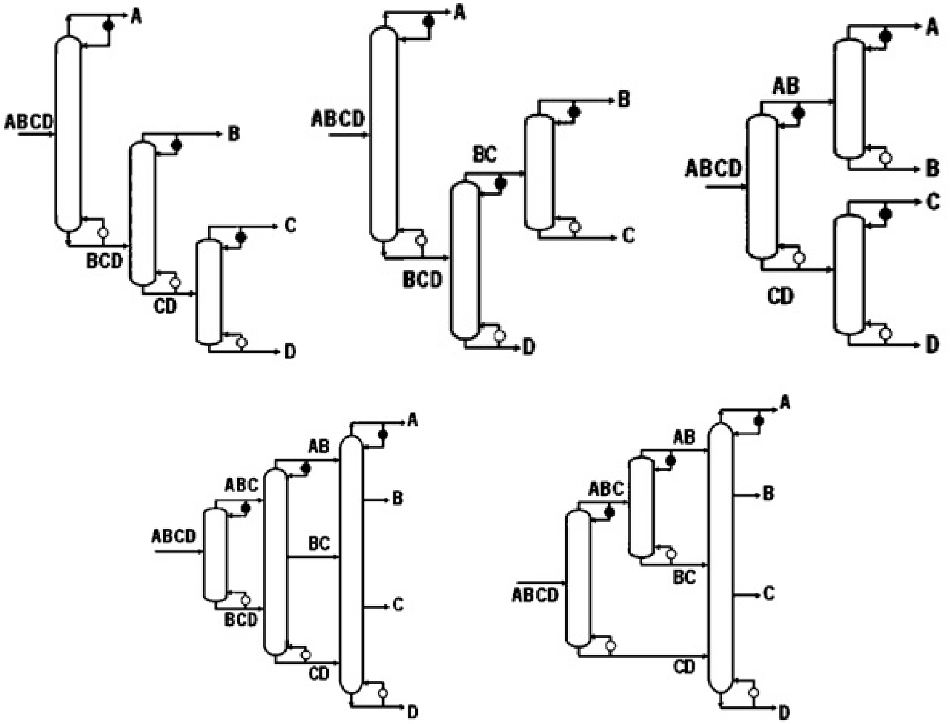


Shah & Agrawal, AIChEJ, 2010

Technical Innovation

- Systematic and easy-to-use method to generate complete set of basic distillation configurations[1]

Number of components in feed	Number of configurations
3	8
4	152
5	6,128
6	506,912
7	85,216,192
8	2.9E+10



Next Step: How to identify low cost configurations?

Technical Innovation

Global Minimization Algorithm (GMA)

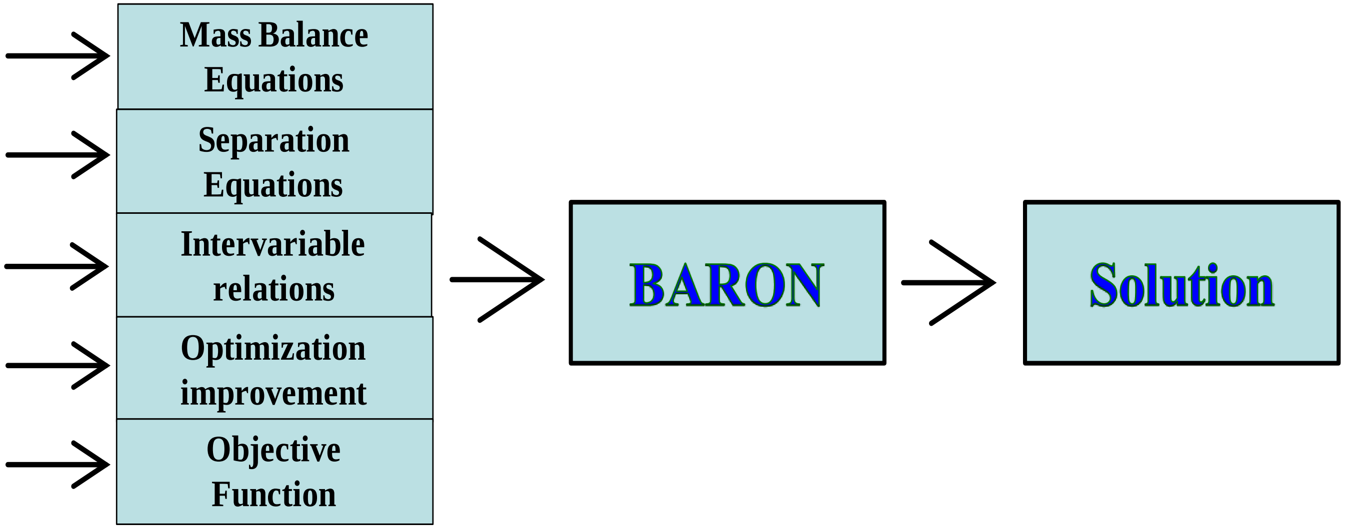
$$f_{i,AB} + f_{i,CD} = f_{i,ABCD}$$

$$\sum_{i} \frac{\alpha_i f_{i,dist}}{\alpha_i - \theta_j} \leq V_S$$

$$LTC_i + VTC_i = FTC_i$$

$$\sum_{i=1:n-1} V_{col,i} \leq V_{transition}$$

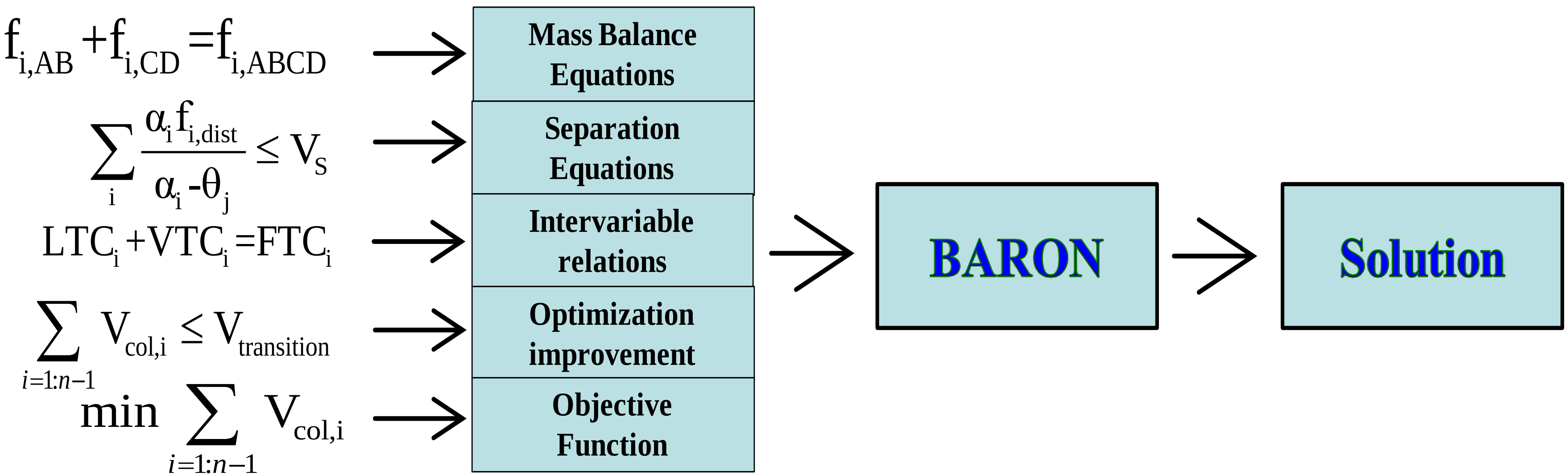
$$\min \sum_{i=1:n-1} V_{col,i}$$



Strategies: Additional (distillation) constraints, variable bounds, initial guesses -> the elusive global optimum attained!!

Technical Innovation

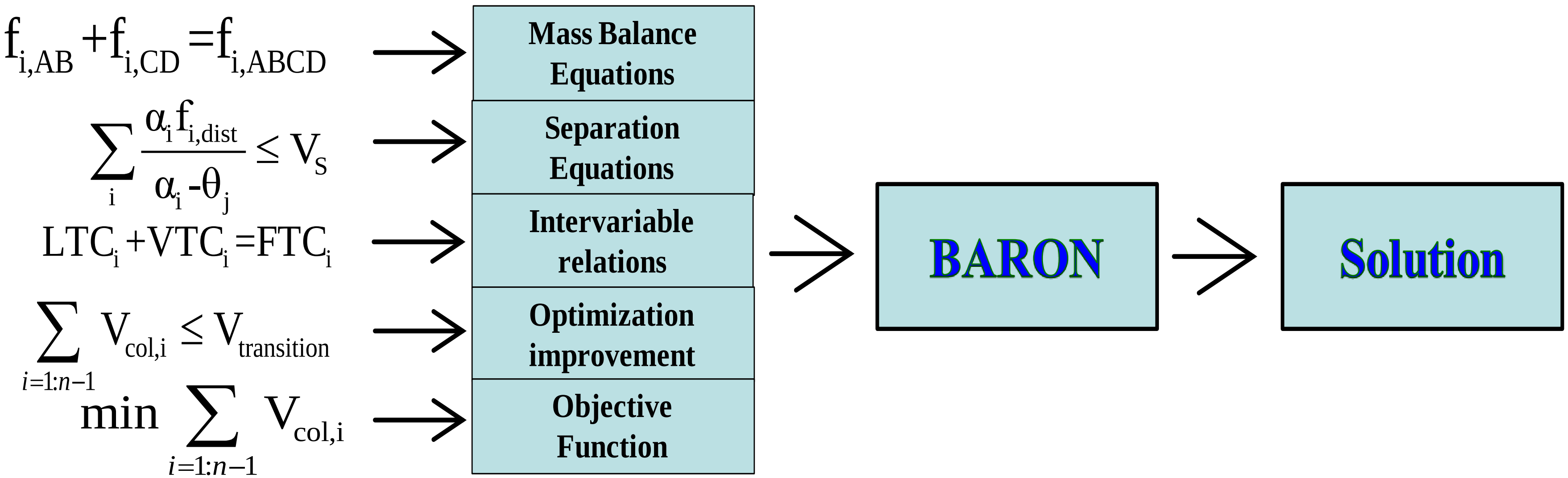
Considerable Progress Under Previous AMO Support



- **Under previous AMO support:**
  - **Developed a model to minimize heat duty**
  - **~6000 out of 6128 configurations for 5-component separations solved in 16+ hours of CPU time**
  - **However, a few (~100) un-converged configurations remained**

Technical Innovation

Now remaining challenges have been solved



- **Under current AMO support:**
  - **Models for both heat duty and total cost completed**
  - **All 6128 configurations solved for energy in 3.5 hours of CPU time!**
  - **First group to identify the global optimum and to rank-list distillation configurations**

Technical Innovation

Petroleum Crude Distillation

Typical fractions obtained by crude distillation:

Naphtha (A), Kerosene (B), Diesel (C), Gas Oil (D) and Residue (E)

Hence, consider crude as 5-component mixture ABCDE

Technical Innovation

Petroleum Crude Distillation

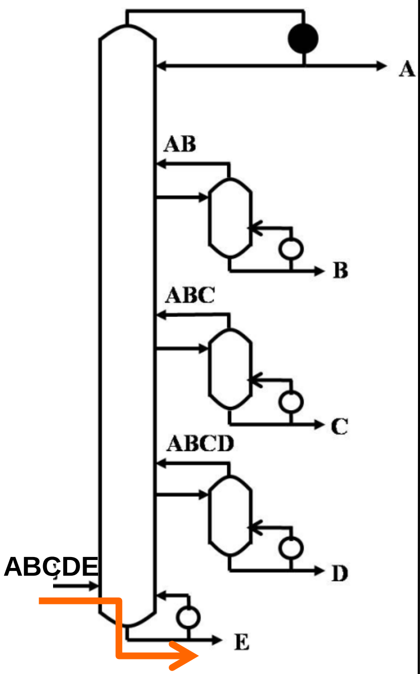
Light Crude

Component	Relative Volatility	Mole %
A	45.3	46.1
B	14.4	19.5
C	4.7	7.3
D	2.0	11.4
E	1.0	15.7

Technical Innovation

Light Petroleum Crude Distillation

Conventional Configuration

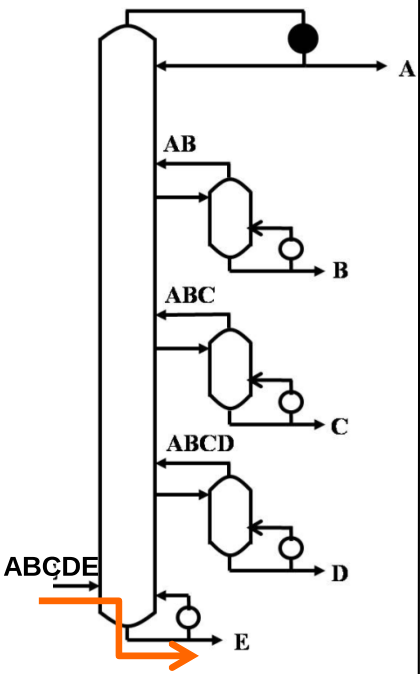


Vap Duty = 1

Technical Innovation

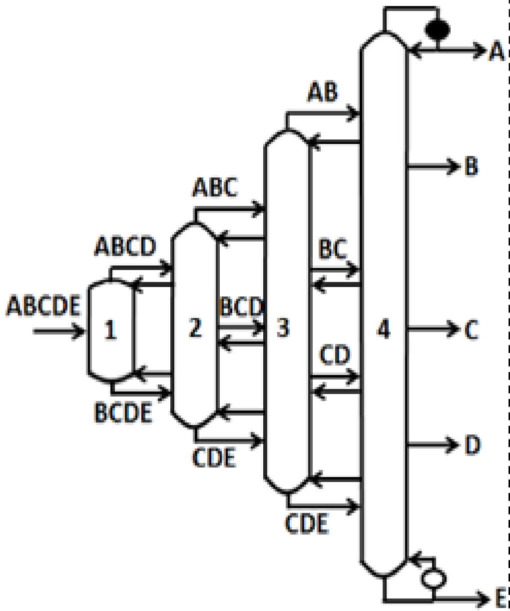
Light Petroleum Crude Distillation (Results from GMA)

Conventional Configuration



Vap Duty = 1

Least Energy Consuming Configuration

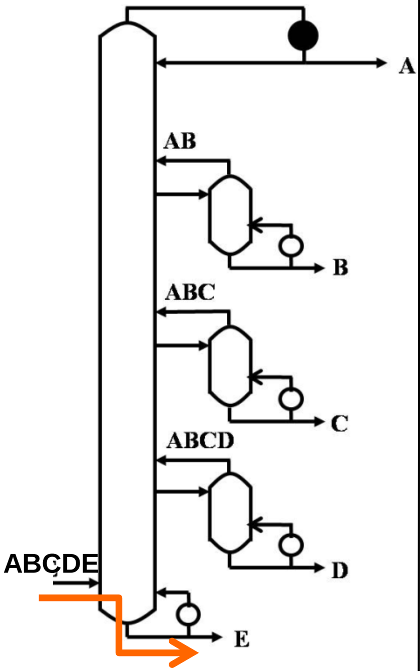


Vap Duty = 0.74

Technical Innovation

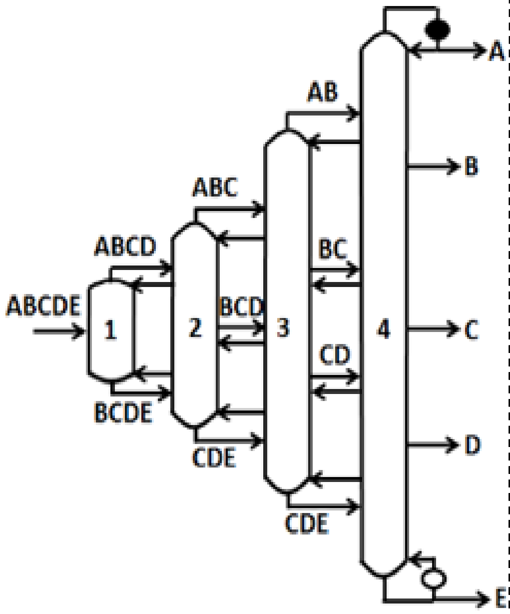
Light Petroleum Crude Distillation (Results from GMA)

Conventional Configuration



Vap Duty = 1

Least Energy Consuming Configuration



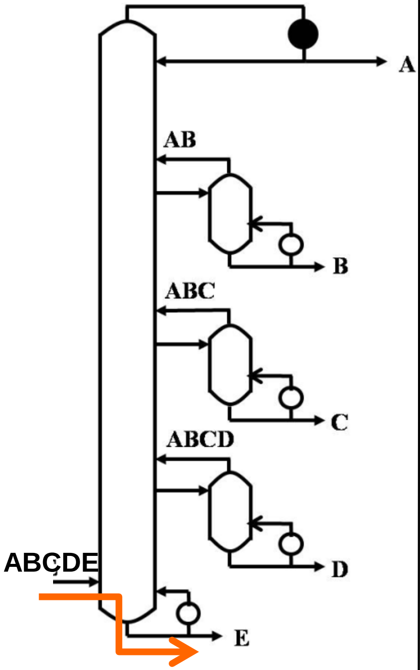
Vap Duty = 0.74

20 sections

Technical Innovation

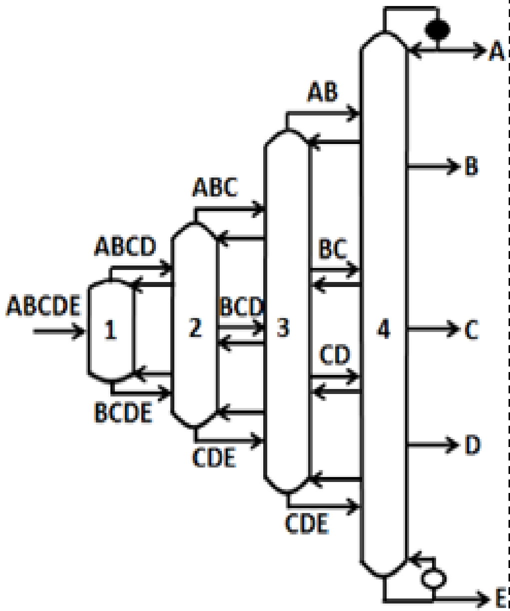
Light Petroleum Crude Distillation (Results from GMA)

Conventional Configuration



Vap Duty = 1

Least Energy Consuming Configuration



Vap Duty = 0.74

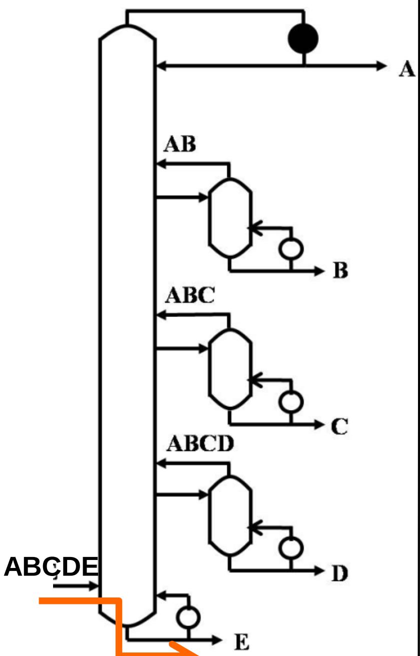
20 sections

Challenge: Keep same energy consumption, but reduce sections?

Technical Innovation

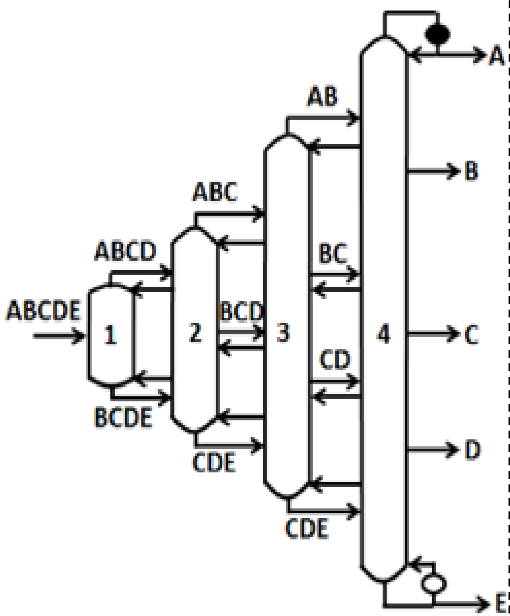
Light Petroleum Crude Distillation (Results from GMA)

Conventional Configuration



Vap Duty = 1

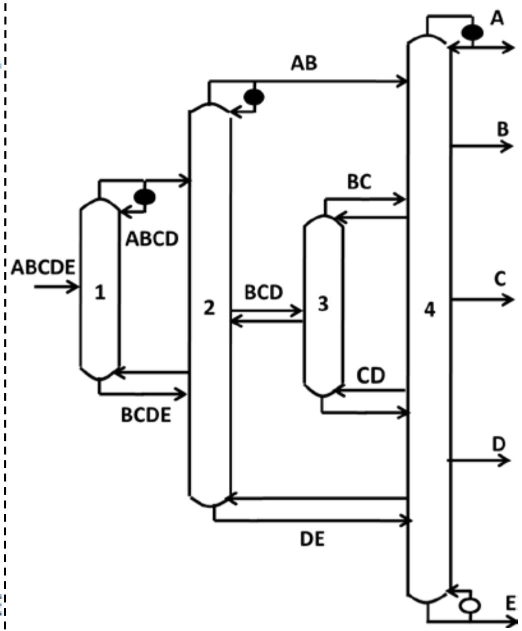
Least Energy Consuming Configuration



Vap Duty = 0.74

20 sections

Challenge: Keep same energy consumption, but reduce sections?



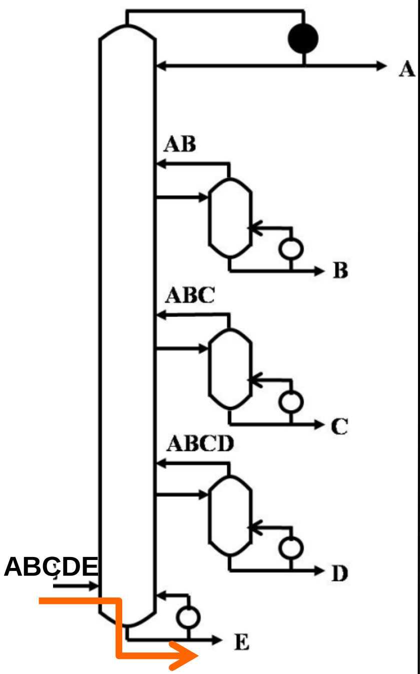
Vap Duty = 0.74

16 sections

Technical Innovation

Light Petroleum Crude Distillation (Results from GMA)

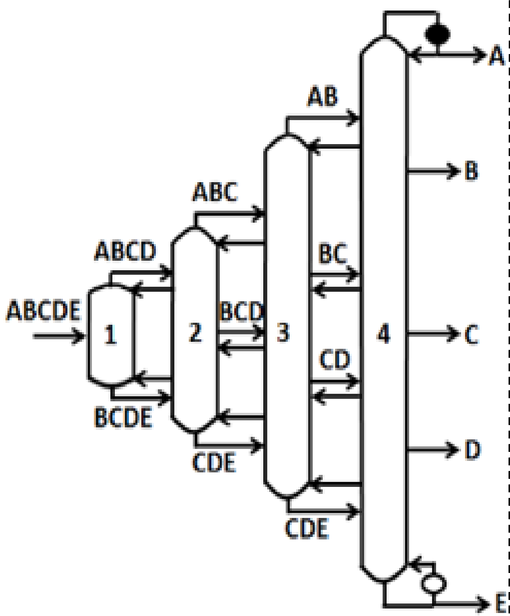
Conventional Configuration



Vap Duty = 1

Total Cost = 1

Least Energy Consuming Configuration

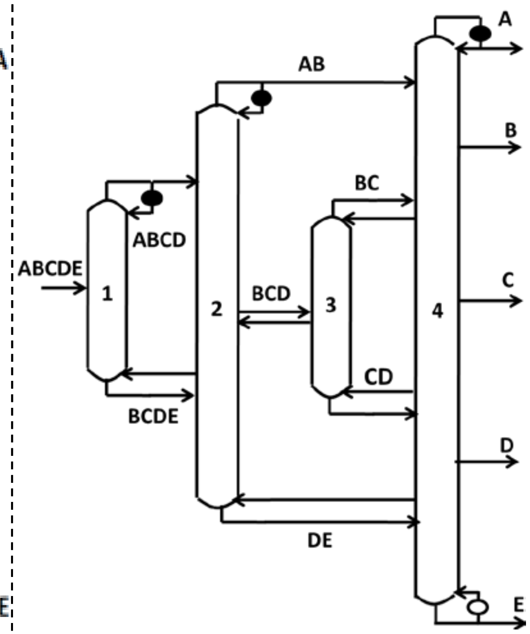


Vap Duty = 0.74

20 sections

Total Cost = 0.614

Challenge: Keep same energy consumption, but reduce sections?



Vap Duty = 0.74

16 sections

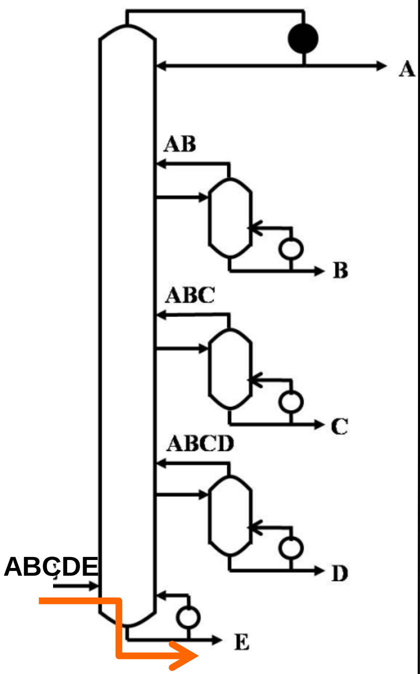
Total Cost = 0.57

(A further 7.1% ↓)

Technical Innovation

Light Petroleum Crude Distillation (Results from GMA)

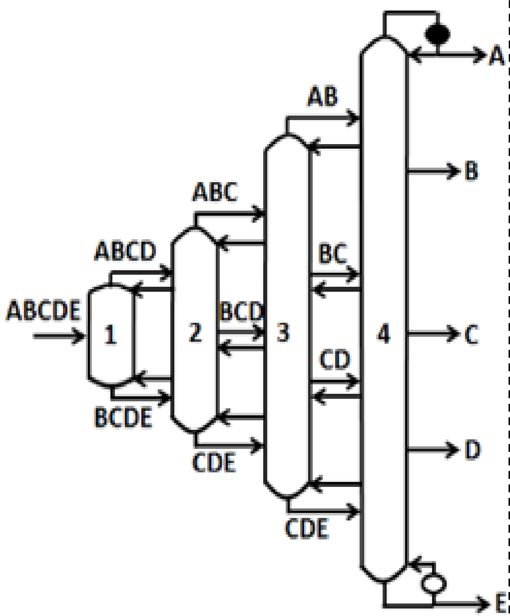
Conventional Configuration



Vap Duty = 1

Total Cost = 1

Least Energy Consuming Configuration

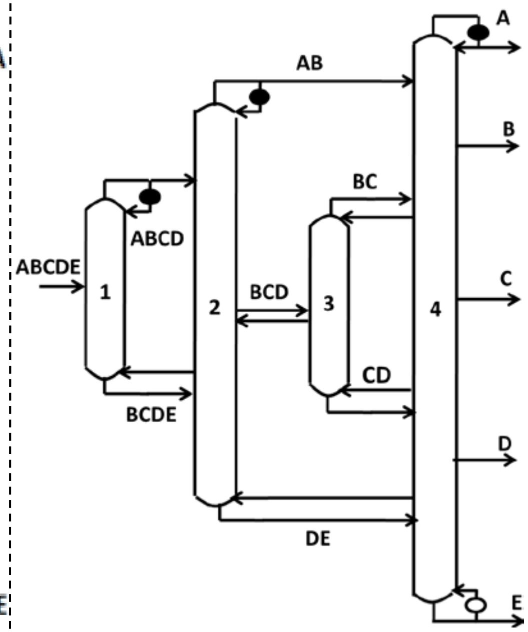


Vap Duty = 0.74

20 sections

Total Cost = 0.614

Challenge: Keep same energy consumption, but reduce sections?



Vap Duty = 0.74

16 sections

Total Cost = 0.57

(A further 7.1% ↓)

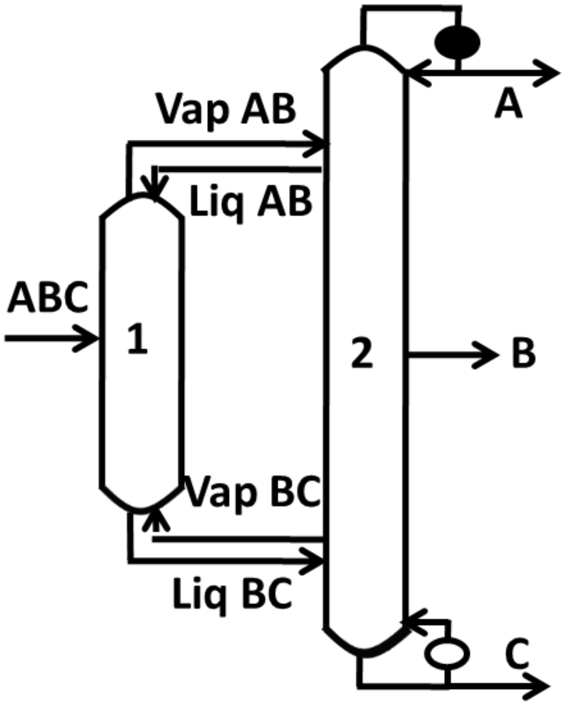
Process Intensification:

New Dividing Wall Columns (DWCs)

Technical Innovation

What is a Dividing Wall Column (DWC)?

A Three-component Configuration

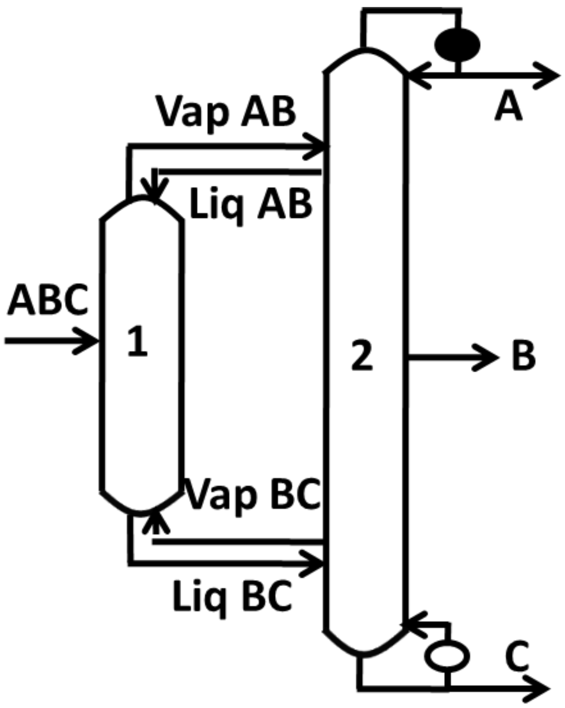


2 Distillation Columns

Technical Innovation

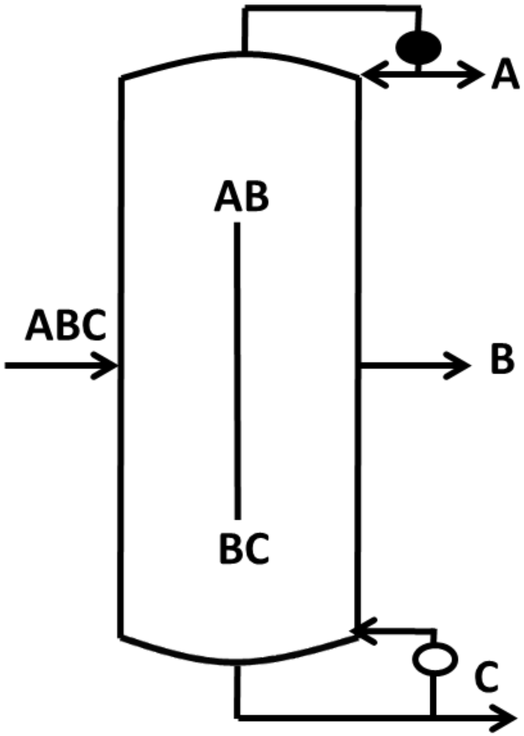
What is a Dividing Wall Column (DWC)?

A Three-component Configuration



2 Distillation Columns

Dividing Wall Column (DWC)



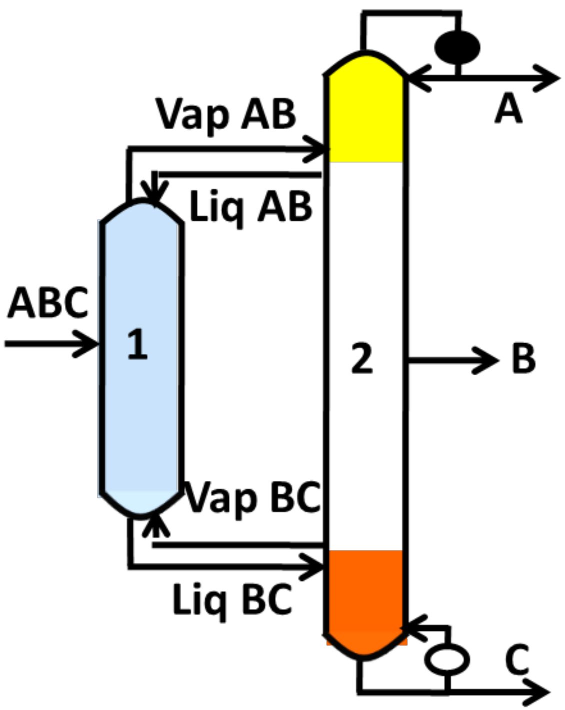
1 Distillation Column

Wright 1949

Technical Innovation

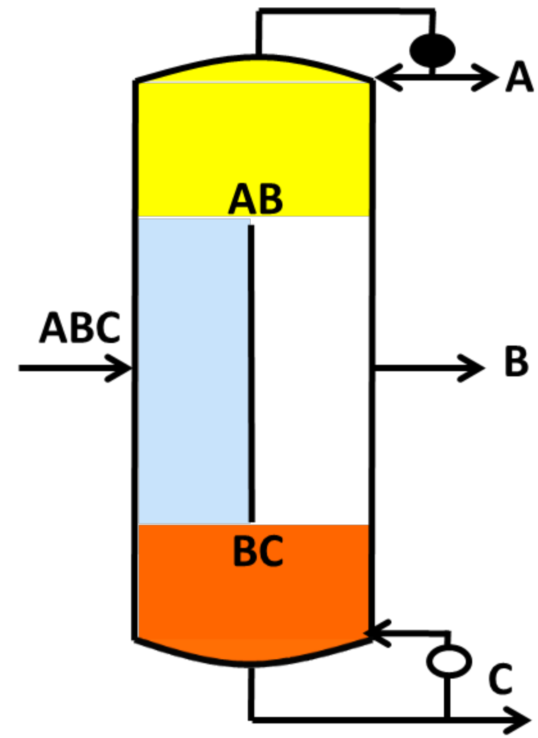
What is a Dividing Wall Column (DWC)?

A Three-component Configuration



2 Distillation Columns

Dividing Wall Column (DWC)



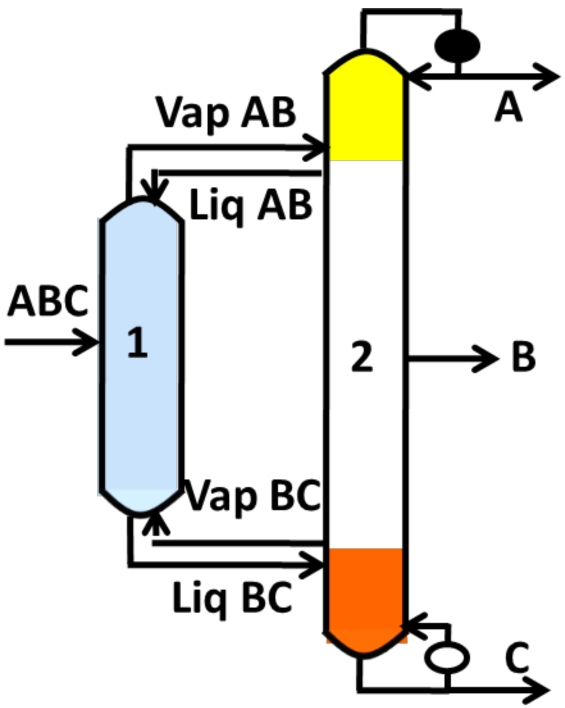
1 Distillation Column

Wright 1949

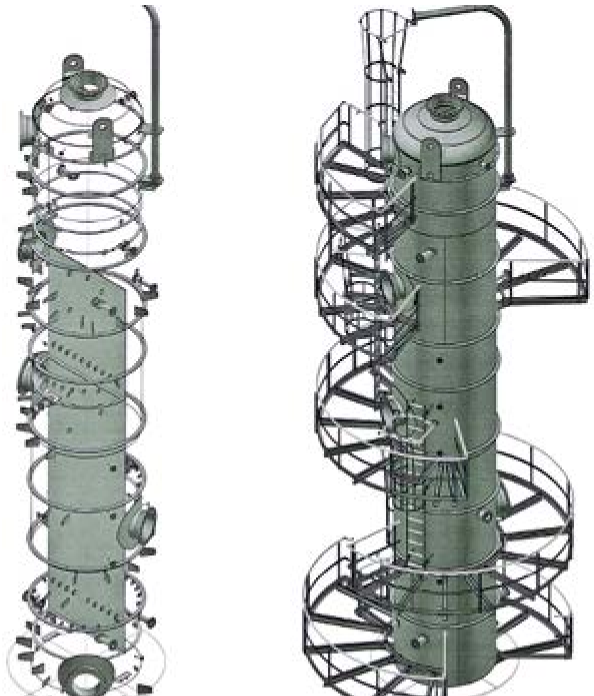
Technical Innovation

What is a Dividing Wall Column (DWC)?

A Three-component Configuration



2 Distillation Columns

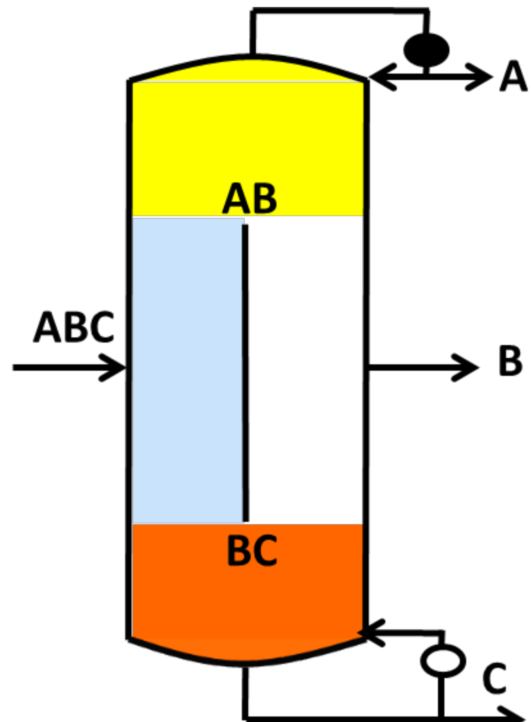


Courtesy: http://www.hydrocarbonprocessing.com/

Courtesy: http://www.cpp-net.com/

Wright 1949

Dividing Wall Column (DWC)

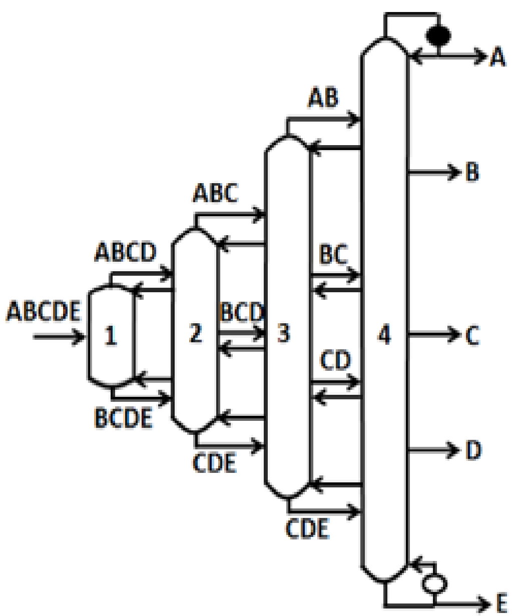


1 Distillation Column

Technical Innovation

We Have Introduced A Method to Draw Operable DWC

Least Energy Consuming Configuration

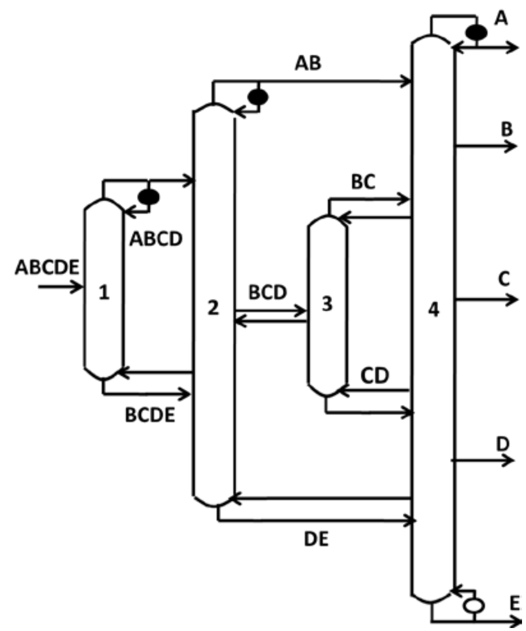


Vap Duty = 0.74

20 sections

Total Cost = 0.614

Challenge: Keep same energy consumption, but reduce sections?



Vap Duty = 0.74

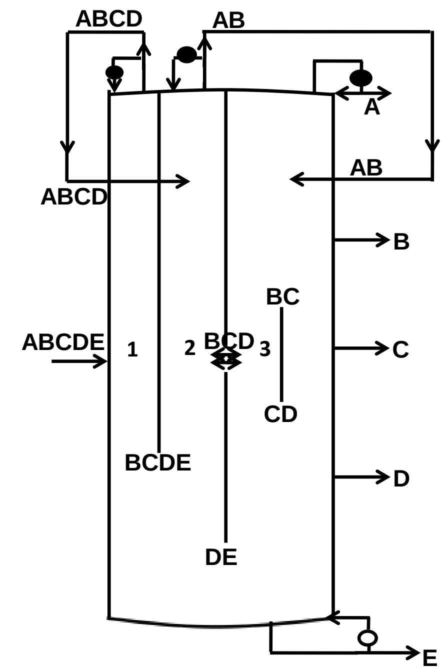
16 sections

Total Cost = 0.57

(A further 7.1% ↓)

Process Intensification:

New Dividing Wall Columns (DWCs)



1 Distillation Column with 16 sections

Technical Innovation

Introduced Additional Process Intensification to Further Reduce Distillation Columns

Technical Innovation

Further Process Intensification

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

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

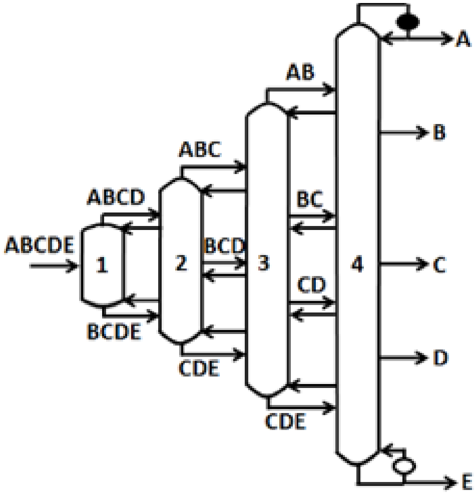
Technical Innovation

Further Process Intensification

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

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

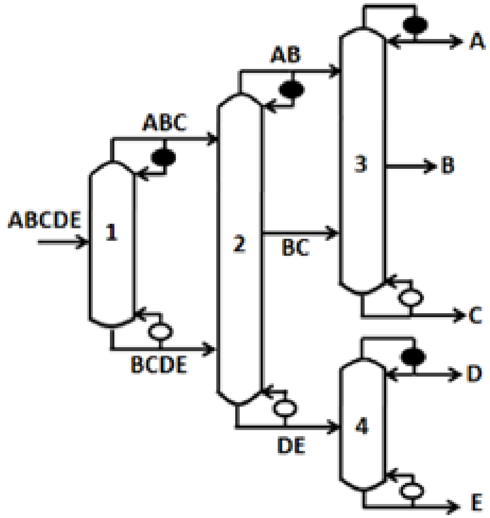
Least Energy Consuming Configuration (from GMA)



Vap Duty = 1

20 sections

From GMA



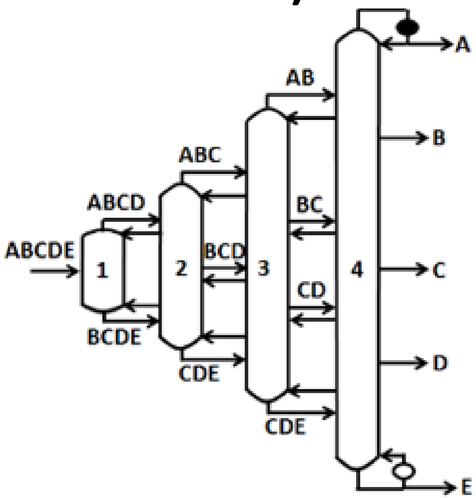
Vap Duty = 1.65

Technical Innovation

Further Process Intensification

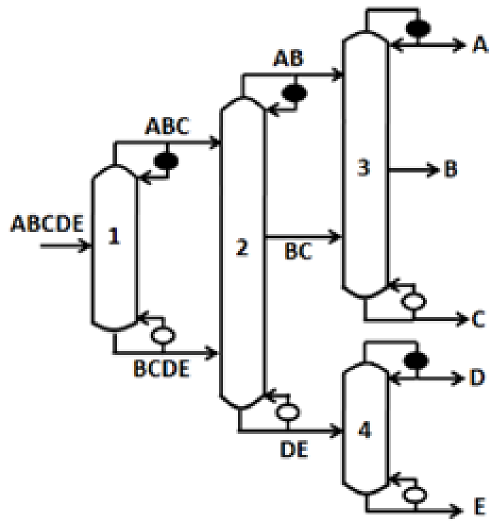
A Case Study -> $\{\alpha_{AB}, \alpha_{BC}, \alpha_{CD}, \alpha_{DE}\} = \{1.1, 1.1, 2.5, 2.5\}$;
$\{f_A, f_B, f_C, f_D, f_E\} = \{0.3, 0.05, 0.05, 0.3, 0.3\}$

Least Energy Consuming Configuration (from GMA)



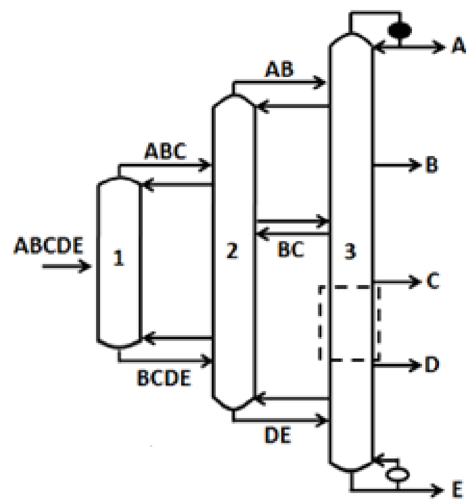
Vap Duty = 1
20 sections

From GMA



Vap Duty = 1.65

Process Intensification:
Combine Columns



Vap Duty = 1
13 sections

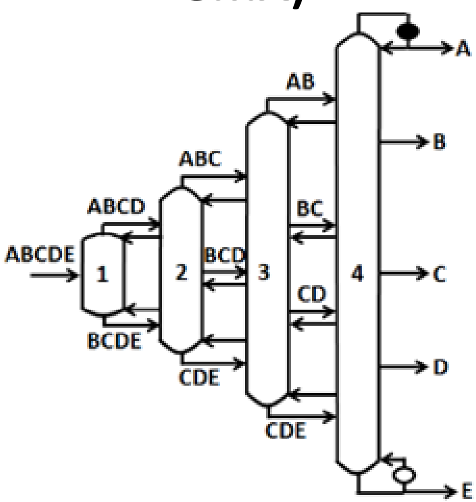
Technical Innovation

Further Process Intensification

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

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

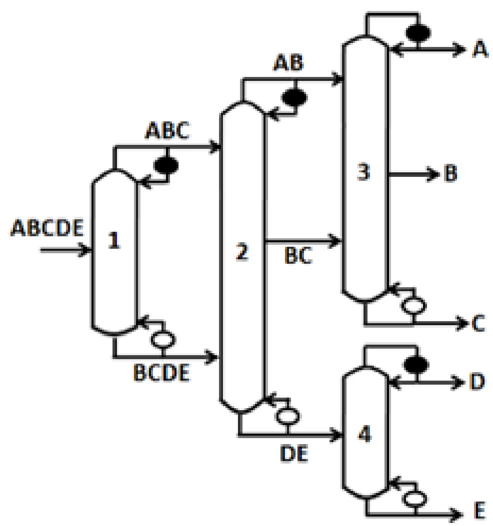
Least Energy Consuming Configuration (from GMA)



Vap Duty = 1

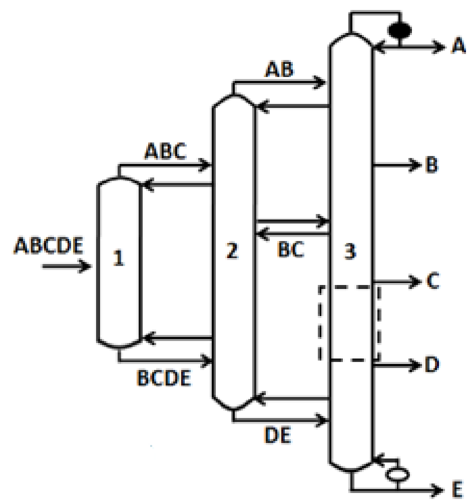
20 sections

From GMA



Vap Duty = 1.65

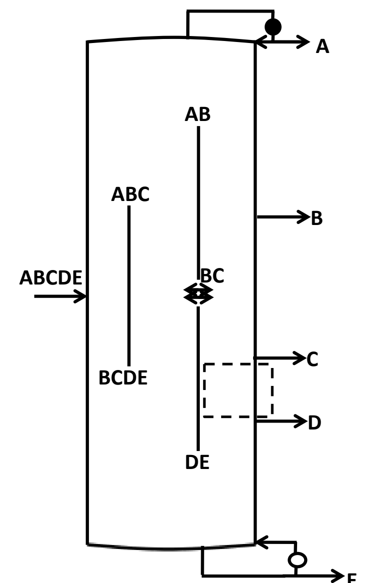
Process Intensification: Combine Columns



Vap Duty = 1

13 sections

Process Intensification: DWC



1 Distillation Column with 13 sections

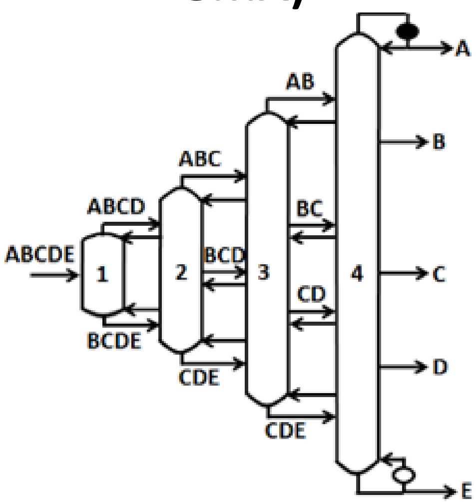
Technical Innovation

Further Process Intensification

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

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

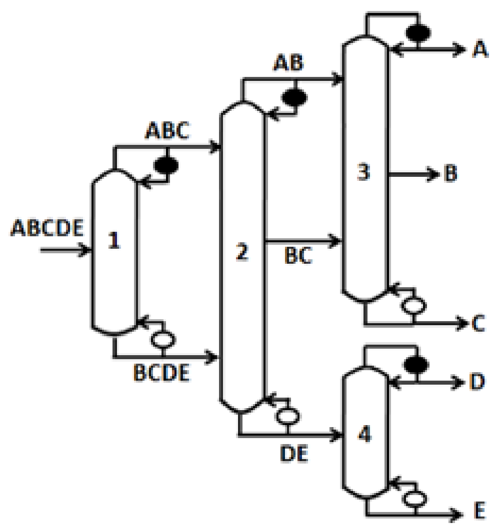
Least Energy Consuming Configuration (from GMA)



Vap Duty = 1

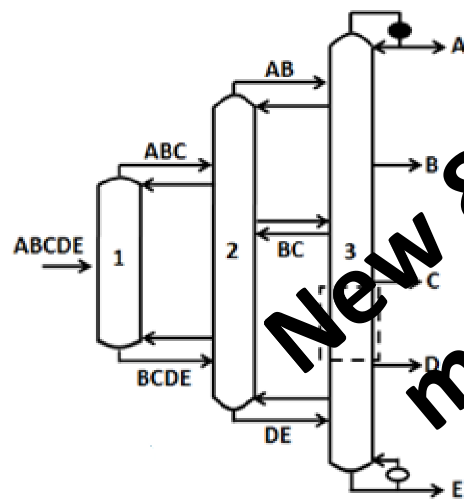
20 sections

From GMA



Vap Duty = 1.65

Process Intensification: Combine Columns

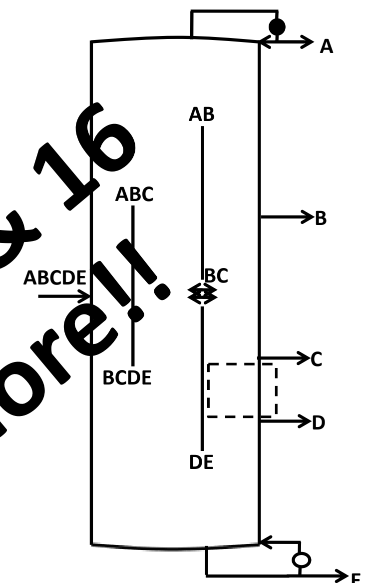


New & 16 more!!

Vap Duty = 1

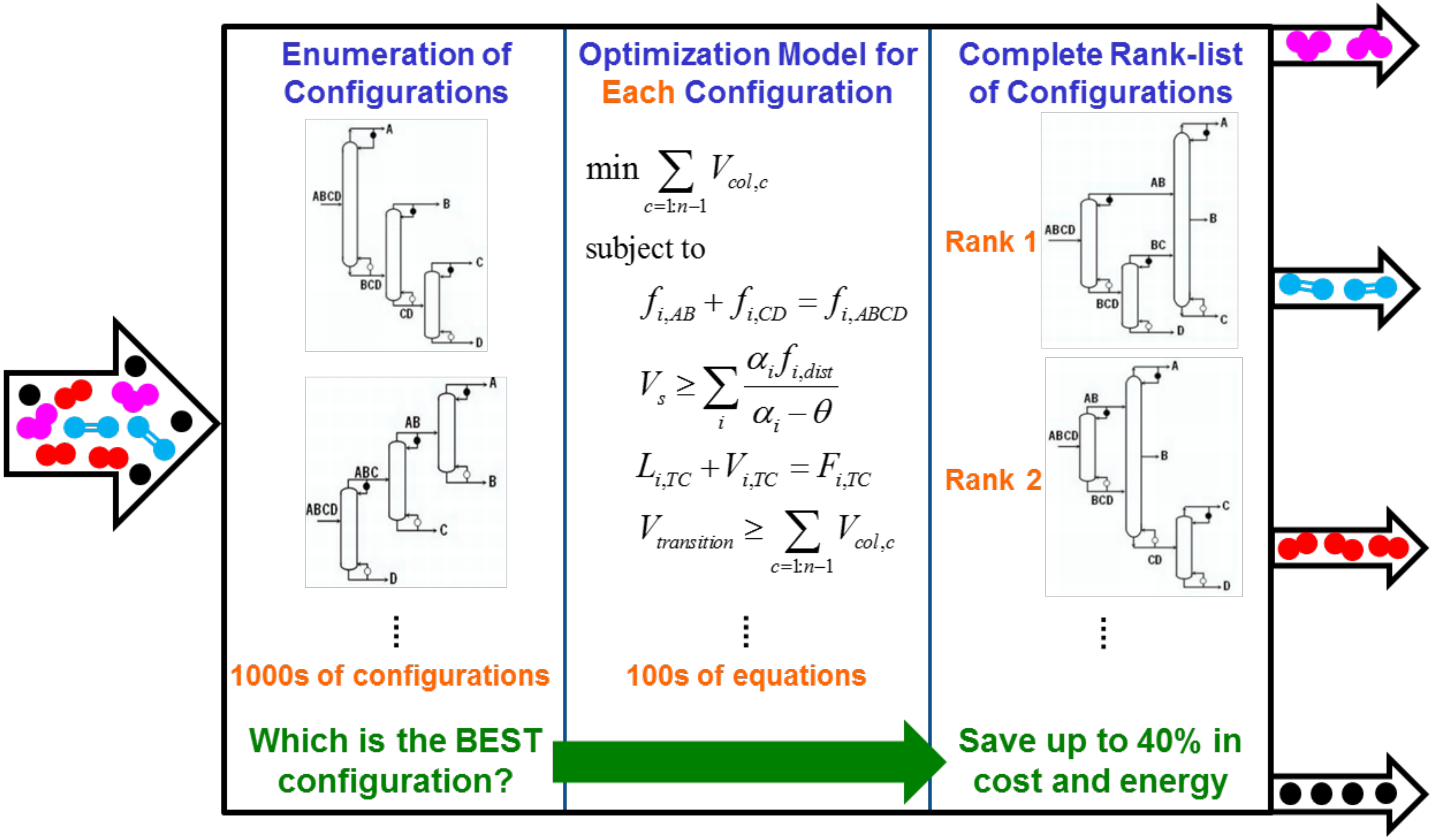
13 sections

Process Intensification: DWC



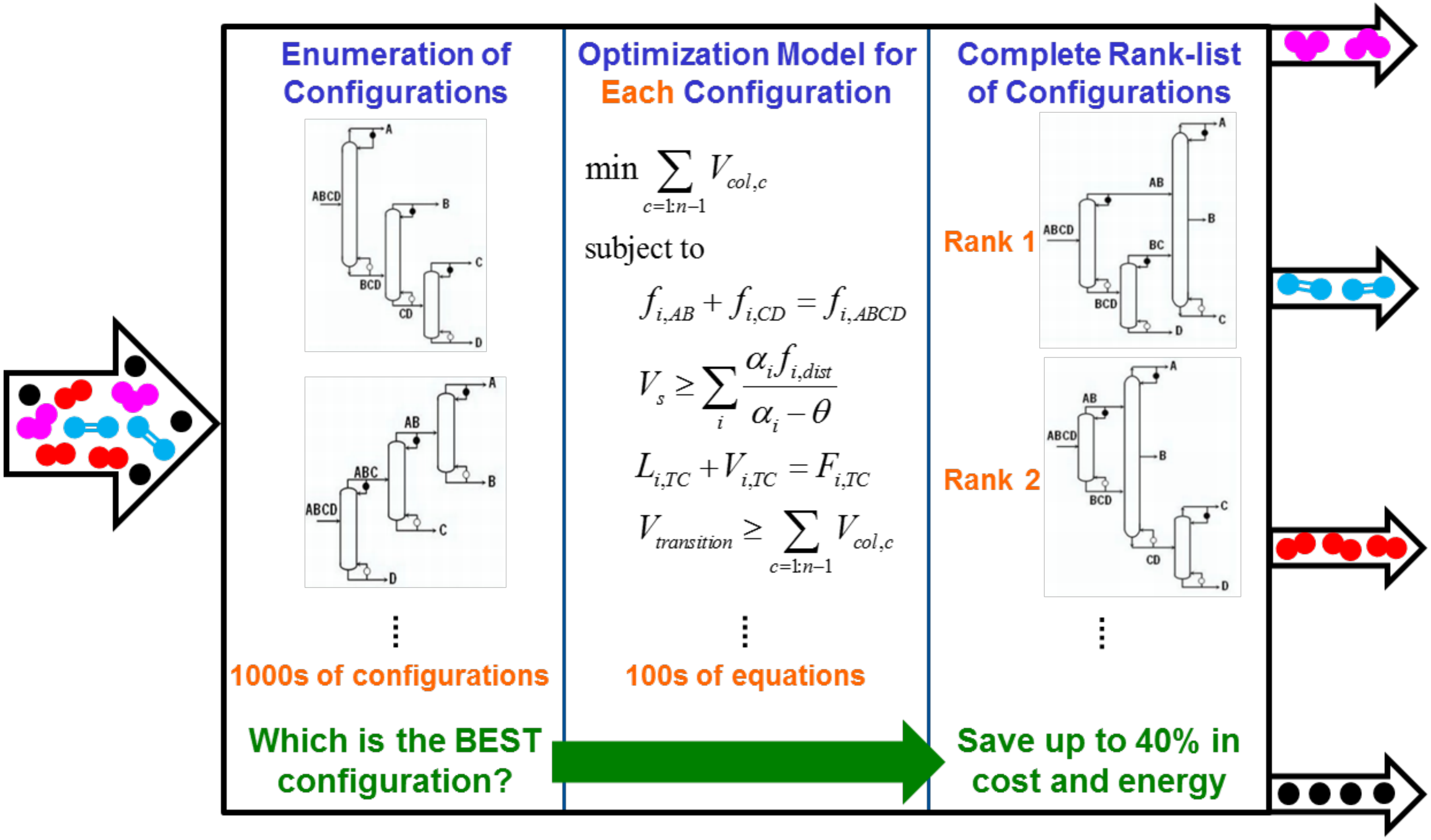
1 Distillation Column with 13 sections

Technical Approach



Thanks to AMO, we are the only USA group performing this research

Technical Approach



Thanks to AMO, we are the only USA group performing this research

Outcome is a quick, rank-listing optimization software tool for industrial practitioners that is easy to use

Transition and Deployment

- 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 production), LNG, Crude Petroleum
  - Biochemicals , e.g. pyrolysis, fermentation, gasification
- Process designers in above industries are prime users
  - New plants
  - Retrofits

Transition and Deployment

- Leveraging commercialization experience of Purdue Office of Technology Commercialization and Purdue Enterprise Company to commercialize our software (e.g., in active dialogue with Dr. Joseph Pekny, Co-founder and Chief Scientist of Advanced Process Combinatorics, Inc.)
- An independent company (Purdue Enterprise Company) to make sales-call
- Hiring a professional developer (Dr. George Applequist) to convert academic software to commercial software
- Made presentation to a number of companies on the capabilities of our software – ExxonMobil, SABIC, Eastman Chemical Company and The Dow Chemical Company, all have shown keen interest
- Will continue to incorporate new methods and tools in the software - continued improvement!

Measure of Success

- New plants with energy-efficient configurations that have never been built before
- Retrofit of new energy-efficient options
- Ultimate impact
  - 30% to 50% reduction in 3% of the total world energy consumption
  - Also 30%-50% cost reduction
  - Significant environmental impact in terms of reduction in CO_2 emissions
- Modular design feasible
- Process intensification through heat and mass integration of distillation columns, and the use of new dividing wall columns

Project Management & Budget

- Duration of the project: Three years (2016 Schedule)

Milestone	Milestone Description	Verification Method	Planned Completion Date
2.2.1	DWCs for any TC configuration	Finish development of the method and write a manuscript.	Q6
3.2	Newly identified heat & mass integrated columns for improved energy efficiency	A method to draw sub column configurations will be made available.	Q5
5.1.1	Exergy optimization software	Computer software with NLP formulation using exergy made available	Q7
6.1.1	Algorithm to identify the TC links with no heat savings	Complete development of the method and comparison on an application with global minimum heat duty	Q7
6.3.1	Development of a method to retain first law benefit from a TC link while eliminating the second law penalty	Complete development of the method and its implementation in the computer software	Q8
7.1.1	Completion of the second internship	Finish second internship and submit a feedback report	Q7
7.1.2	Incorporate feedback from second internship in the software	Incorporate feedback in the computer software	Q8
7.2.1	Identify primary firm and engage discussion on modes of commercialization	Identification of a firm and start of the development of the commercialization terms/needs	Q6
7.2.2	Conclude business model	A business model for distribution of software	Q7
7.2.3	Licensing agreement with Purdue	Executed License from Purdue	Q8

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

Results and Accomplishments

- Our quick-screening optimization tool can lead to new industrial plants and retrofits that are 30-50% more energy-efficient and cost-effective than existing processes
- Completion of internship at Eastman Chemical Company and incorporation of feedback into our optimization tool
- Active efforts to commercialize software
- Ability to draw dividing wall column of any given low-energy configuration, and hence, for the first time, availability of multitude of dividing wall candidates for feed mixtures containing 4 components or more, which can save ~30% operating and capital costs
- Improved energy efficiency and significant equipment (columns, reboilers, condensers & transfer-streams) reduction through process intensification of distillation configurations