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MULTICOMPONENT DISTILLATION CONFIGURATIONS WITH LARGE ENERGY SAVINGS

Vishesh H. Shah and Rakesh Agrawal
School of Chemical Engineering, Purdue University, 480 Stadium Mall Dr, West Lafayette, IN 47907, USA, Email: vhshah@purdue.edu, agrawalr@purdue.edu

Abstract
In industry, many separation processes involve the separation of multicomponent mixtures using distillation. There are many distillation configurations that can carry out the same overall separation process. These configurations use an equal number of distillation columns, but they differ significantly in energy consumption. Therefore a major challenge for a practitioner is the identification of energy-optimal configurations for a given application. We describe an easy-to-use matrix-based framework to identify all feasible candidate configurations for the separation of any non-azeotropic multicomponent mixture. We also describe an optimization framework to rank-list all feasible configurations with respect to energy consumption. We have demonstrated the efficacy of these frameworks by identifying more than 70 new configurations that can lower the energy consumption for petroleum crude distillation by 5 – 48%. We also present a framework to analyze operability of distillation sequences.

Keywords: Multicomponent Distillation, Distillation Configurations, Energy Savings

1. Introduction
To separate multicomponent mixtures into more than two product streams using distillation, a sequence of distillation columns is generally required. Different sequences or configurations of distillation columns can be used to carry out the same overall separation process, but they usually differ significantly in energy consumption and cost. Since large-scale distillation processes such as petroleum crude distillation are highly energy intensive, it is important to choose energy-optimal distillation sequences for multicomponent applications.

The first attempt to identify an optimal distillation sequence from among known sequences probably dates back to Lockhart, 1947[1]. Since then there have been several attempts to generate all possible distillation sequences for the separation of an n-component non-azeotropic mixture into n pure product streams[2-4]. The earlier attempts failed to generate all possible multicomponent distillation sequences. Recently methods to draw basic as well as non-basic configurations have been suggested[5-6]. Through extensive computation, Giridhar and Agrawal found that for four-component feed mixtures, non-basic configurations never had heat duty lower than basic configurations[7]. Only recently, methods were developed to generate all potentially optimal distillation sequences, while not being overburdened by the non-basic distillation sequences that could never be optimal[8-11]. For a detailed discussion about these attempts and some other concepts related to distillation sequencing, the reader is referred to our prior work[11].

In this paper, we focus our attention on identification of energy-optimal distillation sequences that utilize (n-1) distillation columns to separate any non-azeotropic n-component feed mixture into n pure product streams. We also consider thermally coupled distillation configurations in our analysis.

2. Generation of Configurations
We have developed a matrix-based framework to generate all feasible distillation sequences with and without thermal coupling for the separation of any non-azeotropic mixture into n product streams. This framework has been described in detail in our prior work[11]. We describe some of the key steps here:

2.1 Configurations without thermal coupling:
These configurations can be obtained through six easy steps. As an example, consider the problem of obtaining all feasible distillation sequences for separation of a feed mixture into three product streams.

STEP 1: Obtain the value of n, the desired number of product streams, from the problem definition. For our example problem, n = 3.

STEP 2: Generate an n x n upper triangular matrix. All elements in the lower triangular portion are assigned values of 0, while the upper triangular elements are not yet assigned numerical values. Let the components (A, B, C …) be arranged in alphabetical order with respect to their volatility. Therefore A is the lightest component and so on. Each upper triangular element is defined to correspond uniquely to a stream by the following equations:

First component for mixtures in row 'i' = Component 'i' (1)

Number of components for mixtures in column 'j' = n+1-j (2)

$$\begin{bmatrix} ABC & \rightarrow AB & \rightarrow A \\ 0 & \searrow BC & \rightarrow B \\ 0 & 0 & \searrow C \end{bmatrix}$$

Figure 1. Illustration of STEP 2 for the case of n = 3

As seen by the arrows in Figure 1, if we pick any stream in the matrix, possible top products of distillation of the stream can lie only on a horizontal path to the right of the stream. Similarly possible bottom products of distillation of any stream can lie only on a diagonal path to the right of the stream. Therefore, defining correspondence of matrix elements to streams by using equations (1) and (2) includes all possible streams that can be encountered in a distillation sequence and also assigns physical significance to the locations of the matrix elements.

STEP 3: Identify the 'd' matrix elements corresponding to transfer streams. In any distillation sequence, the main feed stream and final product streams are always present and each of these streams is connected to one distillation column. All other streams involve two distillation columns and they are transferred from one distillation column to another. In any n x n matrix, the (1,1) element always corresponds to the main feed stream and the (-,n) elements i.e. all elements of the n^{th} column always correspond to the final product streams. All other upper triangular elements correspond to transfer streams. For our example problem of n = 3, the (1,2) and (2,2) elements of the matrix correspond to transfer streams.

STEP 4: Generate numerical matrices indicating presence and absence of transfer streams. We assign a value of 1 to a matrix element to indicate presence of the corresponding stream in a distillation configuration, and a value of 0 to indicate absence. Hence the (1,1) and (-,n) elements always take values of 1. The 'd' matrix elements corresponding to transfer streams can take values of either 0 or 1. Therefore 2^d candidate matrices need to be generated. Each of these matrices is a candidate distillation sequence.

$$\begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

(a) **(b)** **(c)** **(d)**

Figure 2. Illustration of STEP 4 for the case of n = 3

STEP 5: Eliminate matrices that result in physically unrealizable distillation sequences. This is done using two checks: (i) Except the main feed stream, any stream that exists in a distillation configuration must be produced by another stream; and (ii) in the absence of chemical reactions, all components that enter a distillation column must also leave the distillation column. These checks can be implemented easily because of the physical significance associated with the locations of matrix elements. They can also be easily converted to linear inequalities.

For our example problem of n = 3, the matrix of Figure 2(a) violates check (i). In this matrix the (2,2) element – stream B – is present as indicated by its value of 1. However, since it can only be produced by streams on horizontal or diagonal paths to the left, at least one of the (1,2) or (2,2) elements should have a value of 1. Therefore this check simply means that at least one of streams AB (the (1,2) element) or BC (the (2,2) element) needs to be transferred between distillation columns to produce pure stream B. Since this condition is violated by the matrix in Figure 2(a) it is discarded as a physically unrealizable sequence. All other matrices obey the checks and thus correspond to feasible distillation sequences.

STEP 6: Draw a distillation sequence from a feasible matrix. We start from the (1,1) element corresponding to the main feed stream and move horizontally and diagonally to the right till we encounter the next 1 on each path. These are respectively the top and bottom products of the main feed stream. This describes the first separation split in the sequence. This process is repeated till all the splits have been enumerated. Splits making a common product are then grouped and placed in the same distillation column. Figure 3 illustrates this procedure for the matrix of Figure 2(d). Similarly the matrices of Figures 2(b) and 2(c) correspond to the well-known direct and indirect split sequences.

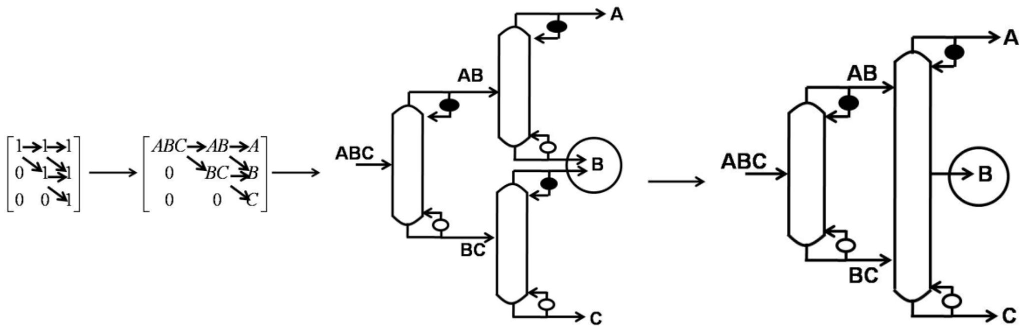


Figure 3. Illustration of STEP 5 for the case of n = 3

Table 1. Number of distillation sequences for mixtures separated into n product streams

n	Sequences without thermal coupling	Sequences with thermal coupling
3	3	5
4	18	134
5	203	5,925
6	4,373	502,539
7	185,421	85,030,771
8	15,767,207	29,006,926,681

2.2 Configurations with thermal coupling:

Once we obtain all feasible sequences without thermal coupling, we can replace reboilers and condensers associated with transfer streams in each configuration by two-way liquid-vapor communications referred to as thermal coupling links. We obtain a large number of configurations with varying extents of thermal coupling. These configurations can significantly lower the energy consumption. They can be easily generated using the information available in the matrix. This procedure has been described in our prior work[11].

2.3 Results:
Table 1 demonstrates that the number of distillation sequences grows rapidly as the number of components in the feed increases. These configurations have been generated using the matrix-based framework and constitute the complete set of potentially energy-optimal distillation configurations.

2. Rank-listing of Configurations

The total minimum vapor duty requirement of a distillation configuration is indicative of its cost and energy consumption. We formulate a general nonlinear programming problem that minimizes the total vapor duty requirement of any distillation configuration with and without thermal coupling. The calculation of minimum vapor duty requirement is based on Underwood's equations[12].

The main decision variables for the nonlinear programming problem are the flows of each component in each stream. There are additional decision variables for sidedraw streams and thermally coupled streams. All decision variables are connected by mathematical constraints that account for the following:

i. Component balance across columns
ii. Feed conditions from the problem definition
iii. Transfer streams that are absent in a configuration are assigned zero flows
iv. Product specifications
v. Absence of components in streams
vi. Connectivity constraints
vii. Thermodynamic equilibrium constraints for sidedraw streams and thermally coupled streams
viii. Distillation constraints

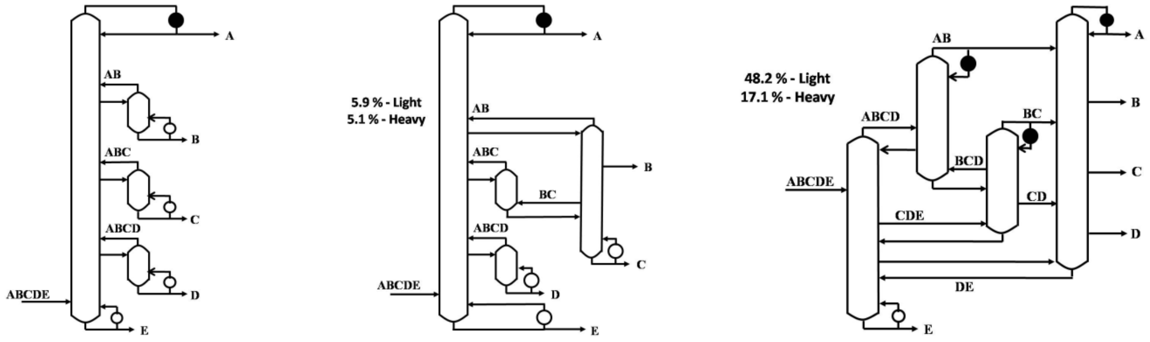
Once we solve for the total minimum vapor duty requirement of each distillation sequence, we can rank-list the sequences in the order of their energy consumption. We can then analyze the best configuration or the top x % configurations in further detail.

3. Case Study – Petroleum Crude Distillation

We have applied these frameworks to crude distillation[11]. Petroleum crude distillation consumes nearly 1.6 million bbl of oil / day[11,13-14] and is a highly energy intensive process. Crude is typically distilled into five fractions: naphtha (A), kerosene (B), diesel (C), gas oil (D) and residue (E). Different refineries process a variety of crude oils, yet they typically use the same distillation sequence.

The current sequence for crude distillation is one of forty well-known sharp split based distillation sequences for separation of a mixture into five products. However our matrix-based framework indicates that there are a total of 6,128 distillation sequences with and without thermal coupling that could carry out the same overall process of separating a mixture such as crude oil into five fractions.

After analyzing the total minimum vapor duty requirements of the forty sharp split sequences, we have found the current sequence to have least vapor demand. This reaffirms the choice of the current sequence for more than 75 years. However, if we consider the complete set of 6,128 distillation sequences, through our rank-listing framework, we have identified more than seventy novel distillation candidates that could potentially lower the energy consumption for crude distillation by 5 – 48%. We have considered a light petroleum crude mixture and a heavy petroleum crude mixture in our calculations. For both crude mixtures, the relative volatilities of A, B, C and D with respect to E are assumed to be 45.3, 14.4, 4.7 and 2.0 respectively. The light petroleum crude mixture is assumed to contain 46.1% A, 19.5% B, 7.3% C, 11.4% D and 15.7% E; while the heavy petroleum crude mixture is assumed to contain 14.4% A, 9.3% B, 10.1% C, 3.9% D and 62.3% E. For both mixtures, the thermal quality i.e. the liquid fraction of the feed is equal to 90% of the heaviest component's concentration. Hence we have considered two-phase feed mixtures. Two attractive configurations with their energy savings have been reproduced from our prior work[11] and are shown in Figure 4.

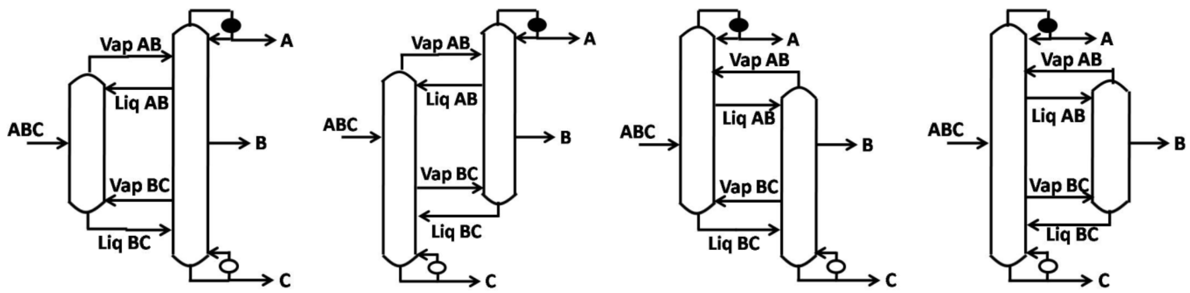


(a) (b) (c)

Figure 4. (a) The conventional configuration for crude distillation, (b) an attractive configuration that is easy-to-retrofit and (c) an attractive configuration for a grassroots refinery

4. Operability of Sequences

Once a distillation sequence has been identified to be optimal, additional rearranged sequences can be derived if the sequence has thermal coupling links[15]. All rearranged sequences have the same minimum total vapor duty requirement as the original sequence. Hence these sequences are identical from an energy perspective, but they differ in terms of operability and capital cost. For instance, for a three component mixture, the configurations of Figure 5 are equivalent from an energy perspective.



(a) (b) (c) (d)

Figure 5. Equivalent rearranged sequences for a three component mixture

In distillation sequences, it is desirable to assign column pressures such that vapor streams flow from a high pressure column to a lower pressure column. If this is not done, then compressors have to be used with some vapor transfer streams thereby increasing the cost of the sequence. Sequences where all vapor transfer streams can flow freely after appropriate assignment of column pressures are referred to as "operable" sequences. The configurations of Figure 5(a) and 5(d) are not operable since vapor streams AB and BC are transferred in opposite directions between distillation columns 1 and 2. However the sequences of Figure 5(b) and 5(c) do not have this problem. Therefore rearrangement of column sections due to thermal coupling can make optimal distillation sequences more operable[15-16].

Many methods have been developed to draw rearranged schemes for thermally coupled multicomponent distillation sequences and to identify operable sequences[15-17]. However there has been no attempt to analyze operability of distillation sequences without thermal coupling because the problem of operability was never thought to exist for configurations without thermal coupling. Since we have obtained the complete set of all feasible distillation sequences, an interesting finding has been that some distillation configurations have operability problem even though thermal coupling is absent. One example is shown in Figure 6. Sidestream CD is transferred between distillation columns and has some portion of flow as vapor, while stream AB is a vapor stream transferred in the opposite direction between the distillation columns. This causes the sequence to be difficult to operate.

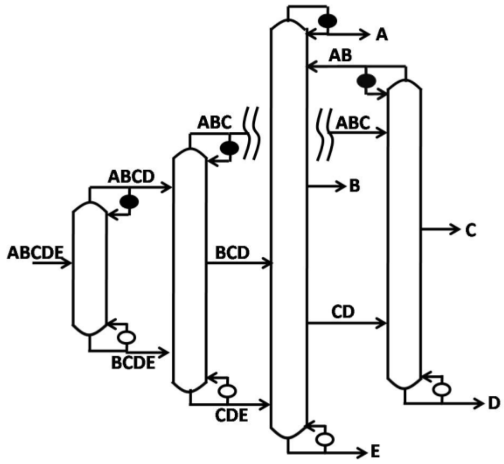


Figure 6. An example of a sequence without thermal coupling that is not operable

5. Conclusions

A matrix-based framework has been developed to elucidate all potentially energy-optimal sequences for distillation of any non-azeotropic multicomponent mixture into n product streams. A nonlinear programming framework has been developed to estimate the minimum total vapor duty requirement of each distillation configuration. This allows us to rank-list all feasible distillation sequences with respect to their energy consumption. The efficacy of this approach is demonstrated by application to the problem of petroleum crude distillation. As can be seen, significant energy savings can be achieved by proper choice of a distillation sequence. Finally operability of distillation sequences with and without thermal coupling has been analyzed.

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