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Estimation of the Number of Distillation Sequences with Dividing Wall Column for Multi-component Separation

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As an important separation unit, distillation column is widely applied in petrochemical and other process industry. For separating multicomponent mixtures, distillation is conducted sequentially in industry. Both individual column and distillation sequence optimization are efficient ways for saving energy consumption. Distillation sequence is usually evaluated by number of distillation subproblems, subgroups and distillation sequences. Distillation sequence has been well studied based on simple column assumption. Dividing wall column (DWC), which is an atypical distillation column for separating a multicomponent feed mixture into three output streams, as a thermally coupled distillation column, has been proposed and applied in distillation sequence. Usually sharp split is also assumed in most literatures on DWCs. A distillation sequence with DWC will give more number of feasible sequences. It is important to estimate the total available number of distillation sequences theoretically. In this work, distillation sequences with both simple column and DWC are considered. Inferential deduction method has been used to explore the number of distillation sequences for multi-component sharp splits. The three general term formulas are obtained with the assumption of sharp split. Under different assumptions, the corresponding numbers of distillation sequences are also discussed.

1. Introduction

Distillation is the primary separation technique widely adopted in process industry, by which final products can be obtained, while most other techniques, such as absorption and extraction, need further processing (Mustafa et al., 2014). Traditional distillation column is assumed to separate one feed stream into two output streams. For the separation of multicomponent mixture, a sequence of distillation columns will be needed. Thus, a large number of columns are applied in process industry. It is reported that there are over 40,000 distillation columns all over the world (Kiss et al., 2013). Despite its flexibility and wide application, one important concern on it is its considerable energy consumption, which can account for more than 50 % of plant operating cost (Kiss et al., 2007). Therefore, many research efforts have been concentrated on energy-efficient distillations in terms of both individual column and distillation sequence.

Distillation sequence synthesis is one of a significant way to save energy in distillation process. The estimation of the number of all possible sequences is very necessary information in searching an optimal distillation sequence in process synthesis. Distillation sequence has been well studied based on simple column assumption (Muhammad et al., 2015), i.e. in each column one feed is separated into two streams without component mixing between two output streams, which is also named as sharp split. The general term formula of the simple column distillation sequence number has been achieved (Thompson and King, 1972). Non-sharp split has also been studied in recent years. Systematic synthesis of functionally distinct distillation systems which including non-sharp splits for five-component separations is presented by a step-by-step enumeration method in the work (Rong et al., 2005). It was conducted for a specific industrial application, and there are more than one solutions for a single case. However, the discussion based on sharp split assumption has theoretical significance to general separation problems.

Dividing wall column (DWC) was first proposed by Wright (1949). It is an atypical distillation column with an internal, vertical partition wall, which effectively accommodates two conventional distillation columns into one

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shell for separating a multicomponent feed mixture into three output streams (Mohamad et al., 2015). As a thermally coupled distillation column, it is reported that about 30 % energy consumption and equipment investment cost can be saved by the application of DWC (Triantafyllou and Smith, 1992). When including DWC, the number of columns in each sequence can be reduced. However, at the meantime, the number of feasible sequences will increase rapidly, almost beyond the speed of exponential growth. Process synthesis in industrial practice showed that the economic performance of the distillation sequence highly depends on the completeness of the sequence alternatives under consideration. The sequence with DWC only at the last separation step was discussed for a five component sequence (Du et al., 2016) by enumeration. More general study on the number of distillation sequences with DWC hasn't been reported yet. Thus, it is important to theoretically estimate the total available number of distillation sequences including both simple column and DWC.

In this work, distillation sequences with both simple column and dividing wall column (DWC) are considered. An inferential deduction to calculate the number of distillation sequences, distillation subproblems, and distillation subgroups for multi-component separation based on sharp split has been presented. Three general term formulas are obtained and discussed under different assumptions.

2. Problem description

Distillation sequence is usually described by the number of distillation sequences, distillation subproblems, and distillation subgroups.

Following the expression used in Analysis and Synthesis of Chemical Process (Zhang et al., 2011), the number of the distillation sequences is defined as S_R which refers to the possible number of sequences for separating R components into R pure products by simple column. The number of distillation subproblems is defined as U which corresponds to a possible number of separation units. Separation sequences are different combinations of subproblems. The number of distillation subgroups is defined as G which is number of streams with adjacent components in a multi-component separation, as the feed or final product of each separator, or subproblem.

In this work, only sharp split is considered in both simple column and DWC. For the convenience of understanding, several new variables are defined in the following discuss.

2.1 Distillation sequences

The recursive formula and general term formula of the number of distillation sequence with simple column only were given in (Seider et al., 1999) as follows:

$$S_R = \sum_{j=1}^{R-1} S_j\, S_{R-j} \tag{1}$$

$$S_R = \frac{[2(R-1)]!}{R!(R-1)!} \tag{2}$$

where R is the number of components ($R = 1,2,3, \dots, n$).

Considering both simple column and DWC, a_R is used to replace the S_R in Eq(1), which represents the number of separation sequence for R component separation if a simple column is picked at the current step, and b_R as the number of separation sequence for R component separation if a DWC is picked at the current step.

Choosing DWC at the current step, there are $(R-2)$ separation choices for the first column. Let the number of components appearing at the top product of the column be j, the number of components appearing at the side product of the column be k, then the number of components appearing at the bottom product of the column will be $(R-j-k)$. Therefore, the recursive formula will be three items multiplication as in Eq(4). The calculation is valid from $R \geq 2$.

$$a_R = \sum_{j=1}^{R-1} S_j\, S_{R-j} \tag{3}$$

$$b_R = \sum_{j=1}^{R-2} S_j \sum_{k=1}^{R-j-1} S_k\, S_{R-j-k} \quad \text{(for } R \geq 2\text{)} \tag{4}$$

The total number of distillation sequences S_R can be calculated as follows:

$$S_R = a_R + b_R \tag{5}$$

For calculation convenience, it is assumed that $a_1 = 1$, while there is actually no column needed if only one component exits, $b_1 = 0, b_2 = 0$, as one or two component separation won't be able to use a DWC. Thus,

$$S_1 = a_1 + b_1 = 1 \tag{6}$$

Obviously, $a_2 = 1$, so that

$$S_2 = a_2 + b_2 = 1 \tag{7}$$

With these initial values, recursive formulas can be executed by *R* programming. The result of the number of the distillation sequence is shown in Table 1.

Table 1: The result of the number of the distillation sequences with DWC

R	2	3	4	5	6	7	8	9	10	11	…
S_R	1	3	10	38	154	654	2871	12925	59345	276835	…

Fortunately, the integer sequence of the result has been studied by Hanna (2005), and the general term formula (10) is achieved. For the expression simplicity, it is assumed that:

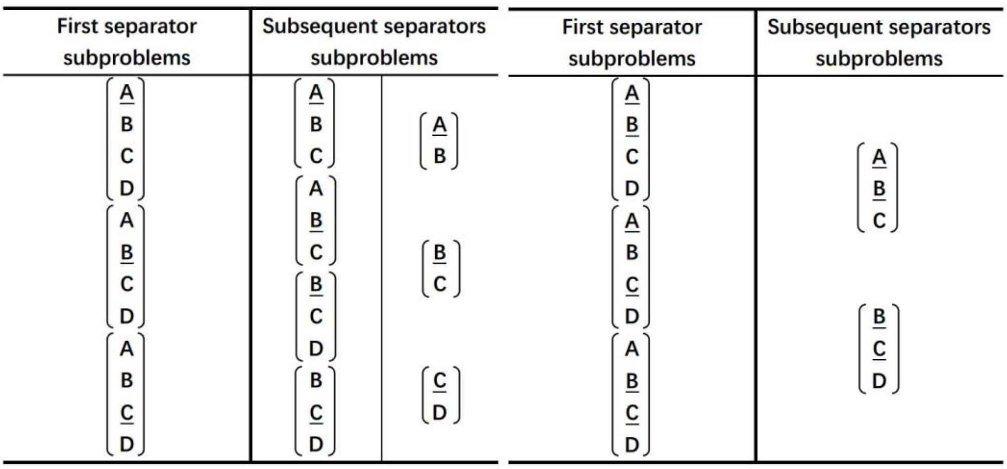
$$R = Q + 1 \tag{8}$$

$$S_R = S_{Q+1} \tag{9}$$

$$S_{Q+1} = \sum_{k=0}^{[\frac{Q}{2}]} \frac{C_{2Q-k}^{Q+k} C_{Q+k}^{k}}{Q+1} \tag{10}$$

2.2 Distillation subproblems

As the four component separation example shown in Figure 1, elements in the first column of Figure 1(a) and 1(b) represent a four component subgroup with different separation choices, i.e. subproblem. Elements in the second column of each subplot represent the outcome of subproblem in its left column; same logic applies in the third column too.



(a) Simple column subproblems *(b) DWC subproblems*

Figure 1: Four component separation subproblems

It can be counted out that the number of subproblems for four component separation with simple column is 10, which can be calculated by the general term formula (Zhang et al., 2011) written as follows:

$$U = \sum_{j=1}^{R-1} j(R-j) = \frac{R(R-1)(R+1)}{6} \tag{11}$$

Considering DWC into the problem, U_a is used to replace the U in Eq(11), which represents the subproblem number with simple column, and U_b as the subproblem number with DWC. So that the U can be calculated as follows:

$$U = U_a + U_b \tag{12}$$

Obviously, at the step of R component separation, there are C_{R-1}^2 ways which is a kind of combination number to apply DWC. Thus, u_R is defined at current separation step.

$$u_R = C_{R-1}^2 \tag{13}$$

When $n < 3$, $u_{b1} = 0, u_{b2} = 0$,$U_b = 0$,

$$U = U_a = \frac{R(R-1)(R+1)}{6} \tag{14}$$

When $n \geq 3$, U_a is remained as Eq(11), while

$$U_b = 1u_R + 2u_{R-1} + 3u_{R-2} + 4u_{R-3} + \cdots + (n-2)u_3 = \sum_{j=1}^{R-2} ju_{R+1-j} \tag{15}$$

So that U can be expressed as the general term formula followed:

$$U = U_a + U_b = \frac{(n-1)n(n+1)(n+2)}{24} \tag{16}$$

2.3 Distillation subgroups

In terms of the definition, the general term formula *of* G (Zhang et al., 2011) is constant no matter which type of column is included.

$$G = \sum_{j=1}^{R} i = \frac{R(R+1)}{2} \tag{17}$$

Take the four component separation as an example, all possibilities are shown in Figure 2.

Table 2: The number of distillation sequences, distillation subproblems, and distillation subgroups

R	S_R	U	G
2	1	1	3
3	3	5	6
4	10	15	10
5	38	35	15
6	154	70	21
7	654	126	28
8	2871	210	36
9	12925	330	45
10	59345	495	55
11	276835	715	66

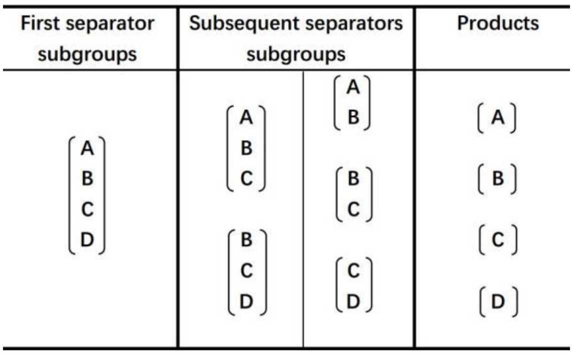


Figure 2: Four component separation subgroups

The number of distillation sequences, distillation subproblems, and distillation subgroups mentioned above can be calculated by the general term formulas. The results are shown in the Table 2.

3. Extension

Three general term formulas are obtained for separation sequence with simple column and DWC. This analysis can be applied if more complicated column structure is considered, e.g. a column with one feed stream and more number of output streams.

3.1 Case for more number of output streams from a column

A special column structure with one feed stream and four output streams is considered as an example here.
Choosing a column with one feed stream and four output streams at the current step, there are $(R-3)$ separation choices for this type of column. Let the number of components appearing at the top product of the column be j, the number of components appearing at the first side product of the column be k, the number of components appearing at the second side product of the column be l, then the number of components appearing at the bottom product of the column will be $(R-j-k-l)$. Therefore, the recursive formula will be four items

multiplication as Eq(18). The S_R can be calculated as Eq(19). The a_R and b_R are defined in Eq(3) and Eq(4) respectively.

$$c_R = \sum_{j=1}^{R-3} S_j \sum_{k=1}^{R-j-2} S_k \sum_{l=1}^{R-j-k-1} S_l \, S_{R-j-k-l} \quad (18)$$

$$S_R = a_R + b_R + c_R \quad (19)$$

$c_1 = 0, c_2 = 0, c_3 = 0$ as one, two or three component separation won't be able to use this type of column. With the initial value $a_1 = 1, a_2 = 1, b_1 = 0, b_2 = 0$, the recursive formulas can be executed by *R* programming. The result of the number of the distillation sequence is shown in Table 3.

Table 3: The result of the number of the distillation sequences with four output streams column

R	2	3	4	5	6	7	8	9	10	11	…
S_R	1	3	11	44	189	850	3951	18832	91542	452075	…

With the same method mentioned in the section 2.1, the general term formula (Vladimir, 2011) can be obtained as Eq(20). The general binomial distribution definition is available at

$$S_R = \frac{1}{R}\sum_{k=1}^{R-1}\left[\sum_{j=0}^{k} binomial(j, R-3k+2j-1)\cdot binomial(k,j)\right]\cdot binomial(R+k-1, R-1) \qquad (\text{for } R \geq 2\ ) \quad (20)$$

From the discussion above, these series of recursive formulas have a possibility to extend to a separator with any number of feed streams and any number of output streams, which possibly exists in practical separation sequence.

3.2 Case for DWC only included at the last separation step

In certain industrial process, pure product is more attractive. Due to the operating challenge, DWC is only used to separate three components into three pure products at the last separation step in a sequence. In this case, G is constant with the Eq(17) as always. U_b in Eq(15) only left with the last item, shown as Eq(21), with the definition of u_R in Eq(13), U_b can be calculated with the result $n-2$. The U can be obtained with the Eq(22).

$$U_b = (n-2)u_3 \quad (21)$$

$$U = \frac{R(R-1)(R+1)}{6} + (n-2) \quad (22)$$

DWC is used only at the last separation step, in other words, DWC is used only in three components separation. Thus, S_R defined in Eq(5) is suitable only when $R = 3$, i.e. the sequence with DWC is only considered when $R = 3$. S_R will be calculated according to Eq(1), as no DWC will be applied at other separation step. Based on Eq(3) and Eq(4), S_3 can be expressed as Eq(23). With the initial value of S_1 and S_2, S_3 can be calculated as follows:

$$S_3 = S_1S_2 + S_2S_1 + S_1S_1S_1 = 1\times1 + 1\times1 + 1\times1\times1 = 3 \quad (23)$$

Set S_3 with the new initial value 3, the recursive formula given in Eq(1) can be executed to get new results by *R* programming, which is shown in Table 4.

Table 4: The result of the number of the distillation sequences with DWC used at the last separation step

R	2	3	4	5	6	7	8	9	10	11	…
S_R	1	3	7	20	63	208	711	2,496	8,944	32,578	…

With the same method mentioned in the section 2.1, the general term formula (Vladimir, 2014) of the number of the distillation sequences can be obtained as Eq(26). The general binomial distribution definition is also available at WolframMathWorld (2017). For the expression simplicity, it is assumed that:

$$R = Q + 1 \quad (24)$$

$$S_R = S_{Q+1} \quad (25)$$

$$S_Q = \sum_{m=0}^{\frac{Q}{2}} \frac{binomial(Q-2m+1, m)\cdot binomial(2Q-4m, Q-2m)}{Q+1-2m} \qquad (\text{for } Q \geq 1\ ) \quad (26)$$

4. Conclusions

The number of distillation sequences, distillation subproblems, and distillation subgroups with both simple column and DWC are discussed under the only consumption of sharp split. Corresponding general term formulas are obtained. The development procedure of recursive formulas can be extended to a separator with

any number of feed streams and any number of output streams, while the number of distillation subgroups remains constant no matter how complicated the column is included. Under the assumption of DWC used only at the last separation step, the corresponding formulas are obtained as well.
If non-sharp split is included in a process, the related work for multi-component separation will be even more complicated, which can be further discussed for a given separation requirement. The impact of thermodynamic properties of components in a separation system hasn't been investigated yet, which could be helpful in reducing the number of feasible separation sequences.

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