Some Complements in Combinatorics of Sharp Separation Systems Synthesis

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The analysis of combinatorics of sequences of sharp separation systems is a problem extensively studied in chemical engineering. Thompson and King (1972) first presented a closed-form expression for determining a number of possible sequences for separating an n-component mixture into pure products by using simple (one input and two outputs) sharp separators. Then, Shoaei and Sommerfeld (1986) showed that this determination could be interpreted in term of Catalan numbers; recently Wahl and Lien (1990) derived this formula from a generating function. This article presents a closed-form expression for a number of different possible separation sequences when complex (one input and three or more outputs) separators are used.

Problem Formulation and Previous Works

The design of sharp separation sequences is one of the most investigated problems in the synthesis of chemical units. It consists in generating all different possible separation schemes when an n-component mixture has to be separated into pure products with the main assumptions:

- Only sharp separators are used, that is, each component of the feed stream exits in only one output stream of the separator.
- The components are ranked in any stream.
- This ranked list of components is invariable.
- Mixture or division of intermediate streams is prohibited.

The number of separation sequences may be defined recursively for sequences involving complex sharp separators (Wahl and Lien, 1990; Domenech et al., 1991).

Sequences of Sharp Separators: Closed Form Formulae

Thompson and King (1972) first presented a closed form expression for the number S_n of sequences involving only simple sharp separators:

$$S_n = \frac{(2(n-1))!}{n!\,(n-1)!} \tag{1}$$

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Shoaei and Sommerfeld (1986) pointed out that this determination is an application of Catalan numbers.

A three-output separator can be illustrated by a distillation column involving a sidestream. The earlier works of Petlyuk et al. (1965), Elaahii and Luyben (1983) or Alatiqui and Luyben (1985) show the interest of this type of separator in practice for small values of n. When two-or-three-output separators are admitted a closed form equation can be derived:

$$S_n = \sum_{i=0}^{E\left(\frac{n-1}{2}\right)} \frac{(2n-2-i)!}{i!\,n!\,(n-2i-1)!} \tag{2}$$

where the function $E(x)$ represents the bracket function.

Indeed, for an n-component mixture, the maximum number of three-output separators is $E[(n-1)/2]$ and the minimum number is null in a sequence. When the number $i\,(0 \le i \le E[(n-1)/2])$ of three-output separators of the sequence is fixed, there is $n-1-2i$ additional simple (one input, two outputs) separators to achieve the separation in the sequence (see Appendix 1). Then, each separation sequence involves:

$3i$ = output streams from three-output separators
$2(n-1-2i)$ = output streams from simple separators
$2n-2-i$ = output streams all in all (excluding feed stream)

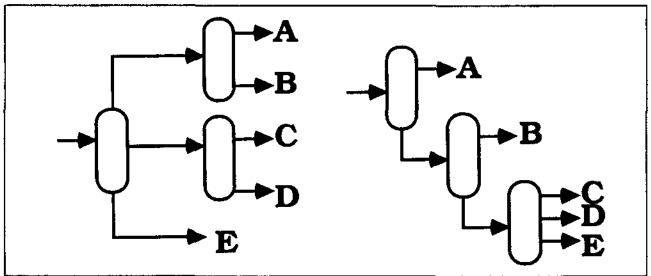

Figure 1. Two sequences of the same structure.

The number of connection streams between separators is then $n-2-i$, because of the assumption of sharp separators (there is only n pure component outputs of the sequence). Thus, the number of possible ways for obtaining such connection is:

$$S_n^i = \frac{\text{no. of choices of connection streams}}{\text{no. of separators}} \quad (3)$$

$$S_n^i = \frac{\binom{2n-2-i}{n-2-i}\binom{n-1-i}{i}}{n-1-i} \quad (4)$$

because the choice of connection streams implies the choice of $n-2-i$ streams between $2n-2-i$ and the choice of i three-output separators between $n-1-i$.

$$S_n^i = \frac{(2n-2-i)!(n-1-i)!}{(n-2-i)!n!i!(n-2i-1)!(n-1-i)} = \frac{(2n-2-i)!}{n!i!(n-2i-1)!} \quad (5)$$

The number of sequences S_n is then:

$$S_n = \sum_{i=0}^{E\left(\frac{n-1}{2}\right)} S_n^i = \sum_{i=0}^{E\left(\frac{n-1}{2}\right)} \frac{(2n-2-i)!}{i!n!(n-2i-1)!} \quad (6)$$

It can be noted that:

$$S_n = \frac{2(n-1)!}{n!(n-1)!} + \sum_{i=1}^{E\left(\frac{n-1}{2}\right)} \frac{(2n-2-i)!}{i!n!(n-2i-1)!} \quad (7)$$

The first term is equivalent to the number of sequences found by the Thompson and King formula and the second term corresponds to the number of sequences where $i\,(i \geq 1)$ three-output separators can appear.

In the general case, the minimum number of separators used to separate n components to be achieved is theoretically one and the maximum number is $n-1$ (in that last case, only simple sharp separators are used). The formulation of a closed form expression, when the number of outputs for each separator is not specified, is a rather difficult task. The enumeration procedure above mentioned is also made.

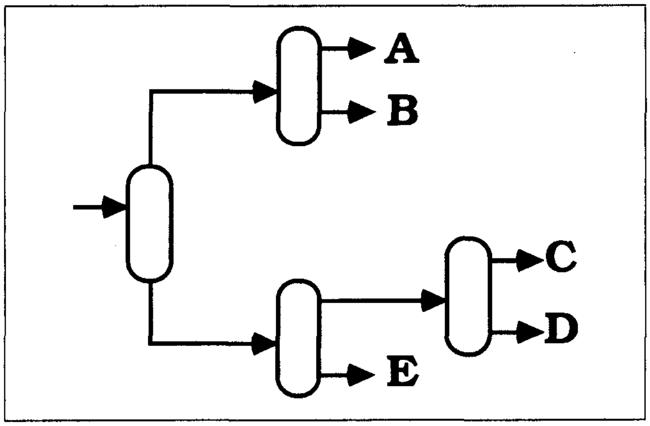

Figure 2. A sequence of different structure.

Let m_i $(0 \leq i \leq n-2)$ the numbers of separators including one input and $(i+2)$ outputs in an admissible separation structure. A structure is a set of sequences involving the same number of the same type separators. For example, the two sequences shown in Figure 1 belong to the same structure (made up of two simple separators and a three-output column) and the one shown in Figure 2 belongs to a different structure.

Then a relation binds the coefficients m_i (see Appendix 2):

$$m_0 + 2m_1 + 3m_2 + \ldots + (i+1)m_i + \ldots + (n-1)m_{n-2} = n-1 \quad (8)$$

Let I_n the set of admissible structures of sharp separators.

$$I_n = \{m_0, m_1, \ldots, m_{n-2} \text{ with } m_0 + 2m_1 + 3m_2 + \ldots + (i+1)m_i + \ldots + (n-1)m_{n-2} = n-1\}$$

Then

$$S_n = \sum_{m_k \in I_n} \frac{\text{no. of choices of connection streams}}{\text{no. of separators}} \quad (9)$$

For an admissible structure, let $m = \Sigma_{m_k \in I_n} m_k$ the total number of separators. Then, each separation structure involves:

nm_{n-2} = output streams for n-output separators
:
. . . .
:
$3m_1$ = output streams for three-output separators
$2m_0$ = output streams for simple separators

that is, $nm_{n-2} + \ldots + 3m_1 + 2m_0 = m + n - 1$ [= output streams all in all (excluding feed stream) from Eq. 8]

The number of connection streams between separators is then $m-1$, from the assumption of sharp separators (there is only n pure component outputs of the sequence). Thus, the number of possible ways for obtaining such connection is:

$$S_n = \sum_{m_k \in I_n} \frac{\binom{n+m-1}{m-1}\binom{m}{m_{n-2}}\binom{m-m_{n-2}}{m_{n-3}}\cdots\binom{m-m_{n-2}-m_{n-3}-\ldots-m_1}{m_0}}{m} \tag{10}$$

$$S_n = \sum_{m_k \in I_n} \frac{\binom{n+m-1}{m-1}}{m} \prod_{m_j \in I_n} \binom{m-m_{n-2}-\ldots-m_{j+1}}{m_j} \tag{11}$$

then:

$$S_n = \sum_{m_k \in I_n} \frac{(n+m-1)!}{n!\Pi m_k!} \tag{12}$$

with the same definition of I_n and m.

The main feature of these expressions is the definition of the set I_n of admissible structures of sharp separation for n components. The definition of I_n involves an integer relation between the numbers m_k of possible separators with $(k+2)$ outputs. When the number of outputs is limited to two (simple separators) or three, then the definition of I_n is a trivial task. It becomes:

- $m_0 = n-1$ and $m = m_0 = n-1$ for simple separators (the number of simple sharp separators for separating an n-component mixture is $n-1$) and relation 12 is equivalent to 1.
- $m_0 + 2m_1 = n-1$ and $m = m_0 + m_1$ for two-or-three output separators. The substitution of m_0 by $n-1-2m_1$ in relation 12 leads to relation 2.

For complex separators (more than three outputs), the use of Eq. 12 needs the resolution in the space of integer numbers of:

$$m_0 + 2m_1 + \ldots + (n-1)m_{n-2} = n-1 \tag{8}$$

The calculation of the number of all integer solutions of such an equation for an important value of n is not an easy task.

Table 1. Enumeration of all the Structures for $n=8$

Structure No.	m_0	m_1	m_2	m_3	m_4	m_5	m_6	m
1	0	0	0	0	0	0	1	1
2	1	0	0	0	0	1	0	2
3	0	1	0	0	1	0	0	2
4	2	0	0	0	1	0	0	3
5	0	0	1	1	0	0	0	2
6	1	1	0	1	0	0	0	3
7	3	0	0	1	0	0	0	4
8	0	2	1	0	0	0	0	3
9	2	1	1	0	0	0	0	4
10	4	0	1	0	0	0	0	5
11	1	0	2	0	0	0	0	3
12	5	1	0	0	0	0	0	6
13	3	2	0	0	0	0	0	5
14	1	3	0	0	0	0	0	4
15	7	0	0	0	0	0	0	7

However, we can enumerate easily, even in a spreadsheet, the elements of I_n corresponding to an equation of this type.

For $n=8$, by example, the enumeration of all the structures of I_8 (that is, all the m_i with $m_0+2m_1+3m_2+4m_3+5m_4+6m_5+7m_6=7$) leads to the Table 1.

The number S_8 is then by relation 12:

$$S_8 = \frac{8!}{8!1!} + \frac{9!}{8!1!} + \frac{9!}{8!1!} + \frac{10!}{8!2!} + \frac{9!}{8!1!} + \frac{10!}{8!1!} + \frac{11!}{8!3!} + \frac{10!}{8!2!} + \frac{11!}{8!2!} + \frac{12!}{8!4!} + \frac{10!}{8!2!} + \frac{13!}{8!5!} + \frac{12!}{8!3!2!} + \frac{11!}{8!3!} + \frac{14!}{8!7!}$$

each term of this sum corresponds to a distinct structure.

Thus, $S_8 = 4{,}279$

This result is clearly the same as previously found by a recursive procedure (Domenech et al., 1991).

Conclusion

A nonrecurrent formulation of the number of sharp separation sequences involving complex separators (that is, separators having more than two outputs) is derived in this article. This derivation requires the numbering of all possible separation structures determined by solving equations in the space of integer numbers.

Thus, it appears that the elucidation of the main combinatoric points will enable in the future the solution of complex sharp separation problems by means of combinatorial optimization techniques, as for example the simulated annealing procedure.

Notation

I_n = set of admissible structures of sharp separators
m = total number of separators in a sequence $= \Sigma_{m_k \in I_n} m_k$
m_k = number of separators with one input and $(k+2)$ outputs
n = number of components to be separated
n_s = number of distinct structures = number of elements of I_n
S_n = number of separation sequences of an n-component mixture

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Appendix 1: Number j of Simple (One Input, Two Outputs) Separators to Achieve the Separation, When Number I $\{0 \leq i \leq E[(n-1)/2]\}$ of Three-Output Separators of the Sequence is Fixed

Excluding the feed stream, the number of streams of the sequence is $2j+3i$. It corresponds to n pure component outputs and $(i+j-1)$ connection streams.

$$2j+3i=n+i+j-1$$

$$j=n-1-2i$$

Appendix 2: Derivation of the Relation 8

Excluding the feed stream, the number of streams in a separation sequence for an n-component mixture, that contains m_0 simple separators, m_1 separators with 3 outputs, ..., m_i separators with $(i+2)$ outputs, ..., and m_{n-2} separators with n outputs is:

$$2m_0+3m_1+\ldots+(i+2)m_i+\ldots+nm_{n-2}$$

It corresponds to n pure component outputs and $(m_0+m_1+\ldots+m_i+\ldots+m_{n-2}-1)$ connection streams.

$$2m_0+3m_1+\ldots+(i+2)m_i+\ldots+nm_{n-2}=n+(m_0+m_1+\ldots+m_i+\ldots+m_{n-2}-1)$$

$$\Rightarrow m_0+2m_1+3m_2+\ldots+(i+1)m_i+\ldots+(n-1)m_{n-2}=n-1 \quad (8)$$

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