Combinatorial Aspects of Sharp Split Separation Systems Synthesis

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Thompson and King (1972) presented a closed form expression for the number of different possible separation sequences arising when an n-component mixture is separated into pure products using sharp component separators with one input and two outputs. Subsequently, Shoaei and Sommerfeld (1986) pointed out that the number of sequences is the series of Catalan numbers (Alter, 1971), but they did not show how to derive the closed form formula. This paper will demonstrate that this may be done using a general mathematical technique—generating functions.

The analysis is extended to combinatorics of sequences of sharp separators with more than two outputs. Finally expressions for the number of distinct separators will be derived.

An underlying assumption throughout the paper is that the components in any stream are "sorted"; components appearing together will always appear in the same order.

Sequences of Two-Output Sharp Separators

A sharp two-output-component separator is a device where a subset of the feed components leave entirely in the separator's top stream and the rest leave entirely in the other, the bottom stream. Thus, the remaining separation problem originating from the top stream will be totally independent of the one originating from the bottom stream. The different separation sequences may be represented as paths in a tree, as illustrated in Figure 1 for a four-component example. It is seen from the figure that this example involves five different paths; five alternative separation sequences are possible.

The number of separation sequences may be defined recursively for the general case: a stream consisting of n components may be split in $n - 1$ different ways in one sharp two-output separator. For each of these alternative splits, the number of different separation sequences is equal to the number of separation sequences originating from the separator's top stream multiplied by the number of separation sequences originating from the separator's bottom stream. A stream with only one component generates exactly one sequence, which consists of zero separators.

With S_n denoting the total number of distinct sequences of sharp two-output separators for a stream with n components, this recursive definition may be stated formally as in Eq. 1 and Figure 2.

$$S_n = \sum_{k=1}^{n-1} S_k \cdot S_{n-k}, \quad S_1 = 1, n \geq 1 \tag{1}$$

Thompson and King (1972) presented a closed form expression for S_n:

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

Generating Functions Used to Derive the Thompson and King Formula

How can a general technique be applied to derive the Thompson and King formula? Suppose that a sequence of unknown numbers $S_0, S_1, S_2, \ldots, S_n, \ldots$ is implicitly defined by a recurrence relation and that it is desired to find a closed form expression for the recurrence relation. One elegant method applicable to many problems in this class is the method of generating functions. The theory of generating functions is based on two mathematical properties of infinite power series:

1. The infinite power series expansion of a given function is unique: if two alternative power series are expanded from the same function, then the two power series must be equivalent.

2. Two infinite power series are equivalent if, and only if, the coefficients in any corresponding pair of terms in the two series are equivalent.

The use of generating functions to derive the Thompson and King formulae which give the Catalan numbers is very often described in combinatorics textbooks (e.g., Townsend, 1987). To

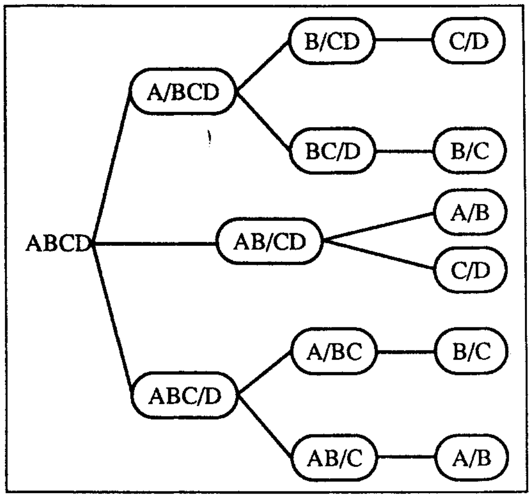

Figure 1. Sequences in a four-component sharp split separation system.

illustrate the elegance of the method, some of the steps are described in the following. The generating function for Eq. 1 may be expressed by the polynomial:

$$g(x) = S_1 \cdot x + S_2 \cdot x^2 + \cdots + S_n \cdot x^n + \cdots \quad (3)$$

where an arbitrary coefficient S_n is defined according to Eq. 1 as:

$$S_n = S_1 \cdot S_{n-1} + S_2 \cdot S_{n-2} + \cdots + S_{n-1} \cdot S_1 \quad (4)$$

Our goal is to find a closed form expression for this relation. This implies that we need to express $g(x)$ as a simple function of x, not as an infinite polynomial. From the pattern in the definition of S_n it may be seen that the square of $g(x)$ gives a very similar pattern:

$$\begin{aligned} g^2(x) &= (S_1 \cdot x + S_2 \cdot x^2 + S_3 \cdot x^3 + \cdots + S_n \cdot x^n + \cdots)^2 \\ &= S_1 \cdot S_1 \cdot x^2 + (S_1 \cdot S_2 + S_2 \cdot S_1)x^3 \\ &\quad + (S_1 \cdot S_3 + S_2 \cdot S_2 + S_3 \cdot S_1)\, x^4 + \cdots \end{aligned} \quad (5)$$

Using the recursive definition of the coefficients from Eq. 1 or 4, this may be expressed as:

$$g^2(x) = S_2 \cdot x^2 + S_3 \cdot x^3 + \cdots + S_n \cdot x^n + \cdots \quad (6)$$

which is identical to the infinite power series for $g(x)$ minus the first-order term $S_1 \cdot x$. S_1 is known, defined to be 1 in the recurrence relation (Eq. 1), so that the closed form expression in the generating function with all unknown coefficients eliminated becomes:

$$g^2(x) = g(x) - S_1 \cdot x = g(x) - x \quad (7)$$

Solving for $g(x)$ gives

$$g(x) = \frac{1 \pm (1 - 4 \cdot x)^{1/2}}{2} \quad (8)$$

From Eq. 3, it follows that $g(0) = 0$, and this eliminates the solution with a plus in front of the square root. This function will need to be expanded to an infinite polynomial in x again, but now the coefficients in front of each term will be expressed only as a function of n—the power x is raised to in the term. Using Newton's extended binomial theorem for the $(1 - 4 \cdot x)^{1/2}$ term this gives:

$$\begin{aligned} g(x) = 1/2 - 1/2 \Bigg\{ &\binom{1/2}{0} + \binom{1/2}{1}(-4 \cdot x) \\ &+ \binom{1/2}{2}(-4 \cdot x)^2 + \cdots + \binom{1/2}{n}(-4 \cdot x)^n + \cdots \Bigg\} \end{aligned} \quad (9)$$

This reveals the unknown coefficients, and only a rewrite of the expression remains:

$$\begin{aligned} S_n &= (-1/2) \cdot \binom{1/2}{n}(-4)^n \\ &= \frac{-(-4)^n \cdot (1/2) \cdot (-1/2) \cdot (-3/2) \cdots (1/2 - (n-1))}{2 \cdot n!} \\ &= \frac{2^n \cdot 1 \cdot 3 \cdots (2 \cdot n - 3)}{2 \cdot n!} = \frac{(2 \cdot (n-1))!}{n! \cdot (n-1)!} \end{aligned} \quad (10)$$

The result (Eq. 10) is the well-known Thompson and King formula.

Shoaei and Sommerfeld (1986) refer to the history behind the sequence of numbers originating from the above formula, known as the Catalan number sequence, and they give credit to Euler for the discovery of the sequence. This is, however, probably not entirely correct. According to Cohen (1978), Euler was not the discoverer of the sequence, he was the first to find the closed form formula. The German mathematician, Johann Andreas von Segner (1704–1777), preceded Euler in the discovery of the recurrence formula, and thus also in the discovery of the number sequence it generates.

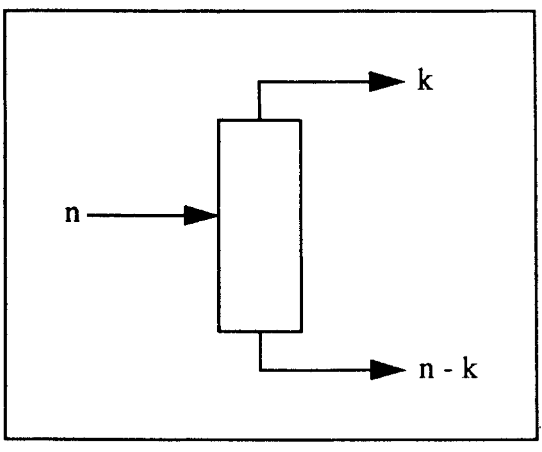

Figure 2. Two-output sharp split separation unit.

Extension to Sequences of Sharp Separators with More than Two Outputs

A separator may, both in principle and in practice, have more than two output streams. Side stream distillation columns and distillation columns with side stream strippers or rectifiers are practical examples of this. It may therefore be useful to extend the analysis to sequences of sharp separators with two or three outputs.

If any of the sharp separators in a sequence is allowed to have either two or three output streams, than a recurrence relation for the number of sequences may be derived using a similar argument as the one used to set up the recurrence relation in the two-output case. Now the recurrence relation must involve the sum of three-term products; and since two or three outputs are allowed, one "empty" output from a three-output separator will be legal, $S_0 = 1$. Generalizing from the two-output case the recurrence relation becomes (Figure 3):

$$S_n = \sum_{k=1}^{n-1} S_k \cdot \sum_{1=0}^{n-k-1} S_j \cdot S_{n-k-j} \qquad (11)$$

The generating function for the number sequence generated by Eq. 11 may be shown to be the analytic real solution of the third degree equation

$$g^3(x) - 2 \cdot g^2(x) + x = -1 \qquad (12)$$

Solving this equation for $g(x)$ gives a function that seems to be too complex to be practically useful for determination of the unknown coefficients by expansion to a power series. It is therefore suggested that the number of two- or three-output sequences of sharp separators is most conveniently computed using the recurrence relation (Eq. 11).

Number of Distinct Separators

The previous sections derived expressions for the number of distinct sequences of sharp separators, while this section derives formulae for the number of distinct sharp separators. From Figure 1 it is seen that the four-component problem has five different sequences. Each of these have three separators, giving 15 separators altogether. But not all of these are distinct, some of them are counted more than once. The formulae derived here count every distinct separator only once.

The relation between the number of separators and the number of sequences may be illustrated as follows. Take the tree from Figure 1 and collapse all instances of the same separator into one. This will transform the tree to a graph, as illustrated in Figure 4. The number of nodes in this graph will be the number of distinct separators for the problem. An expression for this number may be derived inductively. It is evident that there will be exactly one distinct sharp two-output separator for any binary mixture of components. To find an expression for the number of distinct separators for a mixture with any number n of components, it is first assumed that there already exists an unknown number of separators for a mixture of $n - 1$ components. If an expression may be found for the number of new distinct separators introduced when the nth component is added to this mixture, then the total number of distinct separators for any value of n greater than two may be obtained by simple summation.

Addition of an nth component to an n-1 component mixture will introduce the following additional two-output separators as compared to the two-output separators present in the $n - 1$ component case:

$$n = 2 \quad \begin{array}{c} A \\ \overline{B} \end{array}$$

$$n = 3 \quad \begin{array}{ccc} A & A & \\ \overline{B} & B & B \\ C & \overline{C} & \overline{C} \end{array}$$

$$n = 4 \quad \begin{array}{cccccc} A & A & A & & & \\ \overline{B} & B & B & B & B & \\ C & \overline{C} & C & \overline{C} & C & C \\ D & D & \overline{D} & D & \overline{D} & \overline{D} \end{array}$$

$$n = 5 \quad \begin{array}{cccccccccc} A & A & A & A & & & & & & \\ \overline{B} & B & B & B & B & B & B & & & \\ C & \overline{C} & C & C & \overline{C} & C & C & C & C & \\ D & D & \overline{D} & D & D & \overline{D} & D & \overline{D} & D & D \\ E & E & E & \overline{E} & E & E & \overline{E} & E & \overline{E} & \overline{E} \end{array}$$

It is readily seen that if all the n components are present in the separator, one may choose among $n - 1$ locations for the split. Thus, the number of additional splits with all n components present is $\binom{n-1}{1}$. But it is also possible that only $n - m$

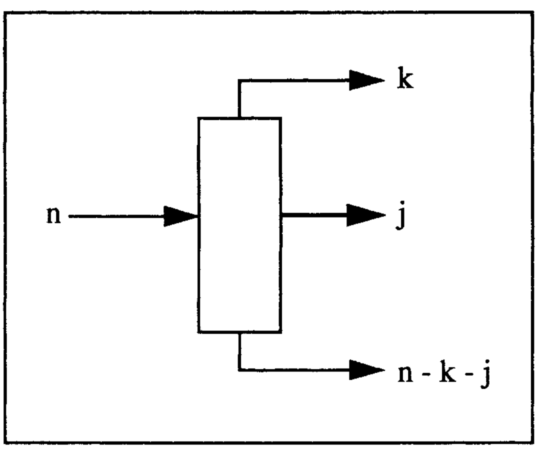

Figure 3. Three-output sharp split separation unit.

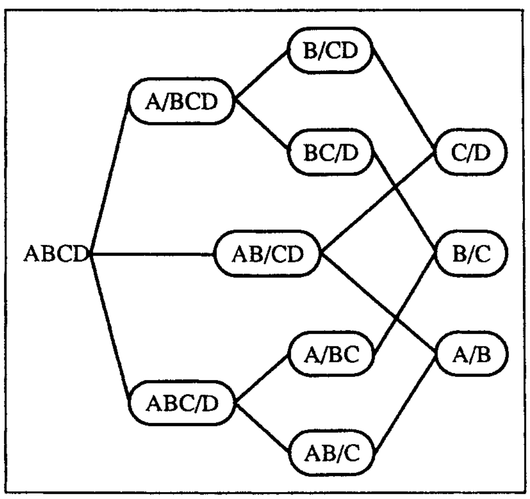

Figure 4. Separators in a four-component sharp split separation system.

components are present, as long as the nth component is among these, with m ranging from 1 to $n-1$. The total number of new splits introduced by addiiton of an nth component to an $n-1$ component mixture will thus be

$$ES(n)_2 = \binom{n-1}{1} + \binom{n-2}{1} + \cdots + \binom{1}{1} \equiv \binom{n}{2} \quad (13)$$

The total number of splits will naturally be the sum of additional splits introduced with each component added to the mixture, counting from two and up to n:

$$TS(n)_2 = \binom{2}{2} + \binom{3}{2} + \cdots + \binom{n}{2} \equiv \binom{n+1}{3} \quad (14)$$

which may also be expressed as

$$TS(n)_2 = \frac{n^3 - n}{6} \quad (15)$$

The latter form, reported earlier for example by Lien (1988), is easier to compute than the former, but the former is more easily generalized to cases with more then two outputs. The procedure for calculation of the number of three-output separators is similar to that for two-output separators, with the only difference that *two* different splits must be placed in $n-1$ places.

The number of extra splits when an nth component is added to an $n-1$ component mixture is thus in the three-output case:

$$ES(n)_3 = \binom{n-1}{2} + \binom{n-2}{2} + \cdots + \binom{2}{2} \equiv \binom{n}{3} \quad (16)$$

This results in a total number of three-output separators equal to:

$$TS(n)_3 = \binom{3}{3} + \binom{4}{3} + \cdots + \binom{n}{3} \equiv \binom{n+1}{4} \quad (17)$$

which may also be expressed as

$$TS(n)_3 = \frac{n^4 - 2n^3 - n^2 + 2n}{24} \quad (18)$$

A generalization to the number of extra splits, if 2,3, . . . or r output streams are allowed, is trivial, since the number of two-output separators is independent of the number of three-output separators,

$$ES(n)_r = \binom{n}{2} + \binom{n}{3} + \cdots + \binom{n}{r} = \sum_{k=2}^{r} \binom{n}{k} \quad (19)$$

Table 1. Numbers of Sequences and Separators for Two- and Three- Output Streams

No. of Comp.	Output Streams: No. of Sequences, 2	No. of Sequences, 2 or 3	No. of Separators, 2	No. of Separators, 2 or 3
2	1	1	1	1
4	5	10	10	15
6	42	154	35	70
8	429	2,871	84	210
10	4,862	59,345	165	495

The total number of splits in this most general case is thus:

$$TS(n)_r = \binom{n+1}{3} + \binom{n+1}{4} + \cdots + \binom{n+1}{r+1} = \sum_{k=3}^{r+1} \binom{n+1}{k} \quad (20)$$

Table 1 illustrates the rapid growth rate of the number of sequences and separators for two- and three-output streams.

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Notation

$ES(n)_r$ = additional number of splits for n components and r output streams
$g(x)$ = generating function
S_n = number of sequences for n components
$TS(n)_r$ = total number of splits for n components and r output streams

Literature Cited

Alter, R., "Some Remarks and Results on Catalan Numbers," *Proc. Louisiana Conf. Combinat., Graph Theory, and Comp.*, Baton Rouge, 109 (1971).

Cohen, D. I. A., *Basic Techniques of Combinatorial Theory*, Wiley, New York (1978).

Lien, K. M., "Expert Systems Technology in Synthesis of Distillation Sequences," PhD Thesis, Univ. of Trondheim, Norway (1988).

Shoaei, M., and J. T. Sommerfeld, "Catalan Numbers in Process Synthesis," *AIChE J.*, **32**, 1931 (1986).

Townsend, M., *Discrete Mathematics: Applied Combinatorics and Graph Theory*, Ben/Cummings Publ., Menlo Park, CA (1987).

Thompson, R. W., and C. J. King, "Systematic Synthesis of Separation Schemes," *AIChE J.*, **8**, 941 (1972).

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