

# Transformation of the Product Set in Separation Sequence Synthesis

Yi-Ming Chen and L. T. Fan

Dept. of Chemical Engineering, Kansas State University, Manhattan, KS 66506

Among other factors, the complexity of a separation sequencing problem is determined by the size of a product set, that is, the number of product streams involved (see, for example, Muraki et al., 1986; Floudas, 1987). Thus, extensive investigation has been conducted to study the possibilities of reducing the size of a given product set without additional separators (Bamopoulos, 1984; Cheng, 1987). One way to accomplish this is to examine the possible linear dependency among the product streams.

Assume that  $P$   $n$ -component product streams are to be produced; each product stream can be visualized as an  $n$ -component vector. Furthermore, suppose that  $p_1, p_2, \dots$ , and  $p_r$  are  $r$  linearly independent product streams [ $r \leq \min(n, P)$ ] and that they form a basis for the product vector space. Then, the remaining  $(P-r)$  product streams can be expressed in terms of these  $r$  product streams in the following vector notation (Amundson, 1966);

$$p_i = c_{i1}p_1 + c_{i2}p_2 + \dots + c_{ir}p_r, \quad i = r+1, r+2, \dots, P \quad (1)$$

where element  $\{p_{ij}\}$  represents the molar flow rate of the  $j$ th component, ranked in descending order of a certain physical or chemical property, in product stream  $i$ ; and  $c_{i1}, c_{i2}, \dots$ , and  $c_{ir}$  in Eq. 1 are constants. If these constants are all nonnegative, the  $(P-r)$  product streams can be obtained by appropriately blending the  $r$  linearly-independent product streams. This appears to be attractive in reducing the size of the original product set, thereby leading to the simplification of the original separation sequencing problem (Bamopoulos, 1984; Cheng, 1987). Nevertheless, little, if any, has been published on the effect of transforming the original product set into the set with  $r$  product streams on the structure and overall cost of the separation sequence. The purpose of this note is to examine this effect for an all-sharp separation sequence producing nonsharp products. It has been found that the maximum extent of stream bypassing for any sequence with  $P$  product streams (the original problem) is greater than that for the sequence with  $r$  product streams (the reduced problem). Consequently, it can be concluded that, in general, the cost

of the optimal sequence for the original problem is less than that for the reduced problem.

## Representations for Original and Reduced Problems

Consider a general separation sequencing problem involving one  $n$ -component feed stream and  $P$   $n$ -component product streams; Obviously, separation is not needed for  $P=1$  since  $f=p$ . For a given feed and  $P=2$ , suppose that  $p_1$  depends linearly on  $p_2$ . Then, both product streams must have the same composition as that of the feed; again, separation is not needed. For  $P \geq 3$ , assume that the maximum number of linearly independent product streams is  $r$ :

$$r = \text{rank}(P) \quad (2)$$

and that they are designated as  $p_1, p_2, \dots$ , and  $p_r$ . For the original problem of producing the specified  $P$  product streams directly from the feed stream, the feed  $f$ , and the product streams,  $p_1, p_2, \dots$ , and  $p_r$ , can be expressed as the vectors

$$f = [f_1 \ f_2 \ \dots \ f_n]^T \quad (3)$$

$$p_i = [p_{i1} \ p_{i2} \ \dots \ p_{in}]^T, \quad i = 1, 2, \dots, r \quad (4)$$

while the remaining  $(P-r)$  product streams,  $p_{r+1}, p_{r+2}, \dots$ , and  $p_P$ , can be expressed in terms of these  $r$  product streams as:

$$p_i = c_{i1}p_1 + c_{i2}p_2 + \dots + c_{ir}p_r, \quad i = r+1, r+2, \dots, P \quad (5)$$

If the constants,  $c_{i1}, c_{i2}, \dots$ , and  $c_{ir}$ , in the above equation are all nonnegative, the product streams,  $p_{r+1}, p_{r+2}, \dots$ , and  $p_P$ , can be obtained by blending the  $r$  linear-independent product streams,  $p_1, p_2, \dots$ , and  $p_r$ . In such cases, the reduced problem can be formed with the same feed as that represented by Eq. 3 and the following product streams.

Correspondence concerning this work should be addressed to L. T. Fan.

$$p_i^* = [p_{i1}^* \ p_{i2}^* \ \dots \ p_{in}^*]^T$$

$$= \left(1 + \sum_{j=r+1}^P c_{ji}\right) [p_{i1} \ p_{i2} \ \dots \ p_{in}]^T, \quad i=1,2,\dots,r \quad (6)$$

The summation in the parenthesis indicates the amounts of the product streams,  $p_1, p_2, \dots$ , and  $p_r$ , that will be converted into the product streams,  $p_{r+1}, p_{r+2}, \dots$ , and  $p_P$ , through blending. When any of the constants,  $c_{i1}, c_{i2}, \dots$ , and  $c_{ir}$ , is negative, however, we cannot obtain  $(P-r)$  product streams without additional separators.

## Maximum Stream Bypassing

For the original problem, the maximum fraction of the feed stream that can be bypassed to product stream  $p_i$ ,  $x_i$ , can be evaluated as (Aggarwal and Floudas, 1990):

$$x_i = \min\left(\frac{p_{i1}}{f_1}, \frac{p_{i2}}{f_2}, \dots, \frac{p_{in}}{f_n}\right) = \frac{p_{iK(i)}}{f_{K(i)}}, \quad i=1,2,\dots,r \quad (7)$$

and

$$x_i = \min\left(\frac{\sum_{j=1}^r c_{ij} p_{j1}}{f_1}, \frac{\sum_{j=1}^r c_{ij} p_{j2}}{f_2}, \dots, \frac{\sum_{j=1}^r c_{ij} p_{jn}}{f_n}\right)$$

$$= \frac{\sum_{j=1}^r c_{ij} p_{jK(i)}}{f_{K(i)}}, \quad i=r+1, r+2, \dots, P \quad (8)$$

In these equations,  $K(i)$  is the index of the component for which the component ratio between product stream  $p_i$  and feed  $f$  is minimum. Thus, the overall fraction of bypassing the feed stream is:

$$BP^{\text{org}} = \sum_{i=1}^P x_i = \sum_{i=1}^r \frac{p_{iK(i)}}{f_{K(i)}} + \sum_{i=r+1}^P \sum_{j=1}^r c_{ij} \frac{p_{jK(i)}}{f_{K(i)}} \quad (9)$$

For the reduced problem, the fraction of the feed stream bypassing to product stream  $p_i$ ,  $x_i^*$ , is:

$$x_i^* = \min\left(\frac{p_{i1}^*}{f_1}, \frac{p_{i2}^*}{f_2}, \dots, \frac{p_{in}^*}{f_n}\right)$$

$$= \left(1 + \sum_{j=r+1}^P c_{ji}\right) \min\left(\frac{p_{i1}}{f_1}, \frac{p_{i2}}{f_2}, \dots, \frac{p_{in}}{f_n}\right)$$

$$= \left(1 + \sum_{j=r+1}^P c_{ji}\right) \frac{p_{iK(i)}}{f_{K(i)}}$$

$$= \frac{p_{iK(i)}}{f_{K(i)}} + \frac{p_{iK(i)}}{f_{K(i)}} \sum_{j=r+1}^P c_{ji}, \quad i=1,2,\dots,r \quad (10)$$

Hence, the overall fraction of bypassing the feed stream is:

$$BP^{\text{red}} = \sum_{i=1}^r x_i^*$$

$$= \sum_{i=1}^r \frac{p_{iK(i)}}{f_{K(i)}} + \sum_{i=1}^r \sum_{j=r+1}^P c_{ji} \frac{p_{iK(i)}}{f_{K(i)}}$$

$$= \sum_{i=1}^r \frac{p_{iK(i)}}{f_{K(i)}} + \sum_{i=r+1}^P \sum_{j=1}^r c_{ij} \frac{p_{jK(i)}}{f_{K(i)}} \quad (11)$$

From Eqs. 9 and 11,

$$BP^{\text{org}} - BP^{\text{red}} = \sum_{i=r+1}^P \sum_{j=1}^r c_{ij} \left(\frac{p_{jK(i)}}{f_{K(i)}} - \frac{p_{jK(j)}}{f_{K(j)}}\right)$$

$$= \sum_{j=r+1}^P \sum_{i=1}^r c_{ji} \left(\frac{p_{iK(j)}}{f_{K(j)}} - \frac{p_{iK(i)}}{f_{K(i)}}\right) \quad (12)$$

From Eq. 7,  $p_{iK(i)}/f_{K(i)}$  is the minimum component ratio between product stream  $p_i$  and feed  $f$ , while  $p_{iK(j)}/f_{K(j)}$  is generally the ratio of the  $K(j)$ th component of product stream  $p_i$  to that of feed  $f$ . Consequently,

$$\frac{p_{iK(j)}}{f_{K(j)}} \geq \frac{p_{iK(i)}}{f_{K(i)}} \quad (13)$$

Thus, we have:

$$BP^{\text{org}} - BP^{\text{red}} \geq 0$$

or

$$BP^{\text{org}} \geq BP^{\text{red}} \quad (14)$$

Because of the constraint expressed in Eq. 13, the equality in the above expression holds only when every term on the righthand side of Eq. 12 vanishes. From the first  $r$  terms on the righthand side of Eq. 12, we have:

$$\frac{p_{1K(r+1)}}{f_{K(r+1)}} = \frac{p_{1K(1)}}{f_{K(1)}} \quad (15)$$

$$\frac{p_{2K(r+1)}}{f_{K(r+1)}} = \frac{p_{2K(2)}}{f_{K(2)}} \quad (16)$$

$$\vdots \quad \vdots \quad \vdots$$

$$\frac{p_{rK(r+1)}}{f_{K(r+1)}} = \frac{p_{rK(r)}}{f_{K(r)}} \quad (17)$$

In other words, all the minimum component ratios for the product streams,  $p_1, p_2, \dots, p_r$ , occur at the  $K(r+1)$ th component; therefore, for all the other components of these product streams, we have:

$$\frac{p_{ij}}{f_j} \geq \frac{p_{iK(r+1)}}{f_{K(r+1)}}, \quad i=1,2,\dots,r; j=1,2,\dots,n; j \neq K(r+1) \quad (18)$$

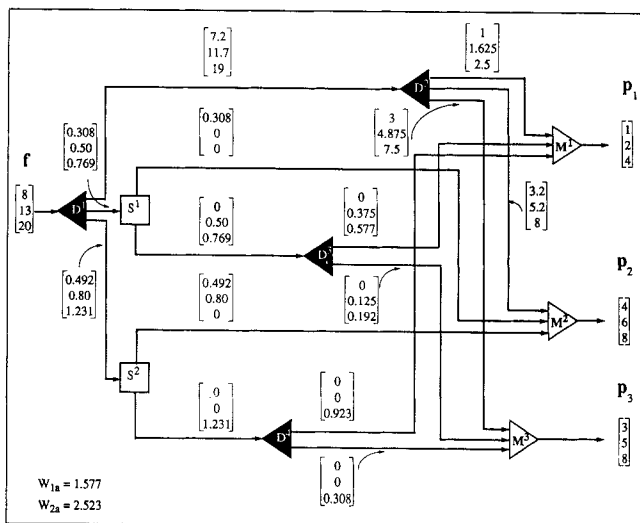


Figure 1. Sequence *a* for the original problem.

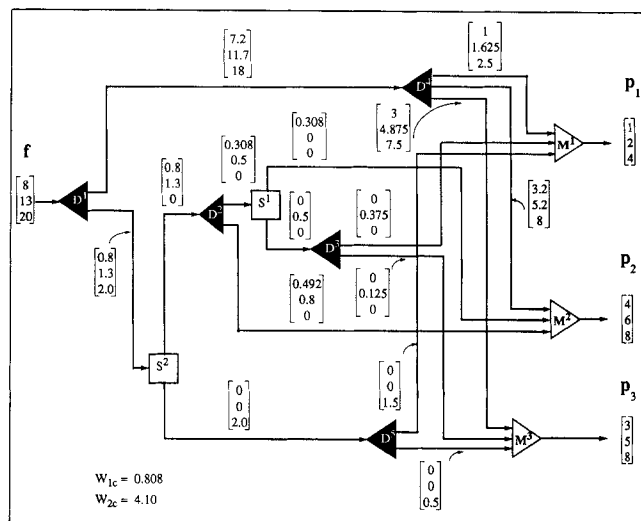


Figure 3. Sequence *c* for the original problem.

or

$$\frac{p_{ij}}{f_j} \left( 1 + \sum_{j=r+1}^P c_{ji} \right) \geq \frac{p_{iK(r+1)}}{f_{K(r+1)}} \left( 1 + \sum_{j=r+1}^P c_{ji} \right) \quad (19)$$

The overall mass balance over the  $K(r+1)$ th component yields:

$$\sum_{i=1}^r \frac{p_{iK(r+1)}}{f_{K(r+1)}} \left( 1 + \sum_{j=r+1}^P c_{ji} \right) = 1 \quad (20)$$

The overall mass balance over the  $j$ th component gives:

$$\sum_{i=1}^r \frac{p_{ij}}{f_j} \left( 1 + \sum_{j=r+1}^P c_{ji} \right) = 1 \quad (21)$$

From the above two expressions,

$$\sum_{i=1}^r \frac{p_{iK(r+1)}}{f_{K(r+1)}} \left( 1 + \sum_{j=r+1}^P c_{ji} \right) = \sum_{i=1}^r \frac{p_{ij}}{f_j} \left( 1 + \sum_{j=r+1}^P c_{ji} \right) \quad (22)$$

In the light of this equation and Eq. 19, Eq. 18 reduces to:

$$\frac{p_{ij}}{f_j} = \frac{p_{iK(r+1)}}{f_{K(r+1)}} \quad (23)$$

Since the righthand side of this expression is independent of  $j$ , we obtain:

$$\frac{p_{i1}}{f_1} = \frac{p_{i2}}{f_2} = \dots = \frac{p_{in}}{f_n}, \quad i = 1, 2, \dots, r \quad (24)$$

The implication is that the product streams,  $p_1, p_2, \dots$ , and  $p_r$ , have the same composition as that of the feed and, therefore, depend on each other, which is in contradiction to the original assumption that these product streams are linearly

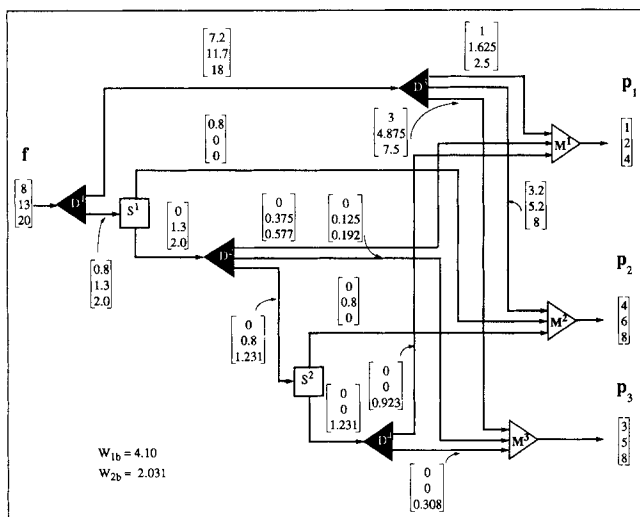


Figure 2. Sequence *b* for the original problem.

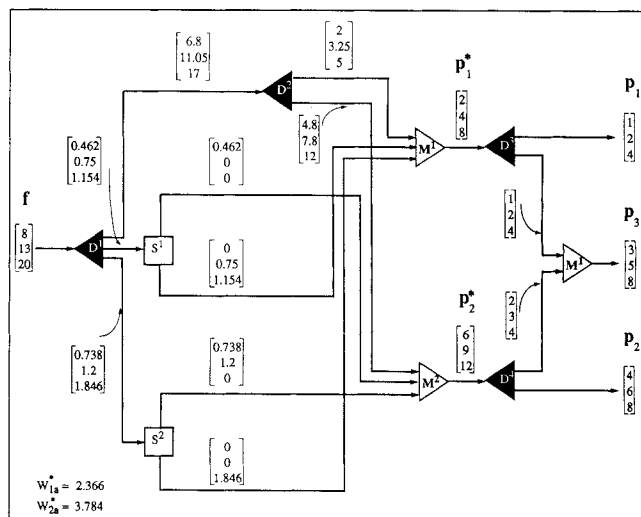


Figure 4. Sequence *a* for the reduced problem.



## Notation

$BP^{org}$  = maximum extent of bypassing for the original problem  
 $BP^{red}$  = maximum extent of bypassing for the reduced problem  
 $D$  = divider  
 $f$  = feed stream  
 $K(i)$  = index of the component at which the minimum component ratio between  $p_i$  and  $f$  is obtained  
 $M$  = mixer  
 $n$  = number of components in the feed stream  
 $p_i$  =  $i$ th product vector of the original problem  
 $p_i^*$  =  $i$ th product vector of the reduced problem  
 $P$  = number of product streams  
 $P$  = matrix with product streams as its column vectors  
 $r$  = maximum number of the linearly-independent product streams  
 $S^i$  = separator in which components  $i$  and  $i+1$ , ranked in decreasing order of a certain physical or chemical property, are light and heavy key components, respectively  
 $x_i$  = maximum fraction of the feed stream that can be bypassed to product stream  $p_i$   
 $W_i$  = molar flow rate of the feed to separator  $S^i$

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*Manuscript received July 17, 1991, and revision received Sept. 30, 1991.*