Feasibility of Partitioning Multicomponent Feeds in the Minimum Number of Splits

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The need to synthesize separation systems arises as a subproblem in the creation of a chemical process flowsheet when one or more multicomponent streams must be fractionated into products with some components in higher concentration. The majority of published works on the problem (Nishida et al., 1981) focus on systems with a single multicomponent feed stream and essentially pure products. Thompson and King (1972a, b) proposed a method to synthesize separation systems in which a restricted type of multicomponent product was allowed. They discovered that when several separation methods were available the determination of the minimum number of separators required to create a given product set was in general not a completely trivial problem. The purpose of the present note is to examine their notion of the feasibility of a product set and to illustrate various complications that can occur with increasing problem size. An algorithm for the determination of product set feasibility is presented. The present intent is not to synthesize flowsheets with difficult product sets; this will be treated in a future paper.

If the products are restricted to those that may be made by performing sharp splits on the feed, then each component in the feed appears in exactly one product in an appreciable amount, but some product(s) may be desired or allowed to contain more than one component. Viewing the feed F as a set of components: $F = \{1, 2, \ldots, m, \ldots, n\}$, then the product subsets $P_1, P_2, \ldots, P_j, \ldots, P_p$ form a partition of the feed, where p is the total number of products. In set-theoretic notation this is stated as:

$$P_j \subseteq F, 1 \leq j \leq p \tag{1}$$

$$P_1 \cup P_2 \cup \cdots P_j \cup \cdots P_p = F \tag{2}$$

$$P_j \cap P_i = \emptyset, 1 \leq j < i \leq p \tag{3}$$

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That is, each product is a subset of the set of feed components, the union of the products is the feed, and no two products have any component in common. Because the products form a partition of the feed, the determination of an optimal sequence of separators, of possibly varying types, to create the products may be called the partitioning problem (the nomenclature is ours).

Thompson and King (1972a, b) developed a heuristic approach to the partitioning problem. An important aspect of their work was an initial analysis step to determine the feasibility of a partition, i.e., whether p desired products could be created using exactly p-1 available splits. An infeasible partition would require more splits as necessary to create a larger feasible partition from which the desired partition could be created by blending. The following discussion presents a review of their insights into a necessary condition for feasibility of a partition which they also believed to be sufficient. While their synthesis method allowed for changes in separation potential order of components, their test for feasibility of a partition had to assume that the separation potential orders were constant. Thus it was quite possible for a feasible partition to later become infeasible with the removal of one or more products, and repeated calls to their feasibility checking routine were necessary as downstream separators were created. Thus the following discussion treats what might be called the static case, that in which all the component separation potential orders are assumed to remain fixed.

Associated with each available separation method is a ranked list s of components in the order of decreasing separation potentials. Every separation method exploits some physical property difference between the components in a feed stream. In the familiar case of ordinary distillation the property is component volatility; therefore, the term "volatility" is used in a generic sense to refer to the component separation potential regardless of the particular separation method. The component highest in separation potential with respect to a particular ranked list is then called the "most volatile."

If a partition is created with a sequence having the minimum number of splits, then it is obvious that no split in that sequence divides any one product into two parts. The problem data may be organized by defining the "span" of a product on a ranked list s as the portion of s bounded by the positions of the most and least volatile components in the product. This can be diagrammed by writing the ranked list and marking the locations of components in a given product with asterisks below. Between the most and least volatile components in the product a line may be drawn to show its span. Two products that span a common split in a ranked list s are said to overlap in s. Given two products i and j which do not overlap in s, if all the splits between the spans of i and j are within the span of product k (or a set of products), then k (or the set of products) is said to span the split between i and j in s; i.e., before i and j can be separated by a split in s, the (spanning) product k (or set of products) must first be removed. Upon such removal i and j are separable by a newly unspanned split. If i and j do not overlap in s, and some split between their spans is not within the span of any other product, then that split is termed "initially unspanned." A sequence of feasible splits does not divide the components of any desired multicomponent product; it begins with an initially unspanned split and continues with initially or newly unspanned splits.

Thompson and King gave the following test for partition feasibility in terms of pairwise separability of the products, restated here using the nomenclature established above.

Product i can be separated from product j by separator s if and only if:
((i and j do not overlap in the ranked list of s) and
(for all multicomponent products MP other than i and j:
(MP does not span (all) the split(s) between i and j in s) or
(for some separator x:
(MP does not overlap either i or j in the ranked list of x)))).

The test worked for all of their examples, but the counterexample shown in Figure 1 appears to pass the test when it is obviously not a feasible partition. That example is not feasible because it has no initially unspanned split, but examination of the six possible pairs of products indicates that they all appear to be splittable by either s_1 or s_2 according to the test. The example appears to be the smallest infeasible partition capable of passing

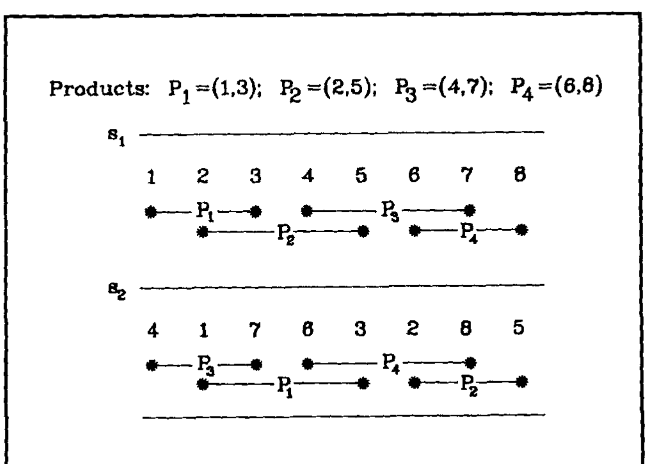

Figure 1. An infeasible partition.

Thompson and King's test for feasibility. Their test will work correctly for any partition with no more than three multicomponent products. It seems unlikely that a feasible partition of any size could be mistaken as infeasible by their test. The fault with the test is that it treats only sets of two and three products at a time when complicated overlaps can occur with sets of four or more products, and it says nothing about initially unspanned splits, of which there must be at least one. A general condition for feasibility must account for all product pairs that are not separable by an initially unspanned split, as in the following.

A partition is feasible if and only if for every product pair (i, j):
((i and j do not overlap in at least one ranked list s) and
((i and j are separable by an initially unspanned split in at least one ranked list s) or
(if i and j are not separable by an initially unspanned split in any ranked list s where they do not overlap, then a sequence of feasible splits exists which can remove all the spanning products in one of those ranked lists so that i and j become separable by a newly unspanned split))).

This test can be applied by the following algorithm, which may involve search.

1. Determine for each product pair (i, j) the ranked lists, if any, in which they do not overlap. (If any pair overlaps in every ranked list, the partition is not feasible.)

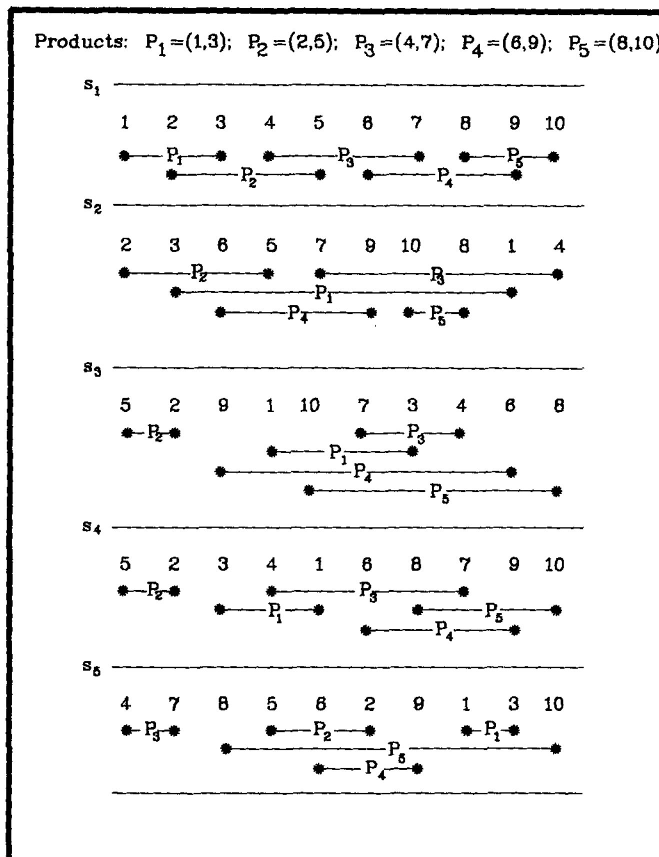

Figure 2. A feasible partition used to illustrate the determination of partition feasibility.

2. Identify all the initially unspanned splits. (If there is none, then the partition is not feasible.)

3. Mark each product pair (i, j) as to whether or not it can be separated by some initially unspanned split. If every pair can be separated, then the partition is feasible. If not, then a depth-firth search (Nijenhuis and Wilf, 1978) for a sequence of feasible splits must be initiated.

4. Locate all subsets (with at least three members) of the set of all products, of which each has the property that all its member products, when taken pairwise, cannot be separated by some initially unspanned split. (Each such subset can be located by finding just one of its member products and testing all the remaining products to see whether they can each be separated from that first product by an initially unspanned split. This is because each initially unspanned split bipartitions the set of products. If products j and j' cannot be initially separated from product i, then they cannot be initially separated from each other.) Place each such "initially spanned" subset on a stack. (This is equivalent to selecting any maximal sequence of initially unspanned splits. Initially spanned subsets with just two members may be ignored, because no product pair overlaps in every ranked list. If the partition had passed the feasibility test of Thompson and King, then initially spanned subsets with three members may also be ignored.)

While the stack is not empty:

5. Remove the last currently spanned subset from the stack. Since this subset of products is now regarded as existing in isolation as an intermediate stream in some sequence of separators, it may contain newly unspanned splits. If so, perform the first one found. The resulting two product subsets must each be checked to see whether they are sufficiently large (according to the criteria of step 4) to require further search for newly unspanned splits. If so, place the affected subset(s) on the stack. If the subset has no newly unspanned split, the partition is infeasible. (The search may be continued to determine all the feasible products.)

The determination of partition feasibility is illustrated for the hypothetical problem of Figure 2 having ten components, five desired products, and five ranked lists. There is no initially unspanned split between product pairs (P_4, P_1), (P_5, P_1), and (P_5, P_4). Thus products (P_1, P_4, P_5) form an initially spanned subset. Of the three initially unspanned splits, two (split 2 in s_3 and split 2 in s_4) are equivalent in terms of the products they separate. Performing two nonequivalent splits creates newly unspanned splits between P_1 and (P_4, P_5) in both s_1 and s_4. Removal of P_1 creates an unspanned split between P_4 and P_5 in s_2. The partition is thus feasible.

Additional discussion of the partitioning problem is given by Mocsny (1986). A computer program for partition feasibility determination is available upon request from the authors.

Acknowledgment

This material is based upon work supported under a National Science Foundation Graduate Fellowship. The authors wish to thank R. W. Thompson for his helpful comments.

Notation

- F = set of feed components
- i, j, k = product indices
- m = component index
- n = total number of components
- P_j = jth required product
- p = total number of products
- s = ranked list of components
- $\subseteq$ = subset relational operator
- $\emptyset$ = the null or empty set
- $\cap$ = set intersection
- $\cup$ = set union

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Manuscript received Aug. 4, 1986, and revision received Nov. 21, 1986.