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Rigorous Algorithm for Synthesizing Azeotropic-Distillation Systems

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The industrial importance of azeotropic-distillation (AD) systems, in general, and heterogeneous AD systems, in particular, has been well known. Most of the available methods for synthesizing such systems resort to some heuristics in order to determine the systems' structures. Thus, it is extremely difficult, if not impossible, to ascertain the optimality of the resultant structures. A highly robust and efficient algorithmic method based on the combinatorial approach is proposed herein for synthesizing a heterogeneous AD system. Each major step of the algorithm is illustrated with the synthesis of the ethanol-water-toluene (EWT) system, which also serves to demonstrate the method's efficacy.

1. Introduction

The importance of optimally synthesizing a heterogeneous azeotropic-distillation (AD) system is well established in chemical and allied industries. Much remains to be done, however, to resolve some of the major difficulties involved. The majority, if not all, of the available methods for synthesizing a heterogeneous AD system resorts to some heuristics in order to determine the system's structure. Nevertheless, counter-intuitive structures may improve the system's performance (Kovacs *et al.*, 1993). Consequently, it is highly likely that a structure, i.e., a network, of the heterogeneous AD system generated by an available method can be far from the optimum if the flowsheet-generation step is neither systematic nor verifiable. The only available systematic method of flowsheet-generation is based on the formulation of the problem of AD-system synthesis as a problem of process-network synthesis problem (Feng *et al.*, 2000); it rapidly generates numerous feasible flowsheets. Nevertheless, the assumptions imposed in the formulation give rise to unduly tight restrictions on the flowsheets that can be generated.

The current work aims at developing an efficient and practical method for the algorithmic generation, i.e., synthesis, of the complete set of flowsheets for a heterogeneous AD system from various types of candidate operating units, which produces the required pure components from the feed, as illustrated in Fig. 1. The development of such a method has been accomplished by merging the virtues of P-graph representation (Friedler *et al.* 1992a), algorithm SSG (Friedler *et al.* 1992b), and the Means-Ends analysis (Siirola, 1996).

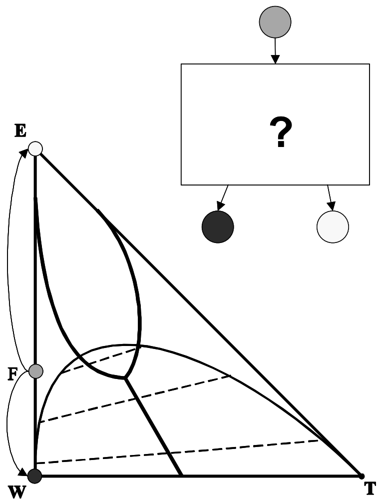

Figure 1. Azeotropic distillation problem.

Initially, the candidate operating units are identified on the basis of the feasible inputs and outputs in the regions of the RCM bounded by thermodynamic boundaries and pinches. This renders it possible to derive analytical expressions of the feasible inputs and outputs in terms of the boundaries' coordinates and to automatically and rapidly examine whether an output from a unit of a certain type can be an input to another. Finally, the feasible flowsheets are exhaustively generated algorithmically; they satisfy the constraints related to the products, raw materials, and feasible inputs and outputs of the operating units; they also satisfy the mass balances around all the operating units of various types. The optimal and near optimal flowsheets can be recovered from the resulting feasible flowsheets.

2. Problem Formulation

Lumped materials are introduced to relax the utmost complexity posed by the infinite number of points on the RCM. A lumped material is mapped to a region, a curve or a point of the RCM, if it represents an input or output of an operation or if it represents the desired pure component or feed stream. Lumped material L_1, shown in Fig. 2., can be an input to a distillation operation with a pure product, i.e., ethanol, as its output stream. Thus, a lumped material is given by a set of concentrations. The candidate operations are identified by the lumped materials representing the feasible regions of their inputs and outputs.

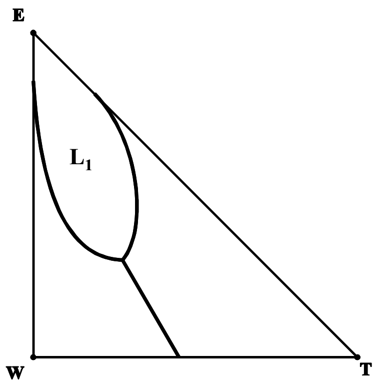

Figure 2. Lumped material L_1.

3. Proposed Algorithm

As mentioned in Introduction, a combinatorial algorithm is proposed, which is based on P-graph representation, algorithm SSG, and the goal oriented solving paradigm known as Means-Ends analysis. It generates feasible flowsheets in terms of combinatorial properties; mass balances; and constraints related to the inputs and outputs of the operating units, as well as the desired system. The algorithm proceeds as follows:

The input to the algorithm is the set of lumped materials representing the desired products, the set of lumped materials representing the given feed stream, and the set of available operations represented by the lumped materials of their inputs and outputs; see Fig. 3(a).

Every step of the algorithm selects an arbitrary lumped material that needs to be produced. An operation is incorporated into the structure if it is capable of producing the selected lumped material, i.e., if the set of concentrations identifying one of its output streams has an intersection with the set representing the selected lumped material. After the operation is included in the flowsheet, the set of lumped materials representing required products are updated as necessary. Figure 3(b) shows that lumped material P_2 produced, which is given by a set of concentrations denoted by a circle, is excluded from the set of products, while the input to the operation producing material P_2 is included.

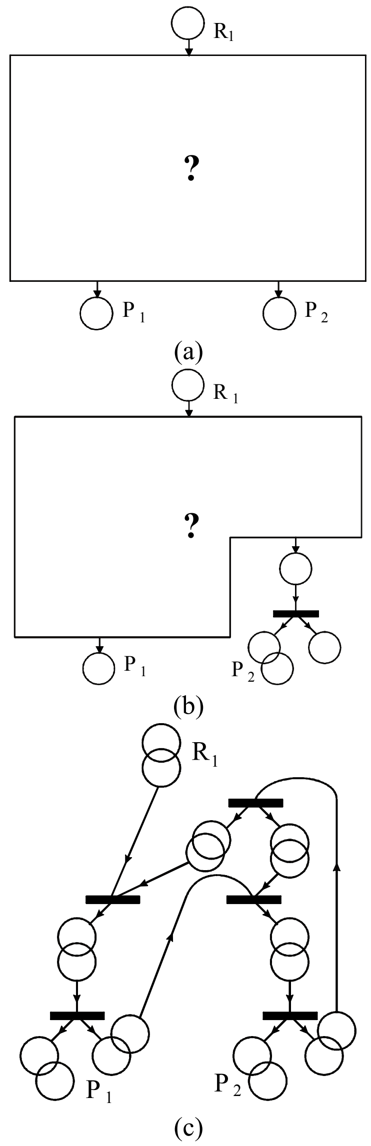

Figure 3. Steps of the algorithm: (a) synthesis problem; (b) subproblem generated in the first step; (c) resultant structure.

The generation continues on every possible branch enumerating all the alternative combinations of operations capable of producing the lumped materials of interest. The algorithm results in a feasible structure on a branch if the flowsheet represents an azeotropic-distillation system where the desired products and inputs to the operating units in the structure are produced, while the given feed stream is consumed; see Fig. 3(c).

4. Implementation

The linearization of the regions representing the lumped materials can accelerate the algorithm. The solutions generated from the resultant linear model should include all the solutions generated with the non-linear model. Thus, each region is linearized such that it contains every point of the original region.

The proposed implementation requires the lumped materials to be represented by convex regions. Hence, the non-convex regions appearing in Fig. 4(a) are segmented and covered by convex ones, as illustrated in Fig. 4(b).

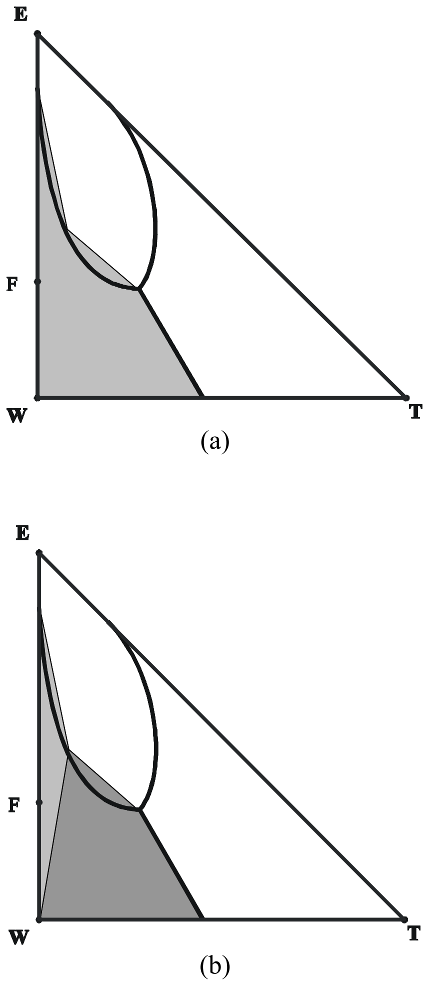

Figure 4. Linearization technique: (a) non-convex region; (b) convex segments covering the non-convex region

5. Application

The well-known Ethanol-Water-Toluene (EWT) problem has been revisited with the proposed method. Twelve lumped materials are identified. The operations, including distillation, decanting and mixing, are deemed to be available. The division of non-convex regions of the RCM gives rise to 7 operations.

The proposed algorithm has yielded 15 flowsheets for the problem with a computational time of 5 minutes on a PC of modest size (900MHz; Pentium II Celeron). These flowsheets include well-known as well as unanticipated flowsheets; see, Fig. 5.

6. Conclusion

A highly robust and efficient algorithmic method has been developed for synthesizing a heterogeneous azeotropic distillation (AD) system. Its efficacy is demonstrated by resolving a well-known problem of industrial importance.

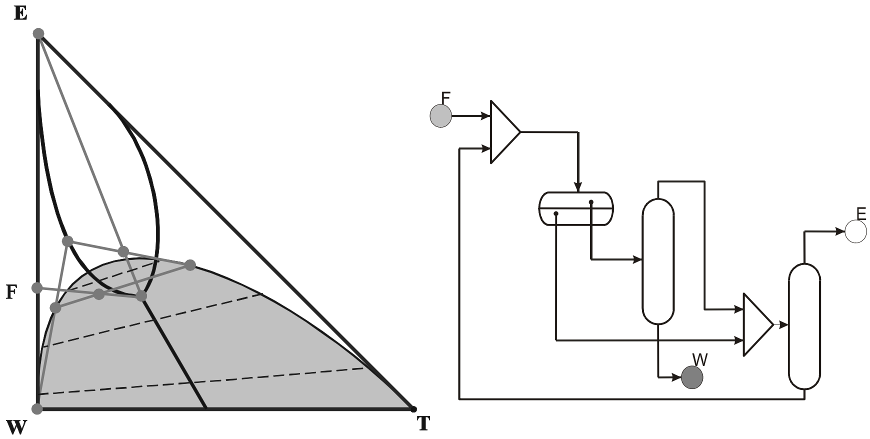

Figure 5. One of the unanticipated solutions for the EWT problem.

7. References

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