

OPTIMAL SEPARATION SEQUENCES BASED ON DISTILLATION: FROM CONVENTIONAL TO FULLY THERMALLY COUPLED SYSTEMS.

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Problem Statement.

Distillation is most widely separation technique used in chemical industry 95% of all separations and purifications are based on distillation and this situation will not change in the next years. Although the study of distillation sequences using conventional columns (one feed, two products, reboiler and condenser) is well established the systematic development of systems considering thermal couples it is still an interesting research activity.

Here we present a model that based on the Fenske-Underwood equations that allow the systematic generation of the best distillation sequence (in terms of total annualized cost) considering all the alternatives from conventional to fully thermally coupled systems going through all the intermediate alternatives. Formally the problem can be stated as follows:

«Given is a mixture of N components that do not form azeotropes, the objective is to generate a separation sequence to get the N pure components (inside some pre-specified tolerance), considering simultaneously all the alternatives from only conventional columns to fully thermally coupled systems and going through all the intermediate alternatives».

Note that the problem could be extended to an M component mixture in which we select N key components to be separated. The objective is then to obtain N streams, in such a way that only one component of the N previously selected is present in each of the final streams. However, we do not lose generality if we constrain to the original case and therefore this will be the criteria we will follow.

Data:

Mixture of five components:

A = benzene; B = Toluene; C = Ethyl-Benzene; D = Styrene E = α -methyl
Estyrene

Relative volatilities assumed constant A = 10.5; B = 4.04; C = 1.76; D = 1.31; E = 1

Feed = 200 kmol/h liquid at its bubble point.

Feed composition (molar fraction): A = 0.3; B = 0.2; C = 0.1; D = 0.2; E = 0.2

Other assumptions: The cost of condensers and reboilers is much lower than the costs of columns and the operating cost. Therefore, a fixed cost of 15000 \$ is added to each heat exchanger. The vapor density is calculated at feed conditions, variations in the density are compensated by the security factors in the calculation of column diameter.

Due to the non-convex nature of the TCD problem it is easy get trapped in local solutions. In order to minimize the effect of non-convexities we take into account the following facts (See also refs^{1,2})

1. For a fixed configuration the resulting NLP usually gets its global optimal solution.
2. Solver based on outer approximation (DICOPT) tend to easily get trapped in local solutions. The reason is that the Master problem is not a lower bound due to the slacks.
3. Solvers based on branch and bound usually get a 'very good' solution (most of the times the optimal global solution). However, the CPU time is too large.
4. The minimum energy consumption is obtained for the fully thermally coupled distillation sequence with the maximum number of column sections. Proved by Halvorsen and Skogestad³
5. The minimum energy consumption for a given sequence of separation tasks is obtained when there are no internal heat exchangers.

Therefore we follow the next heuristic procedure:

- a. First we search in the space of 'basic' configurations without no internal heat exchangers⁴.
- b. For the optimal configuration obtained in step (a) we optimize the heat exchangers (reboilers and condensers) structure.

Note that if the energy is the dominant cost (o at least it has an important contribution) previous heuristic usually get the global optimal solution. In any case, at least a good solution is guarantee. In these two sub-problems the solver SBB is selected.

References

1. Caballero, J. A.; Grossmann, I. E., Design of distillation sequences: from conventional to fully thermally coupled distillation systems. *Computers & Chemical Engineering* **2004**, *28*, (11), 2307-2329.
2. Caballero, J. A.; Grossmann, I. E., Structural considerations and modeling in the synthesis of heat-integrated-thermally coupled distillation sequences. *Industrial & Engineering Chemistry Research* **2006**, *45*, (25), 8454-8474.
3. Halvorsen, I. J.; Skogestad, S., Minimum energy consumption in multicomponent distillation. 3. More than three products and generalized Petlyuk arrangements. *Industrial & Engineering Chemistry Research* **2003**, *42*, (3), 616-629.
4. Giridhar, A.; Agrawal, R., Synthesis of distillation configurations: I. Characteristics of a good search space. *Computers & Chemical Engineering* In Press, Corrected Proof.