

## Design and Optimization of a Hybrid Distillation/Melt Crystallization Process using Genetic Algorithms

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The optimal design of hybrid separation systems is a highly non-linear and multivariable problem, and the objective function (total annual cost, TAC) used as optimization criterion is generally non-convex with several local optimums. Particularly, genetic algorithms optimization methods are very attractive for engineering applications, due to its reliability and simplicity in numerical implementation. In this work, we have studied the design of the hybrid distillation/melt crystallization process with conventional and thermally coupled distillation using as a design tool a multi objective genetic algorithm with restrictions. Results indicate that the energy consumption and TAC of the hybrid separation systems can be reduced significantly using coupled distillation systems. The feasibility of this approach is demonstrated by design of a hybrid distillation/melt crystallization process for separation of a ternary isomer mixture, using thermally coupled distillation sequences.

### 1. Introduction

Sometimes, a combination of various driving forces can ease separation better than a single one, with of course the cost of additional equipment. Feasibility and sequence of such a hybrid separation depends on which different driving forces are more effective and when. Choice of one driving force over another as a mode of separation also depends on the composition. Thus, hybrid alternatives are sought only if conventional methods are not effective in effecting the separation. In recent years, there has been a hybrid process boom in chemical engineering (Berry and Ng, 1997; Franke et al., 2008; Lima and Grossmann, 2009, among others). One example of a hybrid processes is the well-know crystallization operation with the ease of phase separation typical of distillation. They are applicable to solid-liquid-vapor three-phase equilibria. In such systems, the liquid, enriched in the impurities that have not passed into the crystals, vaporizes at a low pressure, near the triple-point pressure of the main component. Therefore, combining all these processes in one installation is expected to raise the separation efficiency without requiring any considerable extra expenses. The hybrid distillation/melt crystallization process combines advantages of the distillation and the melt crystallization in which very high separation factors per stage can be reached. Simultaneously, the combination of distillation and crystallization overcomes the

shortcomings of the individual unit operations, i.e. high energy-consumption at small separation factors and limitation of yield by eutectics, respectively. In the last years, stochastic methods have been successfully applied to process engineering optimization problems. In this context, stochastic optimization methods are playing an important role because they are generally robust numerical tools that present a reasonable computational effort in the optimization of multivariable functions; they are also applicable to unknown structure problems, requiring only calculations of the objective function, and can be used with all models without problem reformulation. To the best of our knowledge, multiobjective stochastic methods have not been reported for design and optimization of the hybrid process with rigorous models. In this work we study the design and optimization of the hybrid distillation/melt crystallization process, using thermally coupled distillation sequences, with genetic algorithms. The design is explained with an industrial process example. The task is to separate a mixture of ortho, meta, and para xylene isomers. The design and optimization was carried out using as a design tool, a multi-objective genetic algorithm with restrictions coupled with the process simulator Aspen Plus<sup>TM</sup>, for the evaluation of the objective function, ensuring that all results obtained are rigorous. A main advantage of this procedure is that instead of obtaining just one optimal design, a set of optimal designs, called Pareto front, is obtained. The results show that this hybrid configuration with thermally coupled arrangements is a feasible option in terms of energy savings (consequently, reduction in greenhouse gas emissions) and capital investment.

## 2. Optimization Methodology

The detailed design of a hybrid separation process is a challenging task because of many degrees of freedom involved. In order to optimize the hybrid distillation/melt crystallization process, using conventional and thermally coupled distillation sequences, we used the multiobjective genetic algorithm with constraints coupled to Aspen Plus<sup>TM</sup>, developed by Gutiérrez-Antonio and Briones-Ramírez (2009). In this context, stochastic optimization methods are playing an important role because they are generally robust numerical tools, which present a reasonable computational effort in the optimization of multivariable functions; they are also applicable to unknown structure problems, requiring only calculations of the objective function, and can be used with all models without problem reformulation. For the conventional and thermally coupled hybrid distillation/melt crystallization process, the multiobjective optimization problem includes, as objectives, the minimization of the total number of stages, the heat duty of the sequence. In the case of the thermally coupled configuration, it also considers the interconnection flows (value and location). In the conventional and thermally coupled hybrid distillation/melt crystallization process, there are four objectives to minimize: the number of stages in each column (i.e., two columns), the volume of the crystallizer, and the heat duty of the sequence. For both systems, the objectives are in competition, so they have to be optimized simultaneously. For the optimization hybrid system, we used 800 individuals and 40 generations as parameters of the multiobjective genetic algorithm with 0.80 and 0.05 for crossover and mutation fraction. These parameters were obtained through a tuning process, where several runs of the algorithm were

performed with different numbers of individuals and generations. The multiobjective genetic algorithm with constraints used allows obtaining the rigorous Pareto front of the conventional and thermally coupled hybrid process: a set of non-dominated, optimal, and rigorous designs that satisfied the purities required.

### 3. Case of Study

The target is to separate a mixture of ortho, meta, and para xylene isomers containing 1% of the low boiling meta component (M), 66% of the intermediate boiling para component (P), and 33% of the high boiling ortho component (O), in mole fraction. For each component, a purity of 99% (in mole fraction) is demanded. For the considered example, distillation alone is feasible, but economically not attractive because of the low separation factors. Note that the separation of the component P and O is especially difficult using conventional distillation, but the combination with melt crystallization offers the advantage of obtaining almost pure product. We analyze four basic configurations obtained according to the rules of synthesis for hybrid systems proposed by Berry and Ng (1997): i) hybrid distillation/melt crystallization processes using conventional distillation arrangement (Figure 1a); ii) hybrid distillation/melt crystallization processes using an indirect thermally coupled distillation sequence (Figure 1b); iii) hybrid distillation/melt crystallization processes using a modified arrangement from the indirect thermally coupled distillation sequence (Figure 1c); iv) hybrid distillation/melt crystallization processes using a Petlyuk column (Figure 1d).

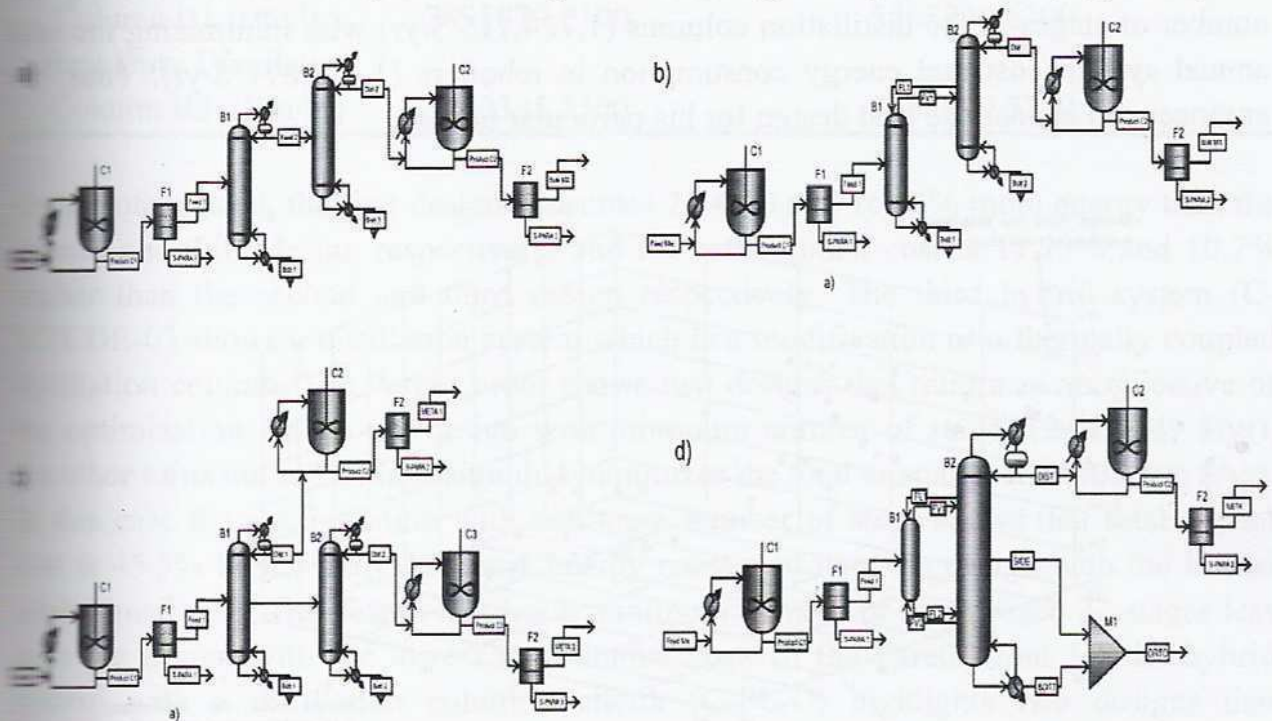


Figure 1: Hybrid distillation/melt crystallization processes, a) using a conventional distillation system; b) using an indirect thermally coupled distillation sequence; c) using a modified arrangement from the indirect thermally coupled distillation sequence; d) using a Petlyuk column.

For this class of systems, thermodynamic models such as NRTL can be used to calculate equilibrium vapor-liquid data and with temperatures and compositions of eutectic points are calculated parameters activity using the Wilson model and to calculate the liquid-solid equilibrium. The design pressure for each distillation arrangement was chosen to ensure the use of cooling water in the condensers. For the crystallizers, we assume that the separation of a pure isomer from the remaining mixture at eutectic composition can be accomplished in one crystallization stage.

#### 4. Analysis of Results

In this section, we analyze the resulting Pareto fronts of the four hybrid configurations analyzed. We calculate the Pareto front using, as design tool, the multiobjective aforementioned genetic algorithm. Figure 2 shows the Pareto front for case C-DSI-C, which includes the objectives to minimize: heat duty and the number of stages of the distillation sequence and total annual cost of the system (equipment costs and service costs). The first observation is that optimal designs satisfy the specified purities and recoveries in the distillation column and crystallizers (Table 1). A second observation is that the Pareto front shows two feasible designs: a design with minimum number of stages in the distillation columns and a design with minimum total annual cost, calculated using the method of Guthrie, and minimum reboiler duty in the distillation arrangement. The two possible designs contrast the objectives of minimizing the number of stages in the distillation columns (1,724,715 \$/yr) with minimizing the total annual system cost and energy consumption in reboilers (1,410,871 \$/yr). Thus, the engineer can choose the best design for his particular needs.

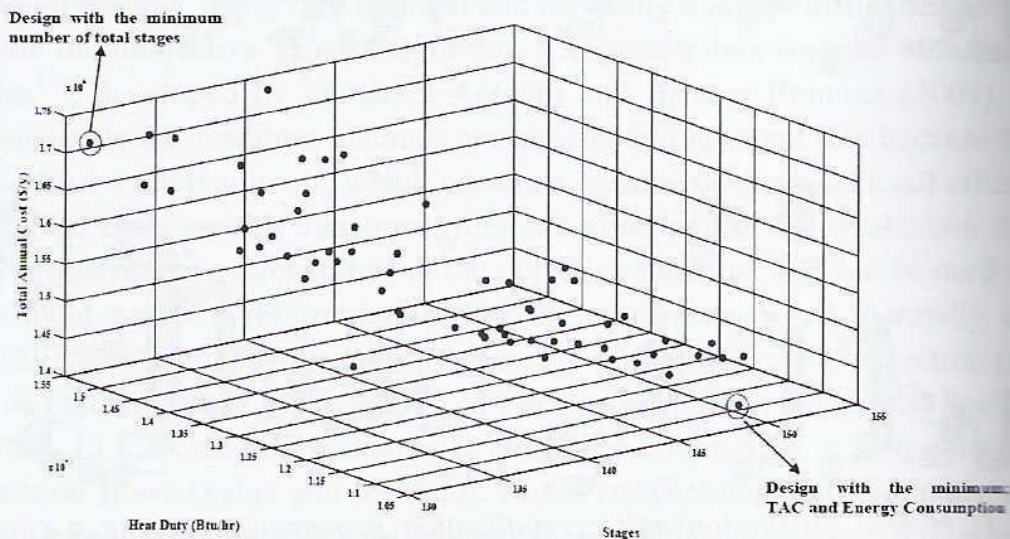


Figure 1: Pareto front of arrangement C-DSI-C.

For the case of system C-TCDS-C, the Pareto front highlights three designs that minimize a design objective. One is the design with fewer stages in the distillation columns, other design that minimizes the total annual cost of the system, and the last represents the design that minimizes energy consumption in reboilers of distillation

columns. The design with minimum number of stages presents a total annual cost of 1,341,946 \$/yr; the configuration with minimum energy consumption in reboilers shows a total annual cost of 1,212,290 \$/yr and the arrangement with minimum total annual cost presents a value of 1,206,375 \$/yr. It is also possible to observe that the design with minimum number of stages used 11 stages less than design with minimum total annual cost and 21 stages less than design with minimum energy consumption in the reboilers.

*Table 1: Optimal design of distillation columns for arrangement C-DSI-C.*

Distillation Sequences [DSI]	Design with the minimum number of Stages	Design with the minimum TAC
Number of Stages		
Column B1	43	58
Number of Stages		
Column B2	87	92
Reflux Ratio Column B1	22.0255	16.3892
Reflux Ratio Column B2	105.2136	78.8435
Feed Stage Column B1	16	15
Feed Stage Column B2	49	53
Heat Duty Distillation		
Column B1 (Btu/hr)	7895879.2100	5465899.5700
Heat Duty Distillation		
Column B2 (Btu/hr)	7260385.3300	5465899.5700

On the other hand, the first design consumes 23.40% and 16.03% more energy than the second and third design respectively, and the total annual cost is 11.23% and 10.7% higher than the second and third design respectively. The third hybrid system (C-MTCDE-C) shows a distillation system which is a modification of a thermally coupled distillation column. The Pareto Front shows two designs that minimize an objective of the optimization, one is the design with minimum number of stages (2,038,549 \$/yr), the other turns out to be the design that minimizes the total annual cost (1,405,896 \$/yr). In this case the configuration with minimum number of steps shows that total annual cost is 45.5% higher and 53% more energy consumed than the design with the lowest total annual cost. The design that has a minimum number of stages used 22 stages less than the design with the lowest total annual cost. In the Pareto front for the hybrid system with a distillation column Petlyuk (C-PC-C) highlights two designs that minimize an objective optimization, one of them is the design with minimum number of stages, and the other is the design that minimizes energy consumption in the reboiler of the column Petlyuk and the total annual cost of the system. All selected designs comply with the restrictions of the purities in the distillation column and the crystallizer. The first design has 6 stages less than the second design, but consumes 7.3% more energy and its total annual cost is 4% higher than the second. So the design selected for comparison is one that shows the lowest total annual cost and minimum energy

consumption. The total annual cost of the design that turns out to be the cheapest is 1,226,443 \$/yr. At this point emerges an important point to highlight. Best hybrid design with a thermally coupled distillation column (C-TCDS-C) has a total annual cost of 1,206,375 \$/yr and a total number of stages in the distillation column of 170 while the best hybrid design with a Petlyuk column (C-PC-C) shows a total annual cost of the system of 1,226,443 \$/yr with a total number of stages 132. The difference between the total annual cost of the system more affordable compared to the more expensive is 1.6%. This result implies that for practical purposes the energy consumption between the two systems is almost similar. However, the difference between the number of stages of the hybrid configuration with the lowest value compared with that that shows the highest number is 28.8%. Given these results, it is possible to conclude that the best design among the four case studies reviewed is the hybrid system that includes a Petlyuk distillation column.

## 5. Conclusions

We have presented a strategy using genetic algorithms for the optimization-based design of cost optimal hybrid separation processes. The methodology is illustrated by an industrial case study, where a ternary mixture of close-boiling ortho, meta and para isomers is separated into pure products by hybrid process of melt crystallization and distillation. The stochastic procedure allows manipulation of continuous and integer variables simultaneously. It was found that the optimum energy consumption design can be related to the minimum total annual operating cost. According to the results obtained in steady state is concluded that the best design option is the hybrid system that uses a Petlyuk column. The benefit our approach lies in the ability to deal with complex hybrid flowsheets and design of optimal process with paramount robustness and efficiency.

## Acknowledgements

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