26TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING

PART A

Edited by
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Economic, Environmental and Dynamic Optimization Applied to Hybrid Processes for the Purification of Biobutanol

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Abstract

Biobutanol is more energy dense and less hygroscopic than bioethanol, resulting in higher possible blending ratios with gasoline. Recently, new developments are focused on diminish the impact in two zones, the strains improvements and the downstream processes. Recent studies conclude that the inclusion of an extractive column can diminish the economic impact. In this study several hybrid designs are compared from a multi-objective optimization perspective where three objective function are evaluated simultaneously, the total annual cost as economic target, theeco-indicator 99 as environmental target and the condition number as controllability index using a stochastic hybrid algorithm, Differential Evolution with Tabu List. Our results indicate that the intensified configuration show the best dynamic behavior in addition with the smallest TAC values with a slightly penalty in the eco indicator values.

Keywords: biofuels, biobutanol, thermal coupling, controllability index.

1. Introduction

Because of depletion of fossil fuels, highly fluctuating market prices in crude oil, and several environmental issues, the biofuels have become a probably source of energy. Among several biofuels, biobutanol has shown great properties such as energy density (27.8 MJ/L), lower vapor pressure at environmental temperature (5.6 hPa) and higher flash point (35 º C). Furthermore, there is no need of any kind of engine modification in order to replace totally fossil fuels with biobutanol (Ranjan et al 2011). After Second World War, butanol productions was totally supplied by the petrochemical industry through the oxo process. Nowadays, the scientific researching have focused efforts on the improvement of complete fermentation process, modifying strains, obtaining cheaper fermentations substrates and improving the purification and recovery techniques. In the field of purification of the broth from the ABE fermentation process, recent studies conclude that the inclusion of an extractive column can diminish the economic impact (Sanchez-Ramirez et al 2015). New sequences can be obtained by the combination of liquid-liquid extraction and distillation columns also introducing thermal couplings and recombining different column sections (Errico et al 2015). In this study several hybrid designs are compared from a multi-objective optimization perspective. Three objective functions are evaluated simultaneously using a stochastic hybrid algorithm, the total annual cost, the eco-indicator 99 and the condition number as economic target, environmental index and controllability index, respectively.

2. Dynamic properties from the point of view of the design

A common approach to the chemical process design and their dynamic properties is to solve in a separated and sequential way (Morari et al 1985). Firstly, the design is performed. Subsequently, the dynamic properties are analyzed. However, trying to analyze this “design-control” methodology, it is evident the existence of a lack the entire design process since both targets are not considered at the begging of design process. Moreover, evaluating the dynamic properties in a separate way do not guarantee that a good and robust design in steady-state would show a good dynamic behavior. Also, it is probably that working out of the optimal operating conditions, the controllability of conventional and complex columns may improve (Serra et al 1999). So, it is quite convenient to use an appropriate strategy which could involve several objectives such as economic, environmental and control targets. This strategy could lead to a suitable operation of the process by improving the profitability, diminishing the environmental impact and enhancing the dynamic properties in order to adapt in an adequate way the changes in the product specifications, and the variations in the raw materials (Skogestad et al 1996).

3. Case Study

Recent studies applied to purification and recovery of the components from the ABE broth have been published by Errico et al. (2015). They claim that the designs showed in Figure 1 have better economic and environmental indexes. The design in Figure 1a) represents the case taken as reference. The other designs represent a thermally coupled design, thermodynamic equivalent design and intensified column in Figure1b), 1c) and 1d), respectively. However, since no control index is involved in the optimization process, the designs obtained do not guarantee a good dynamic behavior. In this case study, all sequences shown in Figure 1 were subject to a rigorous optimization, all those designs were initially simulated using Aspen Plus. The NRTL-HOC model was used for the calculation of the physical property available for the components used at the specified conditions. It was assumed that all process designs have the same stream feeds, it was added hexyl acetate as extractant. The feed composition reported by Wu et al. (2007) was used. The required purities are 99.5 wt% for biobutanol, 98 wt% for acetone, 94 wt% for ethanol and 99.99 wt% for the solvent recovered.

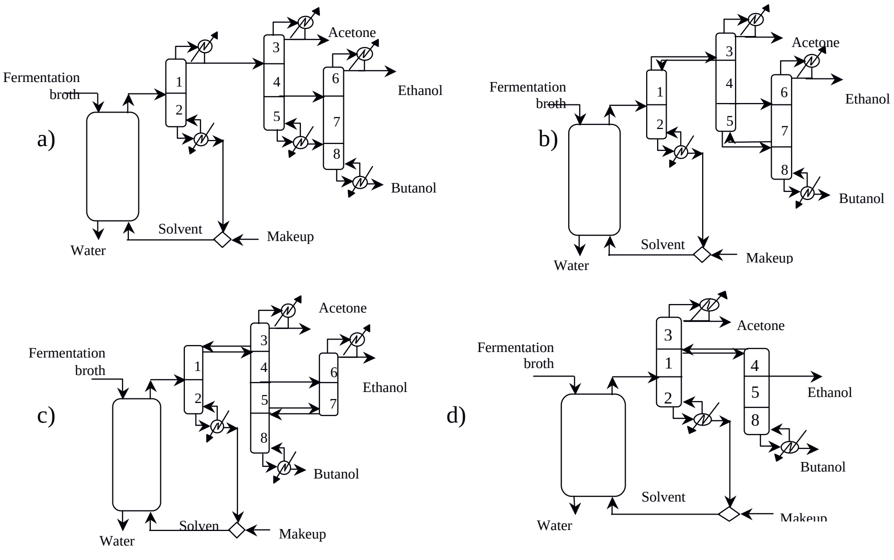

Figure 1 Sequences considered as study cases.

4. Optimization Problem

In this rigorous optimization study, it has been considered three objectives: the total annual cost, the eco-indicator 99 and the condition number. The TAC calculation as economic objective function was performed according to Turton et al. (2009), where TAC is expressed as follows:

$$TAC = \frac{Capital\ costs}{Payback\ period} + Operative\ costs \qquad (1)$$

Also, the calculation of the eco indicator 99 as environmental objective function (Geodkoop and Spriensma, 2001) was stated as follows:

$$Eco\ indicator\ 99 = \sum b \sum d \sum k\ \delta_d \omega_d \beta_b \alpha_{(b,k)} \qquad (2)$$

Where β_b is the total amount of chemical b released per unit of reference flow due to direct emissions, α(b,k) is the damage caused in category k per unit of chemical b released to the environment, ω_d is a weighting factor for damage in category d, and δ_d is the normalization factor for damage of category d.

The calculation of the condition number has been carried out through the singular value decomposition of the relative gain matrix of the design in the nominal point. In this manner, in order to evaluate the dynamic properties of each design, the condition number will be set as a dynamic behavior index since this value has been quite used as a qualitative assessment of the dynamic behavior in a process. The singular value decomposition of the relative gain matrix of a linear system is represented as follows:

$$K = W \sum V^T \qquad (3)$$

Where W and V are unitary matrices and Σ is a matrix whose diagonal elements are the singular values σ. Assuming that *K* is not singular, then the condition number of *K*, γ is a positive number which relates the minimum singular value σ_* and the maximum singular value σ^*, being none of those two zero, the condition number γ, can be estimated as follows:

$$\gamma = \frac{\sigma^*}{\sigma_*} \qquad (4)$$

High values of σ_* and small values of σ^* are desirable in order to claim that the process may assimilate disturbances without system destabilization (Morari et al 1985). The relative gain matrix was obtained by an open loop control strategy for each design. In other words, each design evaluated through the hybrid stochastic algorithm was disturbed in the design variables of each column, note that the selected variable to be manipulated on each column of each design were the closer variables of each product stream, i.e the reflux ratio in Figure 1a) was selected as manipulated variable since is the closer variable to the acetone stream. The magnitude of the step changes in the manipulated variable was defined as a 0.5 % negative change on the values of the manipulated variables in the nominal state, we consider this disturbance small enough to assumed that the response of the system can be approached as a linear response. Once having all the responses for the step changes in the manipulated variables, the relative gain matrix was obtained and the SVD calculation was performed, this calculation provided the condition number value. So, the objective functions were defined as follows:

$$Min\ (TAC, Eco\ 99, Condition\ Number\ \gamma) = f\left(\mathrm{N}_{tn}, \mathrm{N}_{fn}, \mathrm{R}_{rn}, \mathrm{F}_{rn}, \mathrm{F}_{vn}, \mathrm{D}_{cn}\right) \quad (5)$$

$$Subject\ to\ y_m > x_m$$

where N_{tn} is the total column stages, N_{fn} is the feed stages of all streams in column, R_{rn} is the reflux ratio, F_{rn} is the distillate fluxes, F_{vn} is the vapor/liquid flow in interconnections at coupled sequences, $\boldsymbol{F_{ln}}$ is the liquid flow in interconnections at coupled sequences and D_{cn} is the column diameter, y_m and x_m are vectors of obtained and required purities for the m components, respectively.

5. Global stochastic optimization strategy

DETL method was selected as a hybrid multi-objective algorithm. Several results showed that DETL is reliable for solving multi-objective and non-convex problems due to the hybrid nature of the algorithm since the Tabu list is included (Srinivas et al 2010). The methodology of the optimization was made by a hybrid platform using Microsoft Excel and Aspen Plus. The vector of decision variables is sent to Microsoft Excel, where the optimization method is written. In Microsoft Excel, those values are attributed to the process variables that Aspen Plus needs. After the simulation is completed, Aspen Plus returns to Microsoft Excel the resulting vector. Once the design is evaluated in Aspen Plus, the disturbances are set and Matlab performs the SVD calculation, returning the condition number to Excel, and finally, Microsoft Excel analyzes the values of the objective functions and proposes new values of the decision variables according to the stochastic optimization method. The following parameters for the DETL method have been used: 300 individuals, 300 generations, a tabu list of 50% of total individuals, a tabu radius of $2.5*10^{-6}$, 0.80 and 0.6 for crossover and mutation fractions.

6. Results

Figure 2 shows the Pareto front obtained for each case study. In each Pareto front, the three objective function were evaluated and minimized at the same time. Moreover, a tendency is observed, the better condition number values coincide with the highest TAC values, also it happens the same behavior when the Eco 99 and the condition number are evaluated. Considering the TAC values, the tendency is evident, Figure 1a) shows the highest values, which is totally normal, since it is not included any thermally coupling in this design which could diminish the energy consumption and consistent with some authors who claim energy savings and consequently economic improvements when a thermal coupling is included in the configuration (Triantafyllou et al 1992). Furthermore, Figure 1d) shows the smallest TAC values, which again is normal since we are considering an intensified design that includes only two distillation columns. Talking about the environmental impact, Figure 1d) showed a little higher values in comparison with the thermally coupled distillation sequence and the thermodynamic equivalent design, this behavior is normal since the energy required in the reboiler of the intensified design is a little higher, and the environmental impact measured through the eco indicator 99 pays a big emphasis in the use of fossil fuels. In consideration of the condition number, it is clear than Figure 1d) exhibits the better values (smaller values or closer to one) for condition number. This behavior let us note that the inclusion of a thermally coupling in an intensified configuration might improve the indexes evaluated here, such as economic, environmental and controllability indexes. In this scenario, and under this test, we assume than this design presents the best dynamic behavior. This dynamic behavior represents a promissory scenario since this design showed both the best TAC and condition number values.

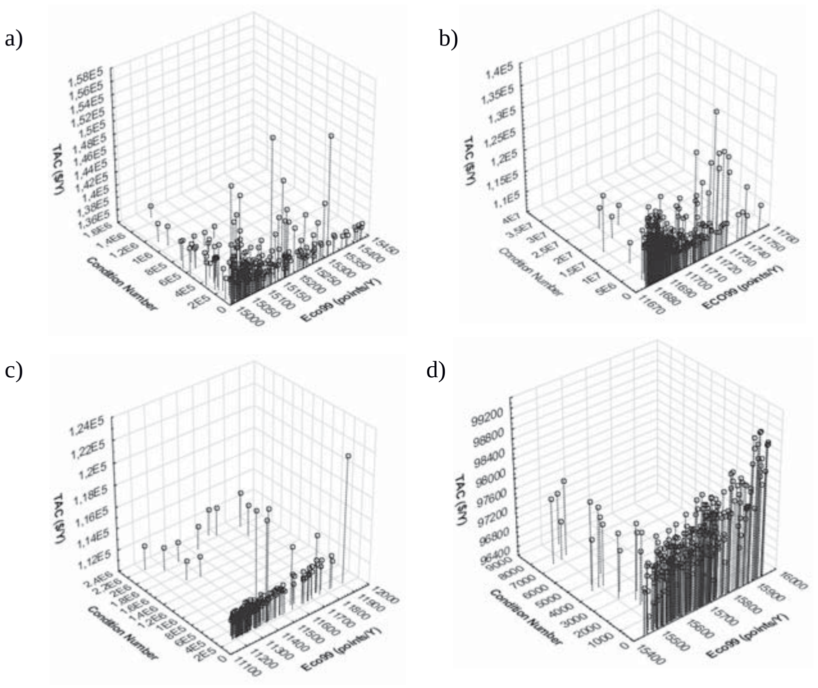

Figure 2 Pareto front of the study cases

In Table 1, it is included the main data of a point of the intensified design which showed the best dynamic index, and consequently the best dynamic behavior.

Table 1 design parameters and comparison indexes for the configuration of Fig. 1(d)

	Liquid-Liquid Extraction Column	C1	C2
Number of theoretical stages	6	57	19
Reflux ratio	---	26.8269	---
Feed stage	1	45	---
Solvent feed stage	6	---	---
Side stream stage	---	---	9
Column diameter (m)	0.335	0.3215	0.3239
Distillate flowrate (kmol h^{-1})	---	0.1333	---
Themal coupling flowrate (kmol h^{-1})	---	2.4291756	---
Side stream flowrate (kmol h^{-1})	---	---	0.0071271
Solvent flowrate (kmol h^{-1})	4.906656	---	---
Reboiler duty (kW)	---	65.238	24.495
TAC (\$ Y^{-1})	96913		
Eco indicator 99 (Points Y^{-1})	15521		
Condition Number	47.7140		

7. Conclusions

A set of four designs for the biobutanol separation has been evaluated through a rigorous optimization methodology with a hybrid stochastic algorithm (DETL). It was included as objective function the TAC, eco indicator 99 and the condition number as economic target, environmental target and control index respectively, all of them minimized at the same time. The inclusion of thermally couplings reduced significantly the TAC and the environmental impact. Our results indicated that Figure 1d), where a thermal coupling and the intensified process is involved, showed the best dynamic behavior. This represents a huge difference comparing with the reference case, which was the second design as concerns to dynamic behavior. In a general way, the inclusion of a control index in the rigorous optimization lead us toward a wider scenarios, where it is possible to guarantee the minimization of the TAC and at the same time, a flexible operability could be reached. This reduction in economic, environmental and control issues, combined with other research efforts, could lead to be more profitable the use of biobutanol as an alternative energy source.

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