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# Flexibility Assessment of a Distillation Train: Nominal vs Perturbated Conditions Optimal Design

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## Abstract

Multicomponent mixtures can be separated into their single components by mean of different distillation train configurations. The standard design procedure consists of the assessment of the optimal columns configuration according to the economic and operational aspects. Anyway this optimal design is strictly related to the operating conditions, i.e. perturbations, when present, can seriously turn the tables. In these cases a flexibility analysis could be of critical importance to assess the operating conditions range of better performance for a system configuration with respect to another one. This is the typical case of biorefineries (and bio-processes in general) where the composition perturbations downstream the fermenter across the year's seasons are completely normal due to the floating nature of the feedstock. Since no similar studies have been found in literature, a brand new ABE/W (acetone, n-butanol, ethanol, water) mixture separation case study has been set up; this mixture derives from an upstream microbial conversion process and the successful recovery of at least biobutanol and acetone is crucial for the profitability of the operation.

Therefore the purpose of this paper is the comparison between the possible distillation train configurations from a flexibility point of view. We are interested in particular in highlighting the differences, if present, between the economic optimal solution and flexibility optimal configuration that sometimes could not be the same, causing this way a very profitable design to be much less performant under perturbated conditions.

The flexibility assessment has been performed with an established procedure introduced in previous papers; all the flexibility indexes proposed in literature have been used both of simple and most complex usage in order to refine the analysis and a flexibility economic assessment has been carried out as well. Finally the two different configurations as well as the two different procedures (operating conditions based vs perturbated conditions based) have been compared both from a design and an economic point of view; then analogies and differences as well as their consequences from a decision making point of view have been highlighted and discussed.

**Keywords:** flexibility analysis, design optimization, distillation, column trains

## 1. Introduction

In refinery operations distillation has always been the leading separation process. In designing a distillation column, given the inlet streams (T, P, partial flowrates), column

top pressure, type of condenser (total or partial) and two design (separation) specifications, one degree of freedom stays unfilled. Either reflux ratio  $R$  (or ratio  $R/R_{\min}$ ) or number of stages  $N$  should be fixed in order to univocally determine the unit design, anyway no physical constraints can help us to make a choice.

The standard decision making process to select the number of stages is indeed an economic-based optimization. Capital and operating costs for given specifications are calculated at different number of stages  $N$  (i.e. reflux ratios); due to the increasing CAPEX and the decreasing OPEX trends with respect to  $N$ , the total cost function shows a minimum for the  $R$  and  $N$  values corresponding to the most profitable column design. However it is worth selecting less profitable solutions whether the optimum point is located close to  $R_{\min}$  or  $N_{\min}$  conditions.

When multicomponent mixtures have to be treated, distillation trains need to be designed. Several distillation train configurations are possible according to the amount of components present in the feed and how many of them are worth to be recovered. For instance the simplest configurations for a multicomponent mixture with two components recovery required are shown in Figure 1. They're namely defined as:

- A) indirect configuration (sequential recovery from the heaviest to the lightest component);
- B) direct configuration (sequential recovery from the lightest to the heaviest component);
- C) midsplit configuration (a preliminary split between heaviest and lightest components is performed, then the separation is refined to achieve specification).

Each single column (and related equipment) is then designed on the basis of the lowest total cost and the cheapest train configuration is selected.

This procedure is well established and it has always worked well so far, anyway it has a main limitation: the economic assessment and equipment design are strictly related to the nominal operating conditions, i.e. they don't take into account feedstock or operating conditions perturbations that could occur. This means that, whether a feed composition perturbation occurs, the system could not be able to achieve the separation specifications or at least a relevant increase of operating costs can be detected causing the most profitable design not to be as profitable as expected.

In refinery's operation these problem are less appreciable since long-term contracts for crude oil supplying and blending processes ensure an almost constant and stable feedstock quality. However, during last 15 years there has been an increasing interest for the production of chemicals and fuels from renewable resources because of growing concerns about global warming and climatic change, increasing crude oil price and existing legislations restricting the use of non-renewable energy sources. The direct consequence of this trend results in an even more increasing demand for bio-based fuels and raw materials, i.e. bio-refinery processes. Anyway bio-processes are highly subjected to composition perturbations downstream the fermenter across the year's seasons due to the floating nature of the feedstock.

Being fermentation usually carried out as a batch process, in order to ensure the desired daily productivity, several fermenters working at the same time are required. On the other hand, even when continuous fermenters are used, their scale up and then the feed flowrate that can be processed have a limit. These conditions cause the fermentation process section to be very expensive, therefore a constantly good performance of the products recovery section is of critical importance for the profitability of the plant.

In the light of the above an a priori flexibility analysis of the different distillation train configurations is non-optional for this kind of separation in order to allow the decision maker to make a multi-criteria-based choice about the optimal design to be selected.

## 2. Objectives and methodology

The purpose of the paper is the economic and flexibility based comparison between different distillation train configurations aimed to the same separation specifications.

As already mentioned, the economic optimal design provided was determined by mean of the usual procedure; capital and operating costs have been estimated using Guthrie (1969) – Ulrich (1984) - Navarrete (2001) correlations.

Flexibility analysis has been performed both from a deterministic (Swaney & Grossmann, 1985; Saboo and Morari, 1985) and a stochastic (Pistikopoulos & Mazzuchi, 1990) point of view and coupled with economics according to the procedure shown by Di Pretoro et al. (2019).

ProSim Plus® process simulator has been used to assess the feasibility of the separation as well as to estimate all process parameters.

Since no former application of flexibility analysis to distillation trains has been found in literature, a new case study referring to the separation of an ABE/W mixture, coming from a fermentation process and a preliminary dewatering operation, has been proposed. The feed composition is listed in Table 1.

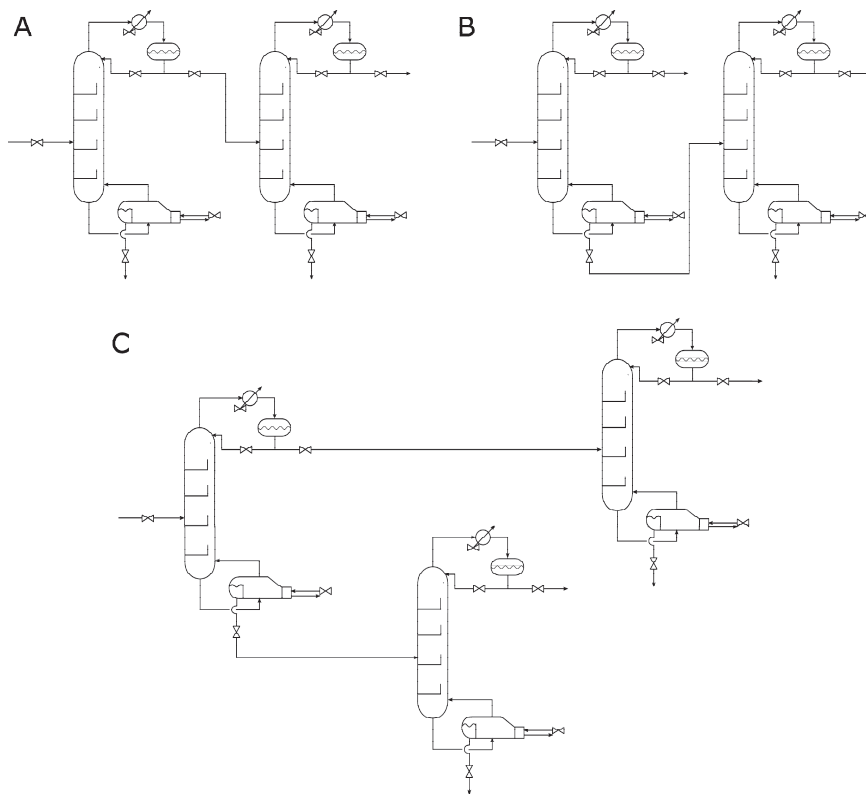


Figure 1 - Distillation train configurations for two components recovery

Table 1 - Feed components partial flowrates

Component	Partial flowrate (mol/s)
Acetone	12.030
Ethanol	3.839
<b>n-Butanol</b>	61.328
<b>Water</b>	12.428

The successful recovery of at least biobutanol and acetone is considered crucial for the profitability of the operation. In order to do this, a minimum of two distillation columns are required and three configurations are possible as previously shown in Figure 1. Midsplit configuration specifications are as follows:

1. Split column:
  - 1.1. Acetone recovery ratio in the distillate: 0.995;
  - 1.2. n-Butanol recovery ratio in the bottom: 0.98;
2. Acetone recovery column (top column):
  - 2.1. Acetone recovery ratio in the distillate: 0.995;
  - 2.2. Distillate acetone mass fraction: 0.995;
3. n-Butanol recovery column (bottom column):
  - 3.1. n-Butanol recovery ratio in the bottom: 0.98;
  - 3.2. Bottom n-butanol mass fraction: 0.99.

Specifications for direct and indirect configuration can be easily deduced from the midsplit ones. The direct configuration has resulted to be highly unfeasible since we should recover in the first column a highly acetone concentrated stream from a feed with a very low acetone molar fraction. Therefore only indirect and midsplit configurations will be compared.

### 3. Optimal design and flexibility assessment

As already mentioned, the standard design procedure has been conducted as usual; optimal number of stages and relative annual total cost for each column are listed in Table 2. With an overall annual cost of 933,509 \$/y vs 1,084,082 the indirect configuration results to be the most convenient with respect to the midsplit one.

The addition of a preliminary column indeed does not substantially affect the acetone column utilities consumption.

Table 2 - Distillation train optimal design

	1 <sup>st</sup> column		2 <sup>nd</sup> column		3 <sup>rd</sup> column	
	N (feed)	Cost (\$/y)	N (feed)	Cost (\$/y)	N (feed)	Cost (\$/y)
Indirect	16 (10)	580,016	50 (46)	353,493	/	/
Midsplit	35 (9)	455,493	50 (47)	352,224	16 (8)	276,365

First of all a flexibility analysis based only on the actual feasibility of the separation (i.e. without taking into account equipment sizing) has been performed. The most critical parameters, as well as the most likely to change, are water and butanol fractions; therefore water and butanol partial flowrates were then considered the uncertain parameters for the analysis.

Despite what usually happens in these situations and what we expected, the midsplit configuration, i.e. the one with one column more, doesn't result to be more flexible than the indirect one as shown in Figure 2. On the contrary it is slightly less performant. For a water vs. n-butanol ratio higher than 0.23 (0.22 for the midsplit) indeed the separation is not feasible at all.

According to the Swaney & Grossmann index ( $F_{SG}$ ), that assesses the highest simultaneous perturbation of all uncertain parameters that the system is able to withstand, the indirect configuration flexibility is about 5% (midsplit about 4%). According to Saboo & Morari the Resilience Index (RI), that defines the largest total disturbance load a system is able to withstand independently of the direction of the disturbance, stays around 8% (midsplit about 7%). Finally, according to the Pistikopoulos & Mazzuchi stochastic flexibility index, evaluating the probability that the system could absorb the disturbance, we find  $SF=77.86\%$  (75.85% for the midsplit) in case of a normal probability perturbation distribution with a 10% variance. These values don't take into account the equipment sizing but thermodynamics only; it means no matter how much we pay for a bigger reboiler or a larger column, no higher flexibility value can be achieved. The same feasibility region has been obtained by changing the columns number of stages between approximately 0.75 and 1.5 times  $N_{opt}$ . Flexibility analysis and economic assessment have then been coupled as shown in Di Pretoro et al. (2019). Total annual costs vs. partial flowrates perturbations have been plotted for the indirect configuration in Figure 3.a. An analogous trend has been obtained for the midsplit configuration.

However, the three columns configuration keeps being more expensive than the two column one, i.e. even under perturbed condition the external duties overconsumption is not compensated by the additional equipment despite what usually happens in standard distillation cases.

Costs result to be higher whether a bigger oversizing is necessary, i.e. positive deviation for both water and butanol flowrates, and along the operating conditions close to the feasibility boundary.

Moreover, the additional cost vs. flexibility plot for the deterministic indexes is reported in Figure 3.b as well; since  $F_{SG}$  represents the flexibility related to the simultaneous deviation of all uncertain variables, it implies a higher cost compared to the same RI value.

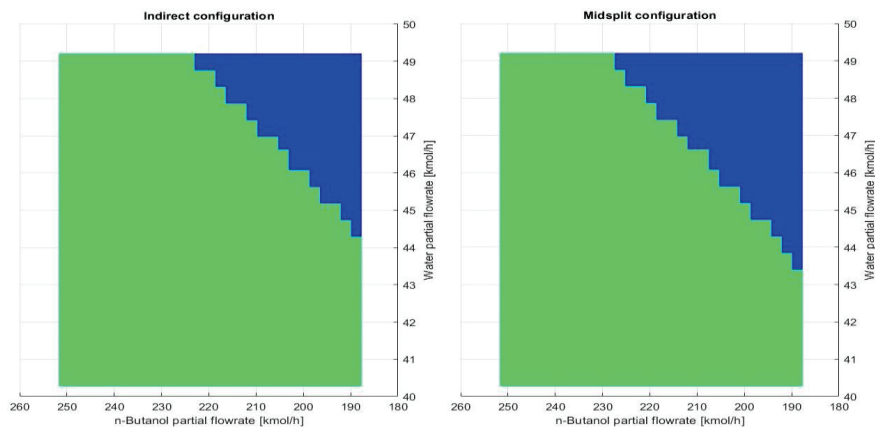


Figure 2 - Feasibility diagrams (Green = Feasible, Blue = Unfeasible)

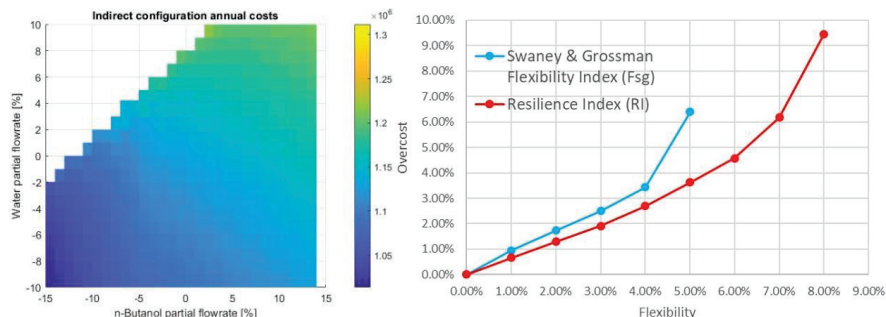


Figure 3 - Economic assessment (Indirect configuration): a. Costs vs. partial flowrates; b. Costs vs. flexibility

## 4. Conclusions

This paper introduces the comparison of distillation trains configurations both on a flexibility and economical basis. Flexibility assessment of distillation trains (involving both series and parallel columns) have been successfully performed with deterministic as well as stochastic indexes. Results have then been coupled with an economic assessment in order to obtain the overcost vs. flexibility analysis plot providing a critical tool to the decision maker.

The indirect configuration, that was the cheapest one, resulted to be also a little bit more flexible than the midsplit configuration, despite the expectation. The economic gap due to the additional column is conserved also under uncertain conditions as well as non-optimal column design. Moreover we can state that beyond a  $F_{SG}=4\%$  or  $RI=7\%$  it is less worth investing since the additional costs line becomes steeper.

However, beside the numerical results that are case-specific, the outcome of general validity is that, in thermodynamically constrained system, the feasibility and flexibility boundaries cannot go over a certain value by adding separation stages to the distillation column or, in general, investing more. An a priori flexibility analysis and economic assessment could then be crucial for making the best design choice and to know the limitation of our system if perturbations are likely to occur.

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