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Genetic Algorithm for Pressure-Swing Distillation Optimisation: Ethanol and Ethyl Acetate Mixture

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In the acetic acid esterification, ethanol (EtOH) in excess is used to produce ethyl acetate (EtAc), which is commonly used as an organic solvent in biochemical and food industries. On the other hand, EtOH is useful considering the growing production of bioethanol for the fuel market. The resulting mixture of EtAc with unreacted EtOH forms an azeotrope which is difficult to separate by conventional distillation. Literature data shows that the azeotropic binary mixture EtOH – EtAc is separated mostly through extractive distillation. Unfortunately, this procedure has some drawbacks, such as high energy cost and environmental concerns (quite related to the extracting agent recovery). However, taking advantage of the azeotrope sensitivity on pressure, the extracting agent use can be avoided. This paper presents an optimal design for the separation of the above-mentioned mixture, using pressure-swing distillation (PSD) as separation process. In order to achieve a fully optimised system in terms of energy and capital, the method followed consists in simulating the process with Aspen Plus® and making use of genetic algorithms (GAs) to optimise the process variables, including, among others, the pressure of the high-pressure column. This process variable is of great importance, and from our point of view, this factor has not been properly studied nor discussed in literature so far. The starting population consists of points that group a set of values for all the design variables. These sets are a mixture of random and calculated values, obtained by application of heuristics, so that the initial population contains some potentially good initial individuals. The optimisation code is written in Visual Basic language and the link between Aspen Plus® and Visual Basic is also programmed so that a continuous connection can assure information flow from the optimisation program to Aspen Plus® and vice-versa.

1. Introduction

Distillation is defined as the process of separating the components of a liquid mixture by its partial evaporation, in such a way that a second phase is obtained from the vapor whose composition is different from the liquid in equilibrium. The equilibrium in both phases is usually assumed, hence, the knowledge of the equilibrium relations is essential to model distillation systems (García and Barreiro, 1986). More important, the equilibrium relationships determine the feasibility of the distillation. Distillation includes conventional distillation for the separation of zeotropic systems and enhanced distillations to separate azeotropic systems. Enhanced distillation methods include pressure-swing distillation, heterogeneous azeotropic distillation, extractive distillation, catalytic distillation among others (Wang et al., 2018).

An azeotrope is a mixture that exhibits the same concentration in the vapor and the liquid phase. This prevents the separation of the pure compounds thorough conventional distillation. To use PSD to separate azeotropic mixtures the azeotropic composition must be sensitive enough to pressure (Xi et al., 2018). Pressure-insensitive binary azeotropes can be separated by distillation itself, but it usually requires the introduction of entrainers. The way in which these entrainers operate is diverse; some of them generate immiscible liquid phases that allow to break the azeotrope (heterogeneous azeotropic distillation) (Li et al., 2021). Others generate a new azeotrope that allows the breaking of the original one (homogeneous azeotropic distillation), and others, “extract” some component from the original mixture, which is separated afterwards from the entrainer (extractive distillation) (Yuan et al., 2015). All these methods require an extra component, the entrainer, that is

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continuously recycled in a system of two columns. These sequences can be thermally integrated (Knapp and Doherty, 1992) but operating with an entrainer is likely to involve an increase in operating cost compared to a separation system that would not require such entrainer.
Pressure-swing distillation prevents the problem of introducing a third component and has gained lots of attention from researchers in recent years, by comparison with the aforesaid methods (Zhu et al., 2016). According to a literature research developed by Risco et. al. (2019), column operating pressures are chosen rather arbitrarily: for a first assessment of a PSD, is usually considered that the azeotropic composition must vary at least 5 percent, over not more than ten atmospheres between the two pressures (Perry and Green, 1998). Luyben (2021) studied the importance of pressure selection since relative volatilities depends largely on the pressure.
The aim of the present study is to optimise the separation process of EtOH and EtAc system by means of the PSD. To do this, the TAC (Total Annualized Cost) function based on Luyben (2012) cost correlations is selected as the objective function to be minimized. The simulation is carried out with Aspen Plus ® and making use of GAs to optimise the process variables, including, among others, the pressure of the high-pressure column (HPC). Yang et al. (2017) optimised the PSD process for the ternary mixture of EtAc-EtOH-Water, not including as design variables any of the pressures. Wang et al. (2018) applied PSD to three case systems, being one of them EtOH-EtAc, most of the variables were optimised but pressures were fixed. Liang et al. (2021) compared extractive distillation and PSD to separate a mixture of water, pyridine and acetonitrile, for the PSD study, pressures were also predefined. The starting points for the GA are a mixture of random and calculated values, which are obtained by application of heuristics.

2. Genetic algorithms

Genetic algorithms (GAs) are an optimisation algorithm that imitates the Natural Selection. It is based on the concept that individuals best adapted to their environments are more likely to survive and reproduce.
GAs have been widely studied by mathematicians, programmers, and engineers due to its versatility and proper performance when solving nonlinear optimisation problems. GAs are executed iteratively on a set of coded solutions (chromosomes), called population, with three basic operators: selection, crossover, and mutation (Tao et al., 2020). To find out the optimum of a problem, GA starts from an initial population, which can be randomly generated, or, on the other hand, it can be a mixture of random and calculated values (as in the case). In each generation the objective function determines the suitability of each solution, and depending on these values, some of them are selected to be “parent” for the mutation and/or the crossover process. The procedure is then more likely to select the best solutions for the next generations, while eliminating the worst (Pal and Wang, 2017).

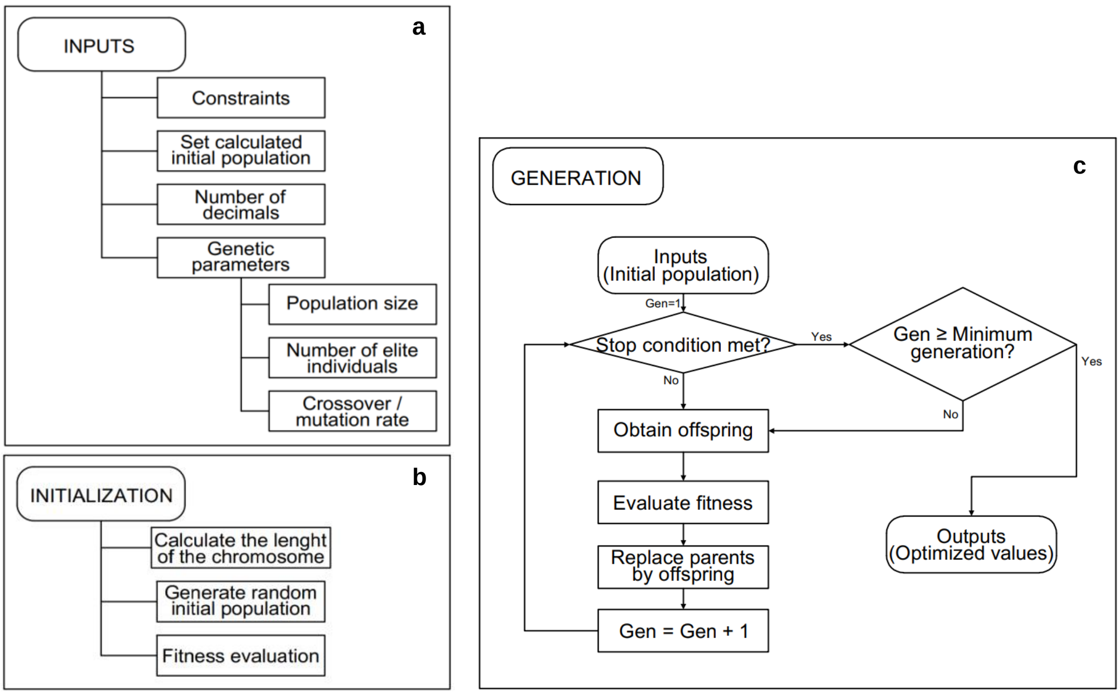

Figure 1: Structure of the GA

The framework of the GA used in this work is made up of three parts:

- Inputs (Figure 1a), where four basic parameters of the GA are defined, i.e., crossover rate, mutation rate, number of elite individuals (those which go through the next generation) and the population size. As well as other parameters such as the number of desired decimals (the more precision the longer the chromosome) and boundary conditions. These values are shown in Table 1.
- Initialization (Figure 1b), where first calculations are made, i.e., the length of the chromosome and the generation of random initial population. In this part, the fitness evaluation of the initial points is also done.
- Generation (Figure 1c), this is the iterative step, the offspring is obtained by mutation and crossover operations, these new points are evaluated, and the new generation is settled. For the stop condition, it is stated that the objective function must vary at least by 1 % between successive generations to keep iterating. If the generation is lower than the "minimum generation" value, although the stop condition is met, the program keeps running. This is done to ensure that there is a minimum number of evaluations, and it does not stop in the first steps.

Table 1: Parameters for the GA

Parameter	Value
Crossover rate	0.80
Mutation rate	0.15
Number of elite individuals	1
Population size	20
Number of decimals (only applicable in continuous variables)	2

3. Materials and methods

The design specifications defined for the problem have been arbitrarily chosen, with the only condition that the feed contains a high concentration of EtAc (resembling a possible case in an EtAc production plant). Table 2 summarizes this data.

Table 2: Design specifications

	Feed	Product 1 (bottoms column 1)	Product 2 (bottoms column 2)
Temperature (K)	293	-	-
Molar flow rate (kmol/h)	100	90	-
Molar fraction EtOH (X_{EtOH})	0.100	<0.010	>0.990
Molar fraction EtAc (X_{EtAc})	0.900	>0.990	<0.010

In addition, it has been assumed that the low-pressure column (LPC) operates at atmospheric pressure, as working at vacuum pressure leads to complications in the design, as well as an increase in the weight and cost of the column.

On the other hand, eight design variables have been chosen to be optimised (Table 3), the remainder being dependent variables, which are calculated trough the simulation software (e.g., the diameter of the columns) or by means of calculations integrated in the optimisation program (e.g., recirculation molar flow rate).

Table 3: Design variables

Name	Type	Name	Type
Number of stages in column 1	Discrete	Stage of feed in column 2	Discrete
Number of stages in column 2	Discrete	Pressure of column 1	Continuous
Stage of fresh feed in column 1	Discrete	Reflux ratio in column 1	Continuous
Stage of feed recirculating from column 2 in column 1	Discrete	Reflux ratio in column 2	Continuous

With regard to GA, 10 out of 20 initial points have been obtained manually by means of heuristic optimisations in the simulation software, fixing the pressures and calculating the rest of variables, considering that the optimum reflux ratio is 1.3 times the minimum. This is done to provide the algorithm some initial points where the optimum is likely to be, in order to improve its convergence.

The simulations were performed using Aspen Plus ® V11 using rigorous models (RadFrac). In the base case scenario, shown in Figure 2, the fresh feed enters the HPC, obtaining 99 % mol EtAc in bottoms, and a mixture on its azeotropic point at the pressure of the HPC in heads. On the second column, 99 % mol EtOH is obtained in bottoms, and a mixture on its azeotropic point at ambient pressure is obtained in heads, which will be pressurized and recirculated to the HPC.

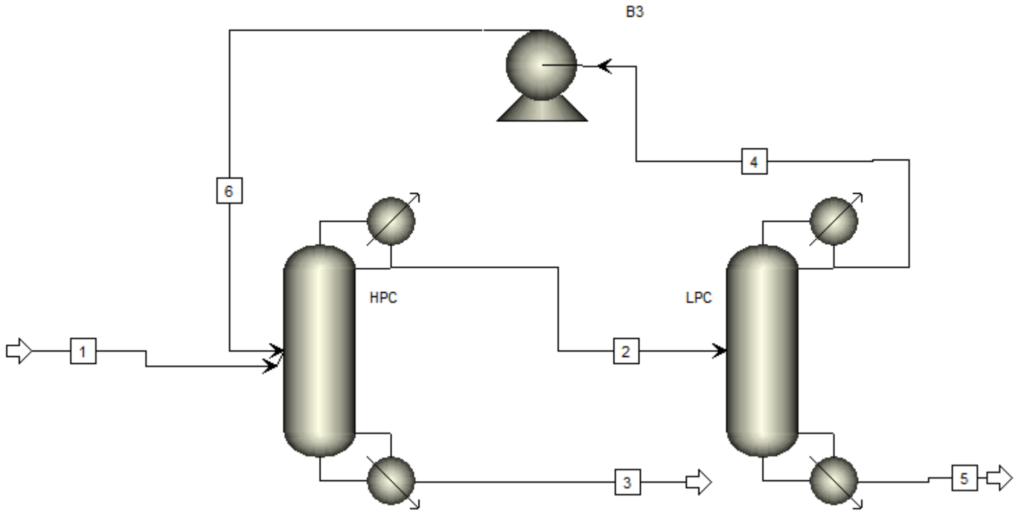

Figure 2: Flowsheet for the PSD process

Concerning thermodynamics, it has been reported that Aspen provides experimental data for the mixture of the study at high pressures, for this reason the UNIQUAC - Redlich Kwong model is selected.

4. Results

4.1 Initial pre-set population

Table 4 presents the values of the design variables for the 10 starting calculated points and their TAC. These points have been obtained (as said in the previous paragraph) applying heuristic rules and will be used along with 10 randomly obtained points as initial data for the GA, giving a total of 20 points initial population.

Table 4: Calculated starting points for the GA

	1	2	3	4	5	6	7	8	9	10
Number of stages in column 1	38	26	24	23	23	23	24	24	24	24
Number of stages in column 2	25	26	26	26	26	25	25	25	25	25
Stage of fresh feed in column 1	31	17	15	14	14	14	14	14	14	14
Stage of feed recirculating from column 2 in column 1	21	7	6	5	5	5	5	5	5	5
Stage of feed in column 2	16	17	17	17	17	16	16	16	16	16
Pressure of column 1 (bar)	4	6	8	9	10	12	14	16	18	20
Reflux ratio in column 1	3.07	2.38	2.31	2.28	2.31	2.33	2.27	2.35	2.45	2.58
Reflux ratio in column 2	1.91	1.87	1.89	1.90	1.91	1.99	1.90	1.91	1.93	1.94
TAC (k$/y)	860.2	717.4	689.6	681.3	716.9	711.2	692.3	691.9	694.2	699.1

4.2 Results

By using the parameters and specifications listed in Table 1 and Table 2 respectively, a series of generations is carried out. Figure 3 plots the TAC of the best (elite) individual for each generation. After 15 generations no noticeable improvement is obtained. The design variables corresponding to the optimum are shown in Table 5. Noteworthy is that this optimum lies in the maximum pressure that has been achieved during the optimisation procedure, which is 20 bar.

The results were as follows: for the HPC, stage number is 16, reflux ratio is 2.32 and feeding stages are 5 and 14; for the LPC, stage number is 25, reflux ratio is 2.19 and feeding stage is 18. The optimum is found at 20 bar on the high-pressure column, in contrast with most of the studies, which is usually established at 10 atm.

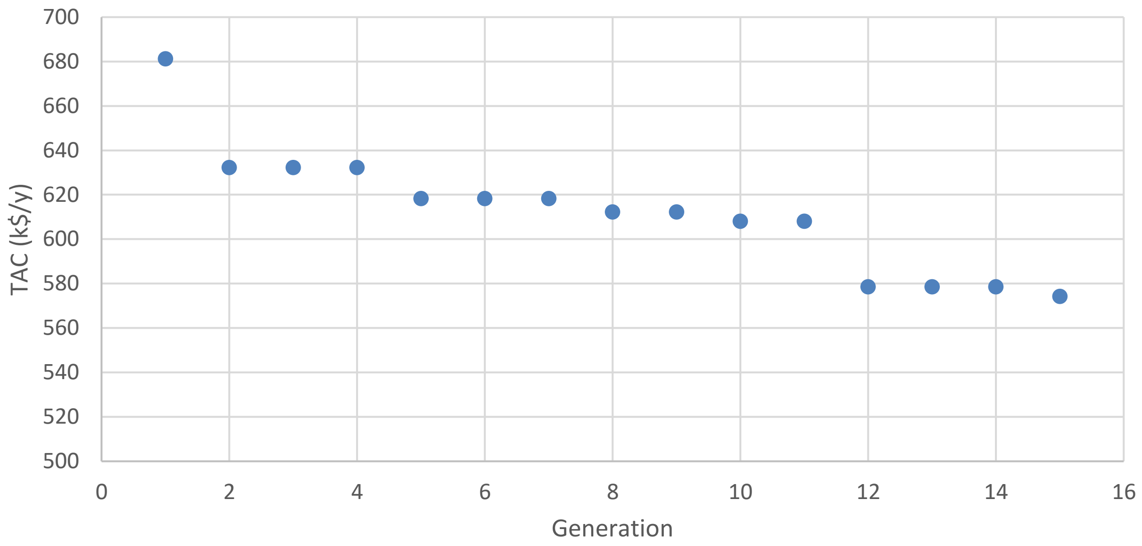

Figure 3: Evolution of the objective function in each generation

Table 5: Values of design variables for the optimum point

Generation	15
Number of stages in column 1	16
Number of stages in column 2	25
Stage of fresh feed in column 1	14
Stage of feed recirculating from column 2 in column 1	5
Stage of feed in column 2	18
Pressure of column 1 (bar)	20
Reflux ratio in column 1	2.32
Reflux ratio in column 2	2.19
TAC (k$/y)	574.2

The simulation results of the major streams are shown in Table 6. Fresh feed (stream 1) is defined as in Table 2 and enters the first column (HPC) at its boiling point, obtaining a distillate (stream 2) corresponding to the azeotropic composition at 20 bars, and a residue (stream 3) whereby EtAc is collected. Distillate stream is fed to the second column (LPC), where EtOH is collected in bottoms (stream 5) and a mixture on its azeotropic composition at 1 bar in top of the column (stream 4), which is pressurized and recirculated to the first column (stream 6).

Table 6: Simulation results of the pressure-swing distillation for EtOH – EtAc

Item / Stream		1	2	3	4	5	6
Temperature (ºC)		200.4	183.7	206.9	71.4	77.6	74.2
Pressure (bar)		20	20	20	1	1	20
Molar flow rate (kmol/h)		100	29.9	90.8	20.8	9.2	20.8
Molar fractions							
	EtOH	0.10	0.62	0.01	0.45	0.99	0.45
	EtAc	0.90	0.38	0.99	0.55	0.01	0.55

5. Conclusions

Genetic algorithms appear to be a powerful tool to optimise complex distillation processes. Linking Visual Basic and Aspen Plus ® provides a way to separately carry out the optimisation procedure and the simulation process, improving the task of finding the optimal solution. Giving some initial good estimations to the initial population increases the convergence pace, for this reason an initial set of simulations based on well stablished heuristics is recommended. In reference to the specific studied case, it has been seen that the best solution lies on the one that implies a maximum pressure in the HPC column, which is 20 bar. The HPC has 16 stages and a reflux ratio of 2.32. The LPC has 25 stages and a reflux ratio of 2.19. Final TAC value for 100 kmol/h of crude feed is 574.2 k€/year.

Nomenclature

EtAc – Ethyl acetate
EtOH – Ethanol
GA – Genetic algorithm
HPC – High-pressure column
LPC – Low-pressure column
PSD – Pressure-Swing distillation
TAC – Total annualized cost

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