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Trichloroethylene Stripping Column Optimal Design by Genetic Algorithm and Multicriteria Decision-Making Strategies

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Abstract: The optimization of stripping processes requires the simulation of correlations for a preliminary analysis of the system behavior while avoiding complex, costly, and time-consuming manipulations on a reduced scale. This study gives a suitable strategy while selecting stripping column packings. The strategic use of the genetic algorithm NGSAIIb allowed for solving the optimization problems based on environmental and technical-economic criteria of the Trichloroethylene (TCE) stripping column. For that, a numerical procedure was developed on MATLAB software. Then MATLAB software was linked by the mean of the COM protocol to the Multigen library that is an add-in for Microsoft Excel. In the developed strategy the decision-making method, TOPSIS is considered to compare four random packings (Flexiring), (Rashig ring), structured packings (Mellapak Y250), and (Sulzer BX). After the implementation of the strategy on all the packings, the Sulzer BX structured packing was selected as the best one. This section was based on two decision criteria that are, the TCE removal rate of 99.99% and the ratio of the liquid flow to the gas flow of 44.38%. The study shows that the Sulzer BX packing is the least expensive and promotes increased mass transfer and low total column pressure drop. The analysis of the evolution of the mass transfer coefficient according to the liquid flow rate showed that an efficient stripping column must have a ratio of the liquid flow to the gas flow rate strictly lower than 50%.

Keywords: Genetic Algorithms (GA), Steam Stripping, Wastewater Treatment, Multicriteria Decision Making

1. Introduction

The problem of treating industrial liquid effluents has been a subject of research for decades. Many mechanical and chemical methods are constantly being improved. The most common mechanical methods are the separation of particles by filtration, the use of cyclones, centrifugation, or decantation [1]. However, the application of applying aeration processes has economic advantages for treating compounds (VOC) [2, 3]. Diffusion processes are based on the mass transfer of molecules from a chemical component to another fluid different from the fluid to which it belongs. These processes are adsorption, desorption, distillation, liquid-liquid extraction, and many others. Most of these techniques are carried out in tray or packing columns with energy input represented by steam, air, or chemical gases [4]. The packed stripping process is the most widely used process for VOC removal from wastewater. The determination of stripping column design parameters involving the prediction of mass transfer coefficients remains a challenge for manufacturers due to a large number of existing correlations. This makes the optimization of the stripping process complex. Several authors have published on the optimization of stripping columns.

Ghoreyshi et al [5] proposed an optimal design and operating conditions for a stripping column using a mathematical model based on film strength at the interface between the phases and Henry's constancy [7]. Nirmalakhandan optimized the stripping column by considering the investment and operating costs with the Onda correlation [6]. Dzombak developed a computer program called air stripper design and cost (ASDC) to optimize the total cost and design of the stripper column by applying the Onda correlation and the Prahl linearization method [7]. Simulation using MATLAB was found to be effective for the stripping process correlations in the literature [8].

The stripper column optimizations presented in the literature are single-objective optimizations. Solving multi-objective problems allows for determining real solutions that simultaneously address several issues. There are many methods for solving multi-objective problems including metaheuristic methods representing stochastic algorithms that progress toward a global optimum by simulating objective functions. Genetic algorithms, simulated annealing, and ant colony algorithms are among them. The different variants of genetic algorithms are (Vector Evaluation Genetic Algorithm) VEGA, (Multi-Objective Genetic Algorithm) MOGA, (Non-Dominant Sorting Genetic Algorithm) NSGA IIb and many others based on the concept of sorting individuals according to their dominance or non-dominance [9]. Parhi et al [10] optimized the use of the reboiler and the reflux rate profiles of the distillation steam recompression in terms of energy and cost savings using NSGA II and TOPSIS. Barakat et al [11] and Leipold et al [12] applied multi-criteria optimization as genetic algorithms on different distillation processes to improve the yield while minimizing the production and investment costs. Several other authors have used multi-criteria optimization on industrial processes [13].

The main objective of the present study is to select the best performing by optimizing the operating conditions of four packings i.e., two random packings and two metal structured packings. Castillo [14] correlation has been used for simulation in MATLAB. The communication protocol allowed for multi-criteria simulations and optimizations such as NSGA IIb Genetic Algorithms.

2. Materials and Methodology

2.1. Multicriteria Optimization

Multi-objective or multi-criteria optimization is a branch of mathematics that deals with problems having several objective functions that are usually contradictory. It determines the extreme solutions of functions defined in a specific space by minimizing or maximizing them. The application of this resolution method favors the consideration of several criteria simultaneously. Thus, the improvement of the operational performance can be associated with the environmental and economic aspects while respecting the safety conditions of the operational functioning. The multi-objective optimization problem (MOOP) is defined as follows [9]:

Min f(x) – function minimum

$x \in D \subset \Re^n$ - Domain defined by constraints

$$D = \begin{Bmatrix} x \in \Re^n, g_i(x) \le 0, i \in I = (1,2 \dots m) \\ and\ h_j(x) = 0, j \in J = (1,2 \dots p), \\ with\ p < n, x_{imin} \le x_i \le x_{imax} \end{Bmatrix} \quad (1)$$

The subset D above groups the set of constraints such as the inequalities g(x), equalities h(x) and constraints at variables x_i bounds.

Multi-criteria optimization leads to a multitude of results whose optimal solutions will be the non-dominated solutions. The notion of non-dominance refers to the Pareto sense. Indeed, the Pareto front represents the result of the non-dominance sorting defined by:

A, and B satisfy the constraints and A dominates B [15]:

In minimization problems, this is expressed as:

$$\forall\, i \in \{1, n\}: f_i(x) \le f_i(y)\ and$$

$$\exists\, i_0 \in \{1, n\}: f_{i_0}(x) < f_{i_0}(y) \quad (2)$$

There are different multi-objective optimization solving methods, among which we can mention the Pareto and non-Pareto methods. The non-Pareto method modifies the problem in mono-objective problems; they are for example the aggregated and lexicographic methods. While metaheuristic methods are applied to black box problems.

This study opted for genetic algorithms (GAs) because of the simplicity of application. Inspired by Darwin's concept of natural selection developed in 1859, genetic algorithms were introduced as an adaptive model by John Holland [16].

GAs simulates the evolution of a population also called Darwinian evolution. The theory suggests that all living species are in perpetual evolution and undergo morphological and genetic changes. This simulation translates into the stages of selection, crossover, and mutation. The initial random solutions are used to obtain improved solutions. This method has been used by several authors [15] for the economic-environmental optimization of utility production systems of the toluene hydrodealkylation process [10, 12]. Several types of GA have been developed, one of the most influential is the Non-Sorted Genetic Algorithm (NSGA IIb) which has the advantage of considering elitism based on the ranking procedure and diversity related to inter-individual distance.

2.2. Numerical Procedure

Mathematical models that describe VOC stripping in packed columns are necessary tools for finding efficient solutions in a short time. Simulation of the models on a process scale ensures the feasibility of the models and validates the experimental data [8]. The simulation of models favors the rapid change of variables or even techniques [17]. The numerical procedure used in this study has been applied in the work of Ouattara et al. [15]. It connected NSGA IIb of Multigen library and MATLAB through a COM protocol. The simulation of the model was carried out in MATLAB through the calculation of the equations by Newton-Raphson's "fsolve" method. The results of the simulation were then communicated to Multigen in VBA language (Visual Basic Application) thanks to the creation of a link between MATLAB and Multigen library that is an add-in in

MICROSOFT EXCEL [18]. GA parameters were the following: an initial population of 200 individuals, 1000 generations, a crossover rate of 0.75, and a mutation rate of 0.02.

2.3. Multi-Criteria Decision-Making Strategies

Multi-criteria decision-making strategies allow the identification of the ideal solution among all the optimal solutions of the Pareto front. These methods are Electre, PROMETHEE II, FUCA, TOPSIS, and many others. The present study chose the TOPSIS (Technique for Order Preference by Similarity to Ideal Solution) method because it allows a simplified application and has a small number of adjustment parameters. It ranks a discrete set of alternatives from multi-criteria decision-making problems by selecting the fitted solution that is closest to the positive ideal solution and farthest from the negative ideal solution [19].

2.4. Stripping Model

Castillo's [14] work presented a model capable of predicting hydraulic parameters and mass transfer for the design of a packed column used for steam removal of volatile organic compounds (VOC) from wastewater. Castillo's [14] model is composed of 22 variables and 22 non-linear equations. This model has the particularity to be applied to random and structured packings [14]. An extension of the Stichlmair model, developed by Engel et al [20] was used by Castillo et al. [14] for the prediction of hydraulic parameters. Also, equations related to mass transfer have been developed on the basis of the model of Gualito et al. [21] while differing significantly from it with the use of the relative effective speed (ULe +UGe) and Reynolds number (Re). These equations were used for the calculation of the local mass transfer coefficient of the liquid phase. A detailed formulation of the correlation is available in Castillo's work [14]. The average Absolute Error (AAE) between the experimental and calculated volumetric mass transfer coefficient was 29% according to Mehta [22].

In the stripping process, solvents rich in pollutants specifically VOCs are heated in the stripper to release VOCs including Trichloroethene (TCE) (Figure 1). In this process, the stripping steam is essentially water vapor. The stripping steam comes into countercurrent contact with the charge-rich feed stream, which absorbs energy from the stripping steam for chemical desorption, while the outgoing steam is condensed at the top of the column in an overhead condenser. The design of the stripper must consider hydrodynamic calculations to determine the column diameter and mass transfer calculations for the effective column height. During operation, mass, heat, and momentum transport occur simultaneously; therefore, both phenomena must be considered together for modeling.

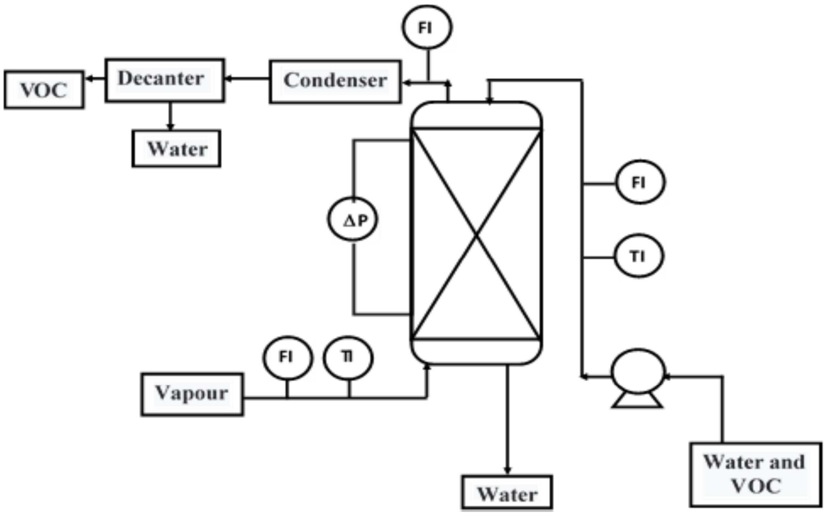


Figure 1. Simplified diagram of a Steam stripper column.

2.5. Multi-Criteria Optimization of Stripping Columns

Castillo's [14] correlation was used to compare the technical-economic and environmental optimization of four packings, i.e., two random and two structured packings. To reduce the TCE concentration at the outlet of the stripping process, the objective functions used are defined as follows:

1) Max K_{La}
2) Min ΔPtot
3) Min Cost (Fixed Investment Cost)

Submitted to

1) Ratio liquid/ steam
2) Total pressure drops in the column

In this study, the liquid-to-gas ratio limit is fixed between 20% and 50%. This limit corresponded to the ratio recommended for the stripping process in the literature [2].

In Table 1, K_{La} describes the mass transfer rate across the vapor-liquid interface. This very important parameter is based on the strength of each liquid and vapor phase film [23]. To increase the mass transfer of solute particles from the liquid phase to the gas phase, K_{La} has to be maximized. The literature evaluates the volumetric mass transfer coefficient of the liquid phase to compare the performance of different types of packing [24]. The objective of minimizing the pressure drop (ΔPtot) was necessary for the safety of the operations. Indeed, pressure control allows the good functioning of the stripping process.

In any industry, investment costs are always minimized. The fixed capital investment cost is calculated as a function of the column diameter and height using the correlations developed by Guthrie and reported in J. Douglas [25] (see Table 2). An update of this cost was carried out thanks to the Marshall & Swift Equipment Cost Index (M&S) available in the journal «Chemical Engineering, January 2022» [26].

Table 1. *Technical and environmental objective functions.*

Technical and environmental objective functions			
Names	**Equations**	**Units**	**Numbers**
Volumetric coefficient of mass transfer (K_{La})	$\frac{1}{K_{La}} = \frac{1}{a_e}\left[\frac{1}{k_L} + \frac{1}{mk_G}\right]$	l/s	(3)
Total pressure loss in the wetted column ($\Delta Ptot$)	$\frac{\Delta P_{tot}}{\Delta \text{Pdry}} = \frac{a_L+a_p}{a_p}\left(\frac{\varepsilon}{\varepsilon-h_{dyn}}\right)^{4,65}$	Pa.s	(4)

Table 2. *Investment cost formulas for the stripping column.*

Economic objective function			
Names	**Equations**	**Units**	**Numbers**
Fixed capital investment	$FCI = \sum_i(Purchase\ cost_i + Installed\ cost_i)$	$	(5)
Purchase cost	$Puchase\ cost = 9{,}201 * \left(\frac{M\&S}{280}\right) * \left(101{,}9D_c^{1{,}066}H^{0{,}802}F_c\right)$	$	(6)
Installed cost	$Installed\ cost = 9{,}202 * \left(\frac{M\&S}{280}\right) * D_c^{1{,}066}H^{0{,}802} * (2{,}18 + F_c) + 0{,}0283168 * \left(\frac{M\&S}{280}\right) * F_c' * \left(\frac{\pi D_c^2 Z}{4}\right)$ with $F_c = F_p * F_m$	$	(7)

The experimental design technic was used to determine the decision variables of this study. These decision variables are the liquid mass flow rate (L) and the steam mass flow rate (G). These optimization variables correspond to the variables used by Narbaitz et al. [27]. In their studies Narbaitz et al [27] demonstrated the influence of the liquid and gas flow rate on the K_{La} coefficient. The liquid and gas mass flow rates also refer to the liquid/vapor ratio. This ratio represents a classical variable in the literature [5- 6, 8, 28].

The limits of the mass flow rates were determined using the limits of the gas surface velocity published in the literature [29].

$$G = U_G * \rho_G * A_c \tag{8}$$

Table 3. *Optimization variables information.*

Column	**Lower bound**	**Upper bound**
Structured packing liquid mass flow rate (kg/h)	2000	15000
Random packing liquid mass flow rate (kg/h)	2000	13000
Structured packing gas mass flow rate (kg/h)	20000	600000
Random packing gas mass flow rate (kg/h)	100000	500000

Regarding the random packings in Table 3, the ranges of the liquid and vapor mass flow rate limits were reduced. Indeed, according to the database presented by Larachi et al. [30] the feed rates of structured packings vary over larger ranges than those of random packings. The lower bound of the liquid mass flow rate was determined by plotting the variation of the liquid flow rate versus the volumetric mass transfer and random packing pressure drop.

Optimization of the structured and random packings indicated an analysis time of one generation varying between 2 s to 5 s on the Multigen interface. The column flooding limits fixed at 70% were considered in the calculations of the diameter of the column by LOBO's linaria correlations (see table 4) [31].

Increasing the liquid-to-vapor ratio affects the driving forces of solute transfer by increasing the concentration gradient between the liquid phase and the interface and then the gas phase.

Table 4. *Column dimension formulas.*

Names	**Equations**	**N°**
Abscissa X	$X = \frac{L}{G}\sqrt{\frac{\rho_G}{\rho_L}}$	(9)
Ordinate Yf	$Yf = e^{-(1{,}023\, ln\, X + 0{,}1065(ln\, X)2 + 3.89)}$	(10)
Specific gas flow rate at flooding (kg/m^2. s^2)	$G_e = 0{,}7 * \sqrt{\frac{Y_f g \rho_G \rho_L}{F_g(\mu_L/\mu_{eau})}}$ with $F_c = F_p * F_m$	(11)
Column section (m^2)	$A_c = \frac{G}{G_e}$	(12)
Column Diameter (m)	$D_c = \sqrt{\frac{4A_c}{\pi}}$	(13)

3. Results

3.1. Optimization Procedure

The numerical procedure was validated on the basis of the example reported by Lopez Toledo [14]. This validation consisted of comparing the simulated values with those of the original example. The relative percentage differences observed between these two studies showed overall low values. The average relative difference was 2.175%. Subsequently, the optimization of the four packings was realized. Pareto fronts obtained allowed the selection of the best optimal packing based on the TCE reduction rate and the liquid-to-gas flow ratio. The specific parameters for each packing are shown in Table 5 [32]:

The four packings selected for this study have been used previously in studies for the pollutants vapor stripping. Mehta et al [22] analyzed the applicability of Wagner and Castillo correlations to determine local mass transfer coefficients in metallic random packing type Rashig ring. Mackowiak et al [33] used nearly a hundred random plastic and metal packing including the Flexiring (Pall ring) metal type to verify a model capable of determining the gas velocity at flooding. Castillo et al [14] experimented and validated a correlation using two random packings and two metallic structured packings of the Mellapak Y250 and the Sulzer BX types.

Table 5. *Characteristics of packings.*

		Random packing		Structured packing	
		Flexiring	**Rashig Ring**	**Mellapak Y250**	**Sulzer BX**
Packing void fraction	ε	0.94	0.924	0,96	0.86
packing Specific surface	aP	215	317	250	450
Stichlmair constant	C1	0.05	40	5	15
Stichlmair constant	C2	1	1	3	2
Stichlmair constant	C3	3	6	0.45	0.35
Liquid particle diameter constant	CL	0.4	0.4	0.8	0.8
Effective specific surface constant	C	0.6298	0.6298	0.7312	0.7312

3.2. Tri-Objective Optimization of the Sulzer BX Packing

Pareto front of 200 optimal solutions obtained with NGSA IIb optimization is shown in figure 2. These 200 optimal solutions were implemented in the TOPSIS spreadsheet for decision-making strategy. This is due to the order to select the ideal compromised solution between Pareto set optimal solutions. The weight of each criterion is identical. The best scenario identified by TOPSIS was scenario 131 in figure 2.

For a better understanding, of the optimization of the Sulzer BX packing, the three-dimensional Pareto front shown in Figure 2 could be observed by 3 curves shown in figure 3 These representations are the projection in two dimensions of figure 2.

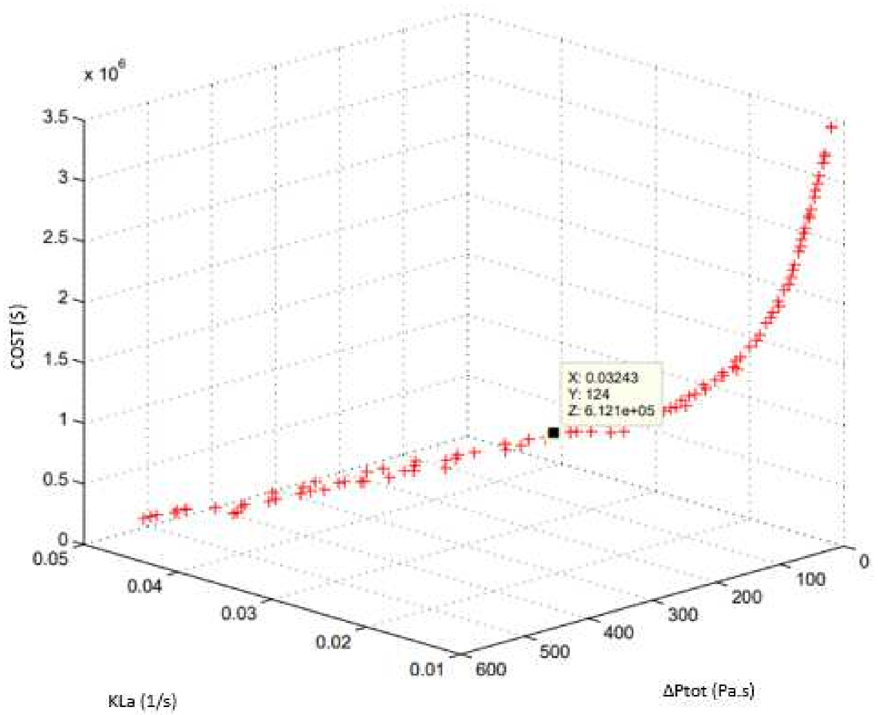
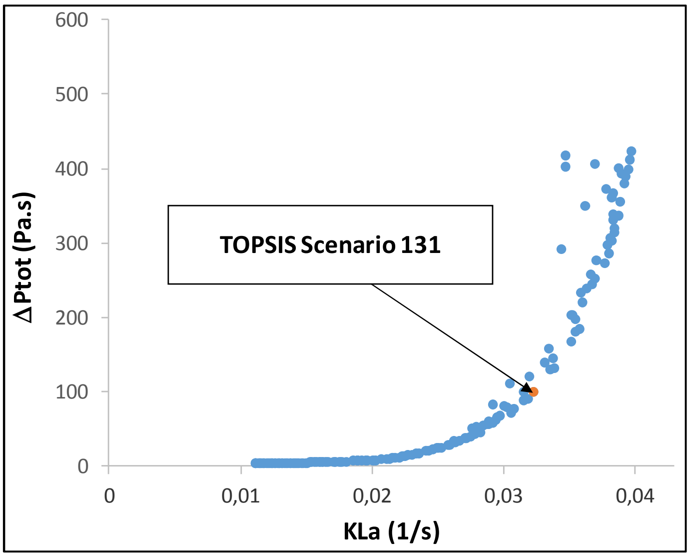


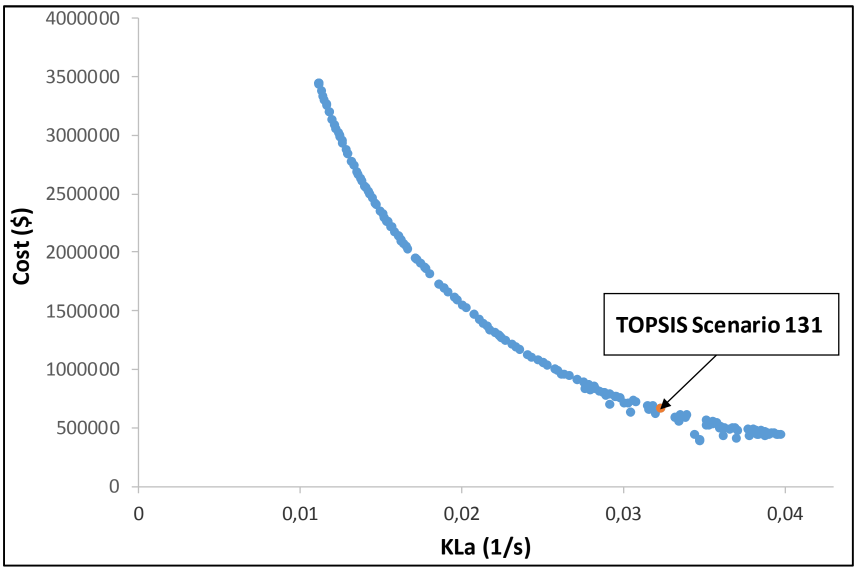
Figure 2. *Multi-criteria optimization of stripping columns with the Sulzer BX.*

Figure 3. a revealed that K_{La} changes from 0.01 to 0.04 (1/s) and ΔPtot from 0 to 450 (Pa.s). In Figures 3. b and 3. c, the cost regressed from 350000 ($) to 500000 ($). Overall, Figure 2 showed that as K_{La} and ΔPtot increased, fixed investment costs decreased. The volumetric mass transfer coefficient is an inverse function of the height of a transfer unit. The height of the column is proportional to the height of a transfer unit and is proportional to the fixed investment cost [33]. Thus, K_{La} is an inverse function of the fixed investment cost. A reduced height column costs less and promotes solute transfer from the liquid phase to the gas phase across the interfacial area. Small height packing column facilitates intimate mixing contact. The contact of the two phases was represented by the interfacial area which was formed by liquid retention [35]. The interfacial surface is dependent on the parameters of the packing, more specifically the specific surface and the operating parameters such as the gas and liquid flow rates. Billet and Schultes [36] represented in a graph the influence of the liquid flow rate on the interfacial surface whatever the correlation used. Thus, a high transfer rate reflects either a large interfacial area or low interface resistances. Indeed, in a stripping process, the most significant resistance is that of the liquid phase. A reduction of the liquid resistance requires an increase in the concentration gradient represented by the local mass transfer coefficient in the liquid phase. At the pressure drop level, the mass transfer evolves with the pressure drop because of the water/steam contacts created by the turbulences in the packing. Narbaitz et al [27] revealed that K_{La} was proportional to ΔPtot. They proposed to integrate the total pressure drop as a variable in the mass transfer correlations. That is due because of its relationship with the packing geometry. Liquid retention influences the pressure gradient above the loading point and thus promotes pressure drop in the column.

The same analysis as that of the Sulzer BX packing was performed on the other three packings. The diagrams were presented below in Figure 4 (a, b, c). The set of diagrams showed that the progression of investment costs was elicited by the decreasing evolution of the liquid phase volumetric mass transfer K_{La} and the total pressure drop ΔPtot.

The ideal solutions found by the TOPSIS method for all packings are in the Tables 6 and 7.





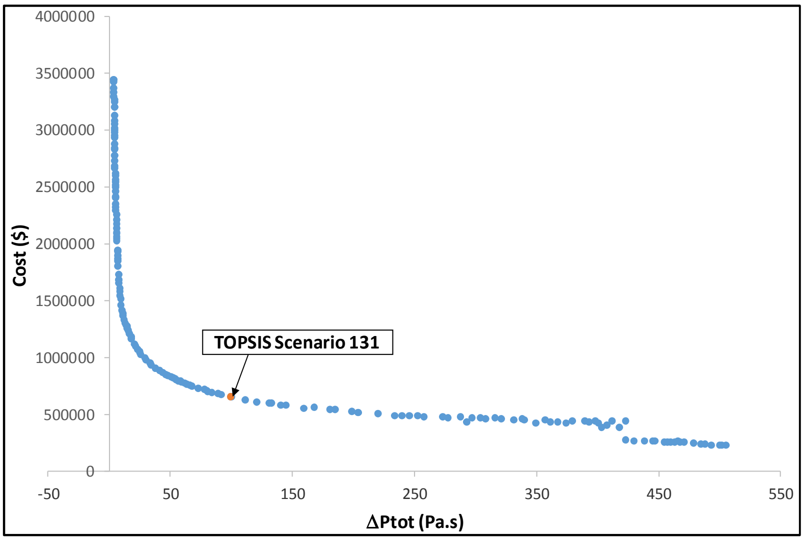
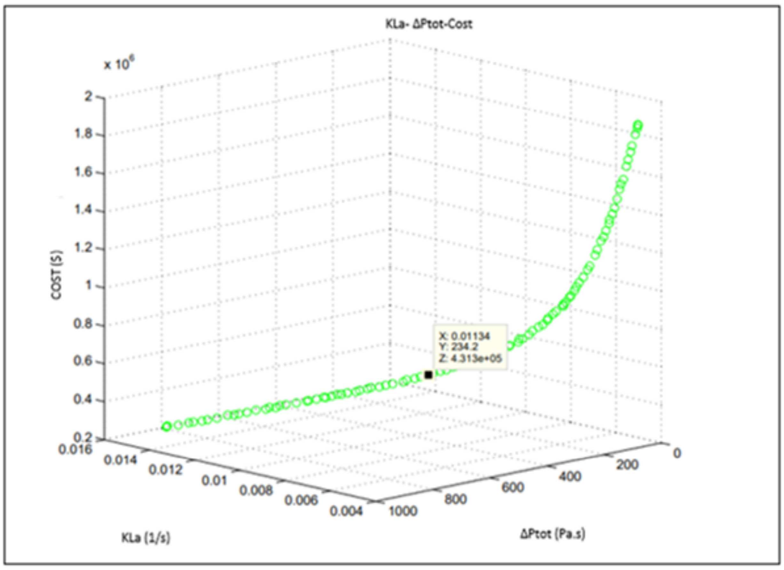
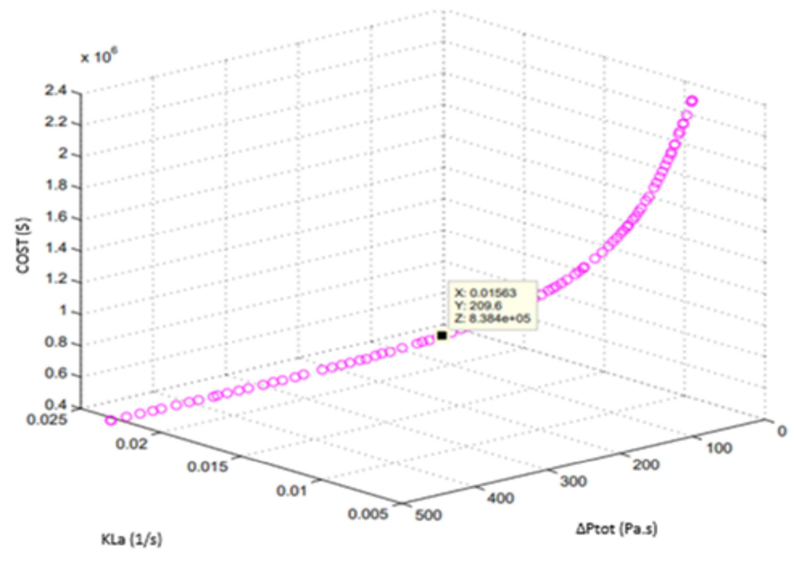


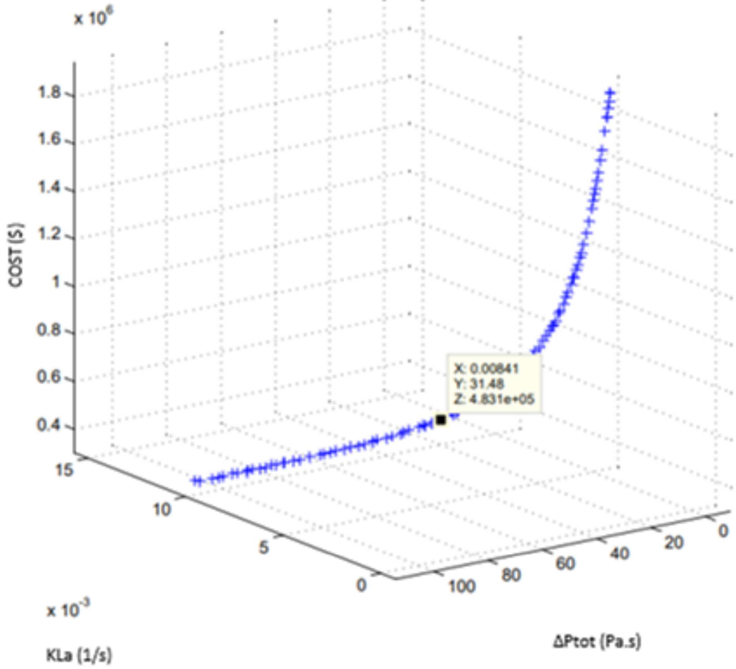
Figure 3. *Tri-criteria optimization of the Sulzer BX packing represented in 2 dimensions.*



(a)



(b)



(c)

Figure 4. *Tri-criteria optimization of stripping columns with the Pall Ring (a), the Rashig Ring (b) and the Mellapak (c) packing.*

Table 6. *Packing comparison by TCE removal rate.*

Packing Type	Material	(Xin-Xout)/Xin	TOPSIS Ideal solutions
Random	Flexiring	79%	43
	Rashig ring	98.25%	83
Structured	Mellapak Y250	77%	74
	Sulzer BX	99.99%	131

Table 7. *Packing comparison by TCE removal rate.*

Packing Type	Material	L/G	TOPSIS Ideal solutions
Random	Flexiring	49,95%	31
	Rashig ring	49,72%	68
Structured	Mellapak Y250	49,56%	12
	Sulzer BX	44,38%	131

Figure 5 displays the influence of the liquid flow (L) on the mass transfer (K_{La}) in the tri-criteria optimization.

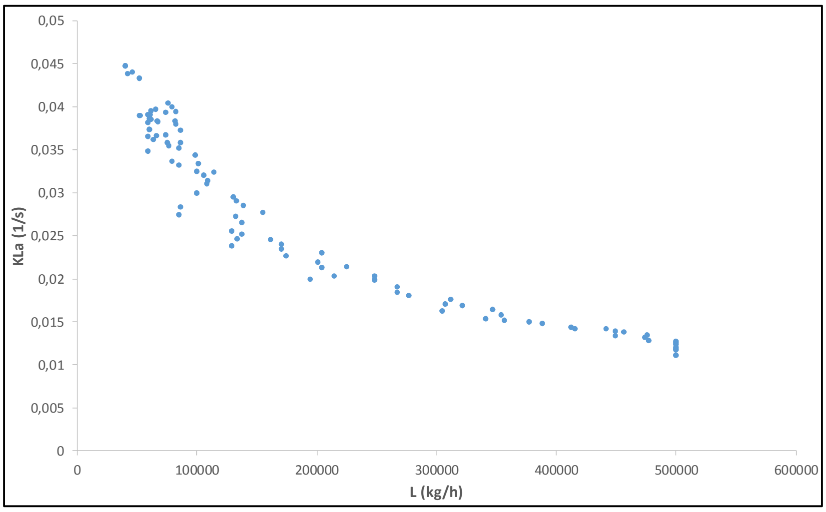


Figure 5. *Volumetric mass transfer coefficient vs liquid flow rate for the Sulzer BX packing.*

4. Discussions

To facilitate the selection of the best packing, the optimal scenarios of each packing were represented in Table 6. Since the objective of this study was to reduce the TCE rate in the wastewater, the criteria for selecting the best packing were the liquid purification rate. According to the table 6, the highest rate was obtained for the Sulzer BX structured packing with a 99.99% of TCE reduction. Sulzer BX structured packing was the best for pollutant reduction in wastewater because the levels of mass transfer criteria, total pressure drop, and fixed investment cost were they optimal. The best packings have specifically high critical surface tension, low packing factor, high nominal size, and high specific surface area according to Almonte et al. [34]. Packing with large diameters and large specific surface areas reduces pressure drop giving by Djebbar et al. [23] and the degree of misdistribution by Stichlmair et al. [37]. It should be noted that random packing is quite expensive as the height of the column has a great influence on the amount of packing. The low degree of inhomogeneity of random packing is a disadvantage because it is a cause of liquid misdistribution in the packing. This hurts the mass transfer in the whole column according to Fair [38].

According to Figure 5, the opposite evolution of mass transfer as a function of liquid flow rate revealed the limitations of excessive liquid increase. An increase in liquid flow rate produces an accumulation of liquid. That is favorable to the formation of a large interfacial area for efficient mass transfer. However, the optimization curves showed a reduction of the mass transfer following the increase of the liquid flow rate with the respect to the limits of the liquid/vapor ratio. Excessive feeding of the liquid reduces the contact time of the two phases and limits the mass transfer of the solute according to Stichlmair et al [37]. An efficient optimization requires a liquid-to-vapor ratio strictly below 50% to ensure sufficient contact between the dynamic liquid retention and the vapor.

The ideal scenario for the Sulzer BX packing found by TOPSIS had a liquid-to-vapor ratio of 44%. This ratio was the lowest scenarios compare to the other three packings.

5. Conclusion

The objective of the study was to compare four different packings using a numerical procedure that integrated Multicriteria optimization Genetic Algorithms (NSGA IIb), MATLAB software, associated with the TOPSIS decision-making method. The optimization criteria were the maximization of the volumetric mass transfer coefficient, the minimization of the total pressure drop in the column, and the minimization of the fixed investment costs. The results of the multi-objective optimization with the multi-criteria decision criteria identified the Sulzer BX structured packing as the packing that has the most favorable volumetric mass transfer coefficients, the lowest total pressure drop, and affordable fixed investment costs. However, the use of structured packings can be difficult due to certain constraints, that are the factors related to fouling, ease of cleaning, and replacement.

6. Recommendation

The investigation revealed that the Sulzer BX structured package was chosen as the best among the four packings studied in this work. However, the use of structured packing can be difficult due to certain constraints. These constraints are factors related to fouling, ease of cleaning, and replacement. Based on this, future research should investigate the study and implementation of a continuous stripping column cleaning system on the one hand, and a strategy for easy replacement of the packing after use on the other.

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