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# PROJETO DE COLUNA DE DESTILAÇÃO PARA PURIFICAÇÃO DE SUSPENSÃO DE NANOPARTICULAS

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***Abstract:*** *The aim of this work is to design batch distillation columns for the the purification of nanocapsules suspension. For that, an optimization procedure was used, considering that there is a fixed annual market demand ($N_B$) for the product. For several $N_B$ and given some specifications (like column pressure, feed load, and product specifications) the column that gives the higher profit is then calculated. For all cases studied the number of stages is not bigger than eight. Additionally, the minimum diameter and the areas of reboiler and condensers were calculated for the best columns. Differently from the work of Miladi and Mujtaba (2004), who proposed to use an exhaustive search algorithm to solve the optimization problem, in this work a very simple strategy was implemented. It showed to be efficient when reasonable initial guesses are provided.*

***Keywords***: *nanocapsules purification, batch distillation, design and optimization.*

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## 1 INTRODUCTION

Batch distillation is, perhaps the oldest operation used for separation of liquid mixtures. For centuries and also today, batch distillation is widely used for the production of fine chemicals and specialized products such as alcoholic beverages, essential oils, perfume, pharmaceutical and petroleum products (Mujtaba, 2004). It is the most frequent separation method in batch processes.

The essential features, as shown in Fig. 1.1, of a conventional batch distillation (CBD) column are:

- A bottom reboiler which is charged with the feed to be processed, that provides the heat transfer surface;
- A rectifying column (tray or packed column), coupled with a total condenser or a partial condenser system;
- A series of product accumulator tanks connected to the product streams to collect the main and/or the intermediate distillate fractions.

Operation of such a column involves carrying out the fractionation until a desired amount has been distilled off or the desirable purity is reached. The overhead composition varies during the operation and usually a number of cuts are made. Some of the cuts are desired products (*main-cuts*) while others are intermediate fractions (*off-cuts*) that can be recycled to subsequent batches to obtain further separation.

One of the main advantages of batch columns is that *nc* components can be recovered in only one column, while in continuous distillation is necessary to have *nc*-1 columns to achieve the same result. Besides, the number of alternatives to operate the sequence of continuous distillations grows exponentially with the number of components. Finally, in pharmaceutical and food industries, product tracking is very important in the face of strict quality control and batch wise production provides the batch identity(Low, 2003).

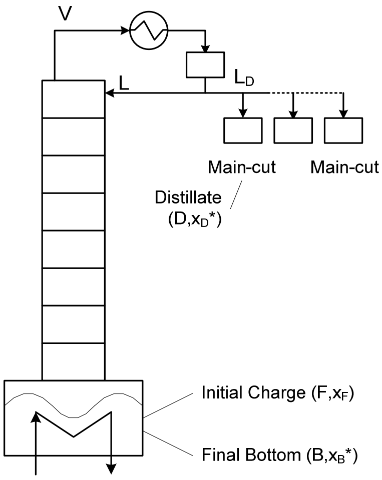

**Figure 1.1:** Batch Distillation Column.

The main objective of this work is to design a batch distillation column capable of eliminate most of the solvent from a nanocapsules suspension, composed mainly by polymeric nanocapsules, acetone (solvent) and water (non-solvent). A method that considers simultaneously the design and operation was then applied (Mujtaba and Macchietto, 1996; Miladi and Mujtaba, 2004).

## 2 MODEL

The column will operate to purify the nanocapsules suspension. The model considers that the feed is a binary mixture composed only by acetone and water, neglecting the effect of the nanoparticles in the thermodynamic equilibrium at the reboiler. The sequence of each one of the $N_B$ batches will be similar.

The model was simulated with MATLAB. As it does not have a thermodynamic toolbox, it was necessary to implement the routines to perform the simulation. Initially, equilibrium predictions of 2 models (Wilson and NRTL) and experimental data (Barnicki, 2002) were compared using Aspen Plus®. The comparison for temperature and composition values can be seen in Fig. 2.1. Since both models describe well the experimental data, Wilson model was chosen because it is simpler to implement than the NRTL model. All the parameters used in the correlation were taken from Perry & Green (1997).

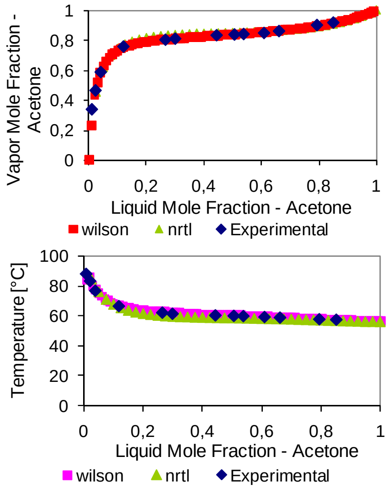

**Figure 2.1:** Comparison among the experimental data (Barnicki, 2002) of composition and Temperature, and the predictions with NRTL and Wilson models.

The following considerations were assumed as true when modeling the column:

- Invariable flow rates of liquid and vapor;
- Constant hold-up in the stages;
- Perfect mixing;
- Fast heat transfer;
- Total condensation;
- Adiabatic column.

Apart from that, the stages are ordered from bottom to top, where the reboiler and condenser were considered as equilibrium stages as shown in Fig. 2.2a.

*Liquid Flow Rate*: $$L = V \Big/ \left(1+\frac{1}{R}\right) \tag{1}$$

*Distillate Rate*: $$D = \frac{L}{R} \tag{2}$$

*Reflux Ratio*: $$R = \frac{L}{D} \tag{3}$$

where:

*L* – Liquid flow rate [kmol/h];
*V* – Vapor flow rate [kmol/h];
*D* – Distillate rate [kmol/h]
*R* – Reflux ratio [-].

### 2.1 *Reboiler*

*Total Mass Balance*: $$\frac{dH_j}{dt} = L - V \tag{4}$$

*Component Mass Balance*: $$x_j \frac{dH_j}{dt} + H_j \frac{dx_j}{dt} = Lx_{j+1} - Vy_j \tag{5}$$

$$x_j (L - V) + H_j \frac{dx_j}{dt} = Lx_{j+1} - Vy_j$$

$$\frac{dx_j}{dt} = \frac{1}{H_j}\left[L\left(x_{j+1} - x_j\right) + V\left(x_j - y_j\right)\right]$$

where:

*H* – hold-up [kmol];
*x* – liquid molar fraction;
*y* – vapor molar fraction;

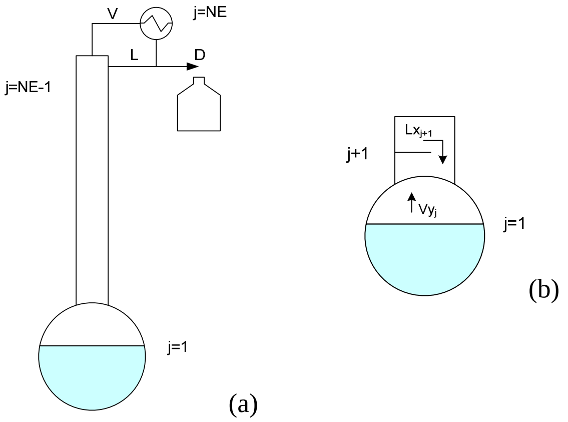

**Figure 2.2:** Schematic Representation: (a) batch distillation column (*NE* is the number of stages), (b) Reboiler.

### 2.2 *Internal Stages, j=2:(NE-1)*

*Component Mass Balance*:

$$\frac{dx_j}{dt} = \frac{1}{H_j}\left[L\left(x_{j+1} - x_j\right) + V\left(y_{j-1} - y_j\right)\right] \tag{6}$$

### 2.3 *Accumulator, j=NE*

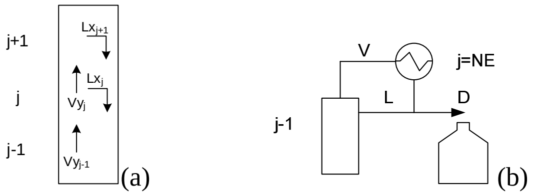

**Figure 2.3:** Schematic Representation: (a) one stage, (b) condenser and accumulator.

*Mass Balance*: $$\frac{dH_a}{dt} = D \tag{7}$$

*Component Mass Balance*: $$\frac{dx_a}{dt} = \left(\frac{D}{H_a}\right)\left(x_j\text{-}xa\right) \tag{8}$$

where $H_a$ is the hold-up in the accumulator.

### 2.4 *Equilibrium*

As explained at the beginning of this section the Wilson activity model (Reid, Prausnitz, and Polling, 1987) is used to calculate the equilibrium for the liquid phase and ideal gas for the vapor phase.

### 2.5 Operation

It was considered that there is a fixed demand for the product; therefore, the number of batches per year ($N_B$) is fixed. Based on the annual operating time ($AOT$) [h/year], the duration [h] of each distillation task is already defined as

$$t_b = \frac{AOT}{N_B} \tag{9}$$

where:
$AOT$ – annual operating time [h/year];
$N_B$ – Number of batches [batches/year];
$t_b$ – total time of each distillation task [h].

The definition of the required number of batches per year is clearly dependent on the market requirements. In this work 6 scenarios were analyzed: from 2500 to 5000 batches/year of same size. Another approach would be to include the number of batches in the optimization problem and in this case one assumes that there is an open market for the product. Not only this is not a realistic assumption but also Miladi and Mujtaba (2004) results proved that when the designs obtained with this approach are now simulated considering fixed demands, in some cases, for a fixed vapor load, the required production is not achieved or there is a negative profit.

Given the initial charge ($x_F$, $F$) and the product specification ($x_B$* and $x_D$*), the amount of D and B to be produced per batch are fixed according to the component mass balance equation:

$$Fx_F = Bx_B^* + Dx_D^* \tag{10}$$

$D$ and $t_b$ in turn fix the distillate rate in the column, as:

$$L_D = \frac{D}{t_b} \tag{11}$$

The internal reflux ratio ($R_{int}$) can then be expressed as a function of $V$:

$$R_{\text{int}} = \frac{L}{V} = \frac{V - L_D}{V} = f(V) \tag{12}$$

Thus, for fixed product demand scenario the set of optimization variables reduces to only $NE$ and $V$.

### 2.6 Optimization Problem

In this work the design was done through a procedure based on optimization as suggested by Miladi and Mujtaba (2004), that is:

| | |
|---|---|
| Given | a binary feed mixture to be separated according to a predefined structure;<br>a set of product specifications;<br>production horizon [h/year];<br>product demand in terms of number of batches of product ($N_B$) |
| Determine | the optimum design (number of stages NE, and vapor load V) and operating decisions (reflux ratio R and batch time, $t_b$) |
| to maximize | the profit P |
| Subject to | any constraints |

Therefore, the mathematical problem to be solved is:

| | | |
|---|---|---|
| Objective Function | Max<br>NE, V, R | P |
| s.t | $x_D \sim x_D^*$ | (inequality constraint) |
| | $x_B \sim x_B^*$ | (inequality constraint) |
| | $N_B$ (fixed) | (equality constraint) |
| | Process model equations | (equality constraint) |
| | Bounds on NE, R, V | (inequality constraint) |

The objective function is the profit obtained per hour with the purification of nanocapsules, as defined by eq. 13.

$$Profit \left[\frac{\$}{h}\right] = (c_1 D + c_2 B - c_3 F) - OC - CC \tag{13}$$

The first term in the right-hand side accounts for the incomes and outcomes due to the cost of raw material and the price of the products. The other 2 terms are the operating (OC) and capital (CC) costs [\$/hour], defined by equations (14) and (15) as proposed by Sharif, Shah, and Pantelides (1998a):

$$OC = 0.0177V + 0.0011(760 - \mathrm{P})^2 + 0.00065Q_c \tag{14}$$

where $P$ is the operating pressure (in mmHg), $V_D$ is the reboiler volume (in L).

$$CC = \alpha_r V_D^{0.6} + \alpha_n V_D^{0.533} NE^{0.802} + \alpha_P (760 - \mathrm{P})^2 \tag{15}$$

where $\alpha_r$ , $\alpha_r$ , $\alpha_p$ are cost coefficients with values of 1.35, 0.0663 and 0.00033 respectively.

Note that both cost equations take into account the effect of the operating pressure, which is important when designing reduced pressure distillation tasks.

The data used in this problem is shown in Table 1.

Tabela 1: Input Data.

Mixture: water and acetone
Column Specifications:
Number of Stages, $NE$ = ‹5 20›
Vapor boilup rate ,$V$ [kmol/h] = ‹5 100›
Condenser hold-up [kmol] = 2% of the feed
Stage hold-up [kmol] = 2% of the feed
Reboiler pressure [bar] = 0.12 bar
Total pressure drop [bar] = 0.1 bar (equally distributed among the stages).
Initial Charge: $F$ = [100 289.5] kmol, $x_F$ = 0.112 (acetone)
Product Specifications:
$x_D$*= 0.95 (acetone)
$x_B$*= 0.05 (acetone)

If one includes the Number of Stages (NE) as an optimization variable, MINLP (Mixed-Integer Non-Linear Programming) algorithm should be used to solve the problem. Instead of this approach, it was decided to repeat the optimization for each NE because at the same time a parameter sensitivity analysis would be then performed.

Thus, we came up with only one optimization variable, $R_{\text{int}}$ or V, depending on how eq. (3) is written:

$$R_{\text{int}} = \frac{V-L_D}{V} = f(V) \quad \text{or} \quad V = \frac{L_D}{1-R_{\text{int}}} = f(R_{\text{int}}) \tag{16}$$

As the values of $R_{\text{int}}$ are restricted to the range [0 1] it was chosen as the optimization variable.

The relationship between $R_{\text{int}}$ and R (eq. (3)) can be written as

$$R = \frac{L}{L_D} = \frac{V \cdot RR_{\text{int}}}{L_D} \tag{17}$$

The optimization was performed as explained by Fig. 2.4. Given the problem specifications – like *NE* (Number of Stages), $N_B$ (number of batches per year), Annual Operating Time, feed amount and concentration, desired purity at the distillate, column pressure and so on – the model is simulated returning the annual profit and the key component purity at the top, among other variables. If the difference between the desired and obtained purity is higher than a certain value (in this work, $3\text{x}10^{-4}$), a new initial guess is calculated and the model is simulated again, until that difference falls below $3\text{x}10^{-4}$. This procedure is repeated several times for different values of F, NE and $N_B$.

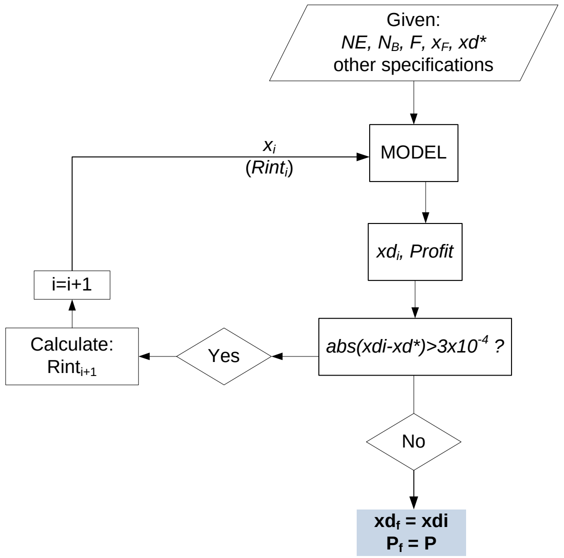

**Figure 2.4**: Optimization Procedure.

In order to calculate $Rint_{i+1}$ one should first detect in which of the five situations showed in Figure 2.5 the last iteration result falls.

In case (a), in any time the purity specification is not reached, therefore the vapor rate should increase, leading also to an increase in the internal reflux ratio. The same happens in situation (c), where at the final time the accumulator concentration is higher than the specification. Also in this case, the internal reflux ratio should increase. On the other side, in case (b), as the vapor rate is too big, the final concentration at the accumulator falls under the specification, then the vapor rate should be reduced. In cases (d) and (e), the distillation proceeds slow due to the insufficient vapor boil up rate. Therefore, one should increase the internal reflux ratio.

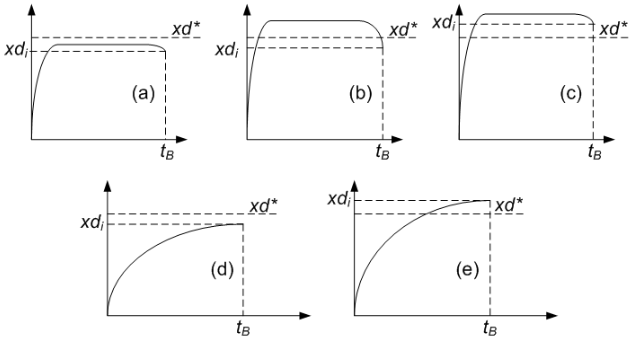

**Figure 2.5:** Possible situations that drive the calculation of $Rint_{i+1}$. ($xd_i$ is the final molar fraction of acetone in the accumulator found in the last iteration step)

All these situations lead to new values of *Rint*, calculated through the following conditional statements (i, time step; j, iteration; matlab code):

```
while abs(xd*-xd_tB,j)>=3e-04
        if xd_end,j<xd_end-1,j
            if xd_end,j < xd*
                max1=find(xd_1:end,j>0.99);
                if isempty(max1)
                    Rint_j+1=Rint+abs(xd*-xd_tB,j)/3;
                else
                    Rint_j+1=Rint-abs(xd*-xd_tB,j)/3;
                end
            else
                Rint_j+1=Rint+abs(xd*-xd_tB,j)/3;
            end
        else
            if xd_end,j < xd*
                Rint_j+1=Rint-abs(xd*-xd_tB,j)/3;
            else
                Rint_j+1=Rint+abs(xd*-xd_tB,j)/3;
            end
        end
end
```

Note that in this work the strategy is to work with a fixed reflux ratio because it is an easy way to analyze several macroscenarios. Another strategy could be to optimize the problem minimizing the energy comsumption to achieve the purity in the required time. In this case, the reflux ratio would be variable, resulting in a problem of optimal control.

### *2.7 Raw Material Cost Calculation (custos.m)*

The constants $c_1$,$c_2$ and $c_3$ were calculated based on the composition and the price of deionized water (US$ 1.00/L), acetone (US$ 5.00/L) and PCL (US$ 300.00/kg), resulting in: $c_1$ = US$ 39.00/kmol, $c_2$ = US$ 65.00/kmol and $c_3$ = US$ 50.00/kmol. Note that the most valuable product is the purified nanocapsules suspension, that is, the bottom product.

### *2.8 Energy Calculations (Al-Tuwaim and Luyben, 2002)*

The following are the equations used in energy calculations.

#### 2.8.1 Minimum Diameter

$$Dia_{\min} = 2\left(\frac{(MW)V'}{\rho_V \pi V_m}\right)^{\frac{1}{2}} \tag{18}$$

where *MW* is the vapor molecular mass, $\rho_V$ is the vapor density and $V_m$ is the maximum allowable superficial vapor velocity [m/s]. Vm is calculated as:

$$V_m = K_V\left(\frac{\rho_L-\rho_V}{\rho_V}\right)^{\frac{1}{2}} \tag{19}$$

where $Kv$ is a empirical constant = 0.09144 m/s for 24in spacing in trays and $\rho_L$ is the liquid density.

In order to calculate $MW$, $\rho_L$ and $\rho_V$, it was considered that the vapor and the liquid inside the column contain mainly the key solvent, with an average mass fraction of 0.98 for the vapor and of 0.94 for the liquid.

### 2.8.2 Utility Flow Rate [m/h]

The utility flow rate is obtained using

$$W = \frac{Q'}{H_V} \tag{20}$$

where $H_V$ is the heat of vaporization [J/kg] of the steam and $Q'$ is the energy consumption [J/h], that is calculated through

$$Q' = V'H_V' \tag{21}$$

The Heat of Vaporization was calculated according to Fish and Lielmézs correlation and Riedel correlation(Reid, Prausnitz, and Polling, 1987).

$$\textit{Fish and Lielmézs}: H_V = \Delta H_{VB} T_R \frac{X+X^q}{T_{BR}\left(1+X^p\right)} \tag{22}$$

where $\Delta H_{VB}$ is the heat of vaporization at normal boiling point, $T_R$ and $T_{RB}$ are the reduced and reduced boiling temperature, respectively and X is defined as

$$X = \frac{T_{BR}}{T_R}\frac{1-T_R}{1-T_{BR}} \tag{23}$$

$q$ and $p$ values for organic and inorganic liquids are 0.35298 and 0.13856, respectively.

$\Delta H_{VB}$ is calculated from the correlation of Riedel:

$$\Delta H_{VB} = 1.093 R T_C\left[T_{BR}\frac{\ln(P_c)-1.013}{0.93-T_{BR}}\right] \tag{24}$$

where $P_c$ and $T_c$ are the reduced pressure and temperature.

For a mixture of acetone and water at 0.12 bar, which molar fractions are [0.112 0.888], $H_V$ calculated using the correlation of Fish and Lielmézs is 1.2288x$10^4$ cal/mol.

### 2.8.3 Heat Transfer Areas

The condenser heat transfer area [m$^2$] is obtained from

$$A_c = \frac{q}{U\Delta T} \tag{25}$$

where $q$ is the heat-transfer rate [J/h] = $V'(H_v')$; $U \equiv$ overall heat-transfer coefficient = 567.83 W/hm$^2$K; $\Delta T \equiv$ temperature gradient = 10 K. The reboiler heat-transfer is similar calculated except that $U$ = 283.91 W/hm$^2$K.

## 3 RESULTS AND DISCUSSION

For different product demands ($N_B$) and for each $NE$, the simulation results in terms of optimum vapor load ($V$), Reflux Ratio ($R$), Operating Cost ($OC$), Annual Capital Cost ($ACC$) and the Profit ($P$) are evaluated. It was assumed that there are 2 sizes of equipments available, that is 300 and 110 kmol, and one should decide which one to buy. Therefore, the analyzed cases were feed loads of 289.5 (Case 1) and 100 (Case 2) kmol of nanocapsules suspension per batch. Of course, when projecting a real plant one should carefully define how much the market will demand in the following years in order to define the size of each batch.

For both cases initially simulations were performed of 5, 10, 15 and 20 stages aiming to find the region where the highest profit is achieved. For case 1, the simulations showed that the column that provides the higher profit is the one with about 10 stages.. However, in order to find the real optimum, further investigations should be done (± 1 stage) until a new optimum value is found or until the confirmation of the original result, that is, 10 stages as the best design. The results for load of 289.5 can be seen in Figure 3.1, while the results for the other option are showed by Figure 3.2.

Analyzing the results it is seen for both cases that the profit increases as the market demand decreases. When more product should be purified, the batch periods are shorter requiring higher vapor loads, which have a direct influence on the operating cost. On the other side, for less demand, the batches are longer leading to lower vapor rates, which decrease the operating cost.

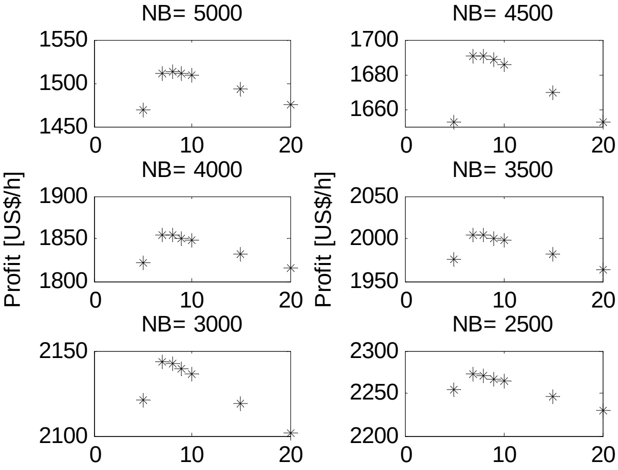

**Figure 3.1**: Profit obtained with the column of capacity 289.5 kmol.

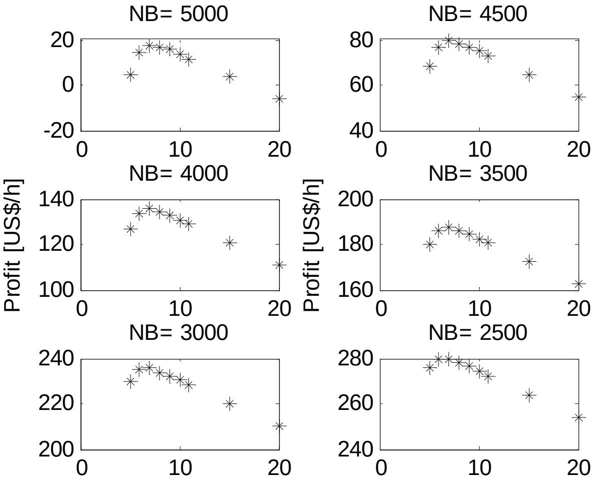

**Figure 3.2**: Profit obtained with the column of capacity 100 kmol.

The effect exerced by the demand is more pronouciable for a feed load of 100 kmol. In the case where NB is equal to 5000, negative values of profit are achieved because the required vapor load leads to prohibitive operating costs. Moreover the profit values in this case are lower than the other.

For each case, if $NE>NE_{opt}$ and $V>V_{opt}$ , the specification will be achieved quicker but leading to unoccupied time and lower profit. On the other side, if V<Vopt the distillation will require larger time and also will not achieve the market demand;

For a given number of stages there is an optimum vapor load, and vice-verse. Therefore, it is not recommended to fix the vapor load and optimize only the number of stages.

In the equation that describes the capital cost the condenser and reboiler areas are not included; however, as they are lower (see Tables 1 and 2 in Apendix) for the smaller design they certainly contribute to reduce the capital costs leading to a possible increase in the profit obtained in this case.

Note that it was considered that the presence of nanoparticles in the feed stream does not affect the thermodynamic equilibrium; therefore, the feed was simplified as a mixture of acetone and water. In the real world, the presence of nanocapsules can contribute to increase or decrease the vapor rate, with effects on the optimum design values found in this work. Besides, as the cost of raw materials and products were calculated based on lab products prices, they can have been overestimated, leading to quantitative errors at profit results.

## 4 CONCLUSIONS

In this work, an optimization procedure was applied in order to design a batch distillation column to purify a suspension of nanocapsules. The purification is the first downstream process when producing solid nanoparticles for controlled drug delivery.

Given the market demand for the product and several specifications, the optimum design in terms of number of stages, vapor rate and reflux ratio, are calculated by maximizing a profit function (eq. 13). Moreover, based on the optimum values the minimum diameter of the column and the condenser and reboiler areas were also calculated.

While Miladi and Mujtaba (2004) proposed to use a exhaustive search algorithm to solve the optimization problem, in this work is proposed a very simple strategy that showed to be efficient when reasonable initial guesses are provided. Furthermore, a modification in the cost functions was done mainly to consider the operation pressure, following the approach proposed by Sharif, Shah, and Pantelides (1998b).

From the simulation results, is possible to conclude that for a given number of stages there is an optimum vapor load, and vice-verse. Therefore, it is not recommended to fix the vapor load and optimize only the number of stages.

In summary, for a feed load of 289.5 kmol, which corresponds to a daily production of 10 kg of purified nanocapsules, the best column is the one with 7 theoretical stages. The profits obtained for a feed load of 100 kmol were lower than the case of higher load, including one case where it is negative.

The process presented by this work can be further improved if the following ideas are tested:

- include the reboiler and condenser areas in the capital cost equations;
- include the reflux ratio, batch time and market demand as optimization variables;
- solve a problem with 2 objective functions, one that intend to maximize the profit while minimizing the energy comsumption;

The first one will be implemented soon.

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# 6 APPENDIX

Table 1: Results of energy calculations of Case 1.

| NB | NE | V [mol/h] | Profit [US$/h] | R | Minimum Diameter [m] | Q' [J/h] | W [kg/h] | $A_C$ [$m^2$] | $A_R$ [$m^2$] |
|---|---|---|---|---|---|---|---|---|---|
| 5000 | 7 | 25070.31 | 1511.43 | 0.321 | 0.2605415 | 1.29E+09 | 605.69 | 63.10 | 126.19 |
| 4500 | 7 | 21576.47 | 1690.17 | 0.276 | 0.2417059 | 1.11E+09 | 521.28 | 54.30 | 108.61 |
| 4000 | 7 | 18379.62 | 1853.66 | 0.235 | 0.2230824 | 9.46E+08 | 444.04 | 46.26 | 92.51 |
| 3500 | 7 | 15439.00 | 2004.04 | 0.198 | 0.2044592 | 7.94E+08 | 373.00 | 38.86 | 77.71 |
| 3000 | 7 | 12722.34 | 2143.01 | 0.163 | 0.1856012 | 6.55E+08 | 307.37 | 32.02 | 64.04 |
| 2500 | 7 | 10209.29 | 2271.53 | 0.131 | 0.1662627 | 5.25E+08 | 246.65 | 25.69 | 51.39 |

Table 2: Results of energy calculations of Case 2.

| NB | NE | V [mol/h] | Profit [US$/h] | R | Minimum Diameter [m] | Q' [J/h] | W [kg/h] | $A_C$ [$m^2$] | $A_R$ [$m^2$] |
|---|---|---|---|---|---|---|---|---|---|
| 5000 | 7 | 8658.712 | 17.52 | 0.321 | 0.153 | 4.45E+08 | 2.09E+02 | 21.792 | 6.495 |
| 4500 | 7 | 7451.699 | 79.28 | 0.276 | 0.142 | 3.83E+08 | 1.80E+02 | 18.754 | 5.84 |
| 4000 | 7 | 6349.76 | 135.60 | 0.236 | 0.131 | 3.27E+08 | 1.53E+02 | 15.981 | 5.196 |
| 3500 | 7 | 5333.036 | 187.61 | 0.198 | 0.120 | 2.74E+08 | 1.29E+02 | 13.422 | 4.544 |
| 3000 | 8 | 4384.244 | 233.95 | 0.162 | 0.109 | 2.26E+08 | 1.06E+02 | 11.034 | 3.865 |
| 2500 | 7 | 3527.032 | 279.97 | 0.131 | 0.098 | 1.81E+08 | 8.52E+01 | 8.8767 | 3.246 |