

THERMAL MODELING OF A DISTILLATION COLUMN OF AN AMMONIA/WATER ABSORPTION REFRIGERATION CYCLE

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Abstract. *The aim of this paper is to present an analysis of a segmented weir sieve-tray distillation column in steady state conditions for a 5 TR absorption refrigeration cycle working with ammonia/water. The distillation column is to provide ammonia vapor at a high degree of purity to ensure that the refrigeration cycle work properly. Balances of mass and energy of the column were performed based on the method of Ponchon-Savarit, where ideally four plates were calculated with the feeding system in the column above the second plate. A sensitivity analysis indicated that reflux is an important parameter in the economic analysis project, since it depends on the initial high cost of building the column, or the largest expenditure spent on fuel in the operation cycle. Vapor and liquid pressure drop and the mass flows ratios have resulted in the internal geometry of the column, which resulted satisfactorily for the design parameters recommended, even though the work was based on correlations used in the area of petroleum, petrochemical and distillation of alcoholic beverages. The distance between trays is a measure of compaction of the column and was very dependent, as well as other dimensions of the tray, the height of the weir, which was found to be optimal for values between 4 mm and 8 mm. The geometry of the tray turns out to be sensitive to the charge of vapor, and to a lesser extent, to the load of the liquid, being insensitive to the diameter of the hole. The efficiency of the column takes into account transport phenomena in the tray that deviates from the condition of ideality. It was calculated a column efficiency of 50%. This low value is mainly due to the low value of the slope of the equilibrium ammonia/water curve in the early section of stripping and low molar ratio of vapor flow and liquid flow, in this section.*

Keywords: *distillation, heat and mass transfer, ammonia/water, refrigeration, absorption*

1. INTRODUCTION

Worldwide population increase is closely associated with a considerable increase in consumption of electricity and other sort of energy as well. The electricity consumption in air conditioning and refrigeration is elevated, growing in summer and at the peak hour. The decrease in green areas caused by population growth together with the increase in energy consumption, mainly originated from the burning of fossil fuels, have brought the concept of rational and efficient use of energy, in which interest in using absorption refrigeration cycles is located. These cycles need very little electricity for its operation. The thermal energy needed to power these cycles can be supplied by waste gases heat from thermal processes, also by solar energy, among others. If one includes an absorption refrigeration cycle in a cogeneration or trigeneration system, i.e., the generation of electricity, heat and cold from a single source of energy, this concept of integrated power plant becomes a more efficient, economical and environmentally friendly. The most common working fluids in absorption refrigeration cycles are the pairs of fluids ammonia/water and lithium bromide/water, being the first ones natural fluids. An ammonia/water absorption refrigeration cycle (AARC) achieves cooling temperatures below subzero, since the refrigerant is ammonia, while the lithium bromide/water cycle is limited to temperatures above 0 °C, being water the fluid refrigerant.

A critical element of any AARC is the distillation column in which a simultaneous heat and mass transfer process takes place in the two-phase mixture of ammonia/water. The column must provide high purity ammonia vapor. Otherwise, if the ammonia vapor is too wet, the water content can accumulated continuously in the evaporator causing a degradation of the cycle COP (Fernandez-Seara and Sieres, 2006a; Fernandez-Seara and Sieres, 2006b). Ahachad et al. (1992) compared the COP of an ammonia/water simple effect refrigeration cycle operating with and without a purification system. In place of the rectifier they tested a vapor bubble purifying system. The COP of the absorption chiller with vapor bubble purifying system improved from 15% to 35% and the required area of solar collectors, used as a heat source, was lower by 10%; the highest COP obtained was 0.4.

There is an evaporation temperature increase related to binary solutions such as ammonia/water during a phase change process, it compartment is called temperature glide. If the evaporation temperature keeps raising, the system will reach a point where it will be no longer possible to cool the medium of interest. This temperature behavior avoids the use an ammonia/water mixture at substantial concentrations of water (Fernandez-Seara and Sieres, 2006a; Herold et al. 1996). At higher concentration of water, more significant will be the temperature glide. Therefore, removing water from the ammonia vapor that exits the generator ensures the reliability and efficiency of ammonia/water absorption

refrigeration systems (Bogart, 1982). It has been suggested that a purity of approximately 99.9 wt% of ammonia as the limiting concentration for a proper CRAA operation (White and O'Neill, 1995).

Herold et al. (1996) and Kuehn (1998) presented a conceptual design analysis of distillation columns of AARC without any in-depth study of working parameters such as reflux, feed position of strong solution as well as heat fluxes involved in the generator and the rectifier. Anand and Erickson (1999) analyzed a tray distillation column of a 8 TR AARC emphasizing design parameters such as flooding prevention, hole tray weeping and geometry of the column. Sieres et al. (2009) have made experimental studies of purification systems for an AARC with random packing of *berl*, *raching*, *novalox*, and *pall* types and structured packing *mellapak plus* and *sulzer* types. Their tests showed that the *pall* packing type needed height for a desired purity. Lower heights for the same purification load was found for the *novalox* type than that for a spray column (Mendes, 2008).

This paper studies the distillation process of the ammonia/water solution to obtain a high purity ammonia vapor. The analysis provides geometrical details to achieve pre-established purity values. This study chose a sieve tray column, since its design is simple, besides being economical, having a plain cleaning maintenance, low pressure drop, and it is suitable for most applications. Multiple entrances and exits are more flexible in tray columns when compared with the packing column ones.

Studies on gas-liquid direct contact trays propose two methods for carrying out a mass and energy balance: Ponchon-Savarit and McCabe-Thiele. Treybal (1981) showed that the former method is more accurate, since the other one considers a liquid and vapor constant flow. By using the Ponchon-Savarit method the conservation and constitutive equations were solved using the EES software (Engineering Equation Solver) to solve the nonlinear system of coupled equations.

2. DISTILLATION COLUMN DESCRIPTION

A simplified scheme of an AARC is shown in Fig. 1a. It can be observed the distillation column in thick black line. There exists a reservoir of liquid ammonia/water solution inside the distillation column (Fig. 1b) called "the generator". When heat is supplied to the generator, part of the solution becomes vapor rich in ammonia, given that it is the most volatile component. Wet ammonia vapor rises up the column in a countercurrent direction to the descending liquid solution. Those two flow streams are mixed on the plates located inside the column, occurring a simultaneous heat and mass transfer. As the vapor rises up through the column it will increase its purity (higher concentration of ammonia) while the descending liquid have a lowering in ammonia concentration. When the vapor reaches the top plate (numbered 1 in Fig. 1b) still containing some water vapor content, it passes through an partial condenser called rectifier, where heat is removed and part of the water vapor is condensed along with ammonia. The liquid and vapor are directed to the accumulator where they are separated: the liquid is driven to the top of the column (reflux) and the saturated vapor exits the piece of equipment in direction to the condenser.

3. THERMODYNAMIC MODELING

Figure 1b shows the variables involved in the mass and energy balance in the distillation column. The control volume (CV) allows exchanges of mass and energy with the surroundings. The overall control volume VC-3 allows feeding the column and the label "j" is assigned to it; the solution output is labeled "w", and the saturated vapor is labeled "d". Kuehn et al. (1998) name the sections of enriching and stripping section as "analyzer". In Fig. 1b, L and V are the liquid solution and vapor outlets respectively; "r" is for the reflux. In the column there are N_i plates (ideal), of which n are the enriching section and $N_i - m + 1$ are the stripping section. According to the control volume CV-1, the mass and energy balance yields to:

$$\frac{\dot{m}_{L,n}}{\dot{m}_{V,n+1}} = \frac{x_d - x_{V,n+1}}{x_d - x_{L,n}} = \frac{h'_d - h_{V,n+1}}{h'_d - h_{L,n}} \quad (1)$$

where

$$h'_d = h_d + \frac{\dot{Q}_R}{\dot{m}_d} \quad (2)$$

The relationship between the mass fraction and specific enthalpy in Eq. (1) represents an operation line. The balances of mass and energy from plate 1 to plate n provide operation line in the $x - h$ axis, and they all coincide at the point (x_d, h'_d) . The flow of liquid and vapor coming out of each plate are at equilibrium. The projection of the mass fractions $(x_{L,n}, x_{V,n+1})$ corresponding to the operating line in the $x - h$ diagram, on the $x_L - x_V$ diagram provides a point that belongs to the operation curve. The projections of all mass fractions of the operating lines provide the operation curve corresponding to the side of enriching.

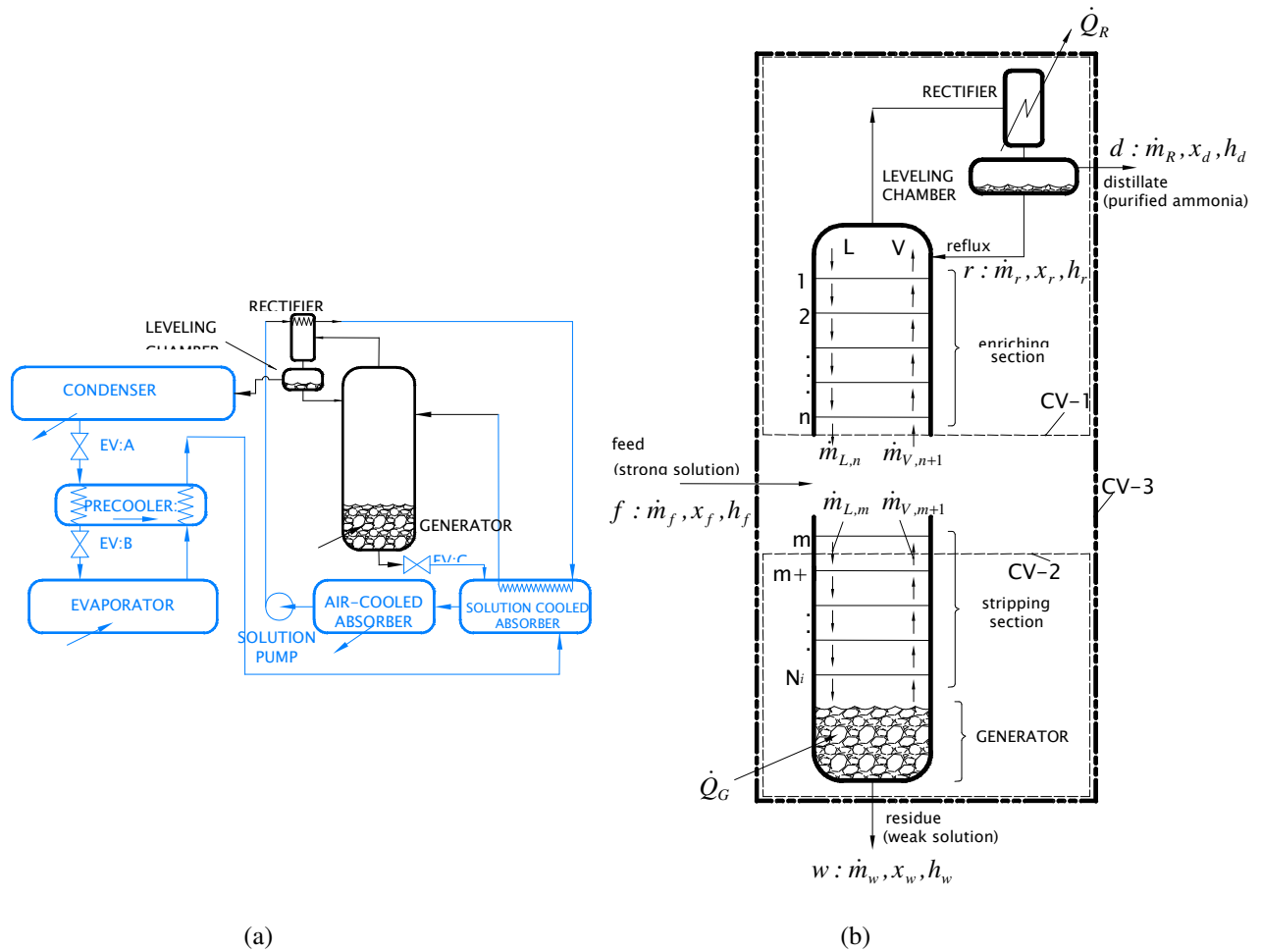


Figure 1. (a) Distillation column (in black line) forming part of an AARC; (b) Variables for the mass and energy balance in the distillation column.

It is defined as reflux ratio R (or external reflux ratio) the ratio of the mass flow of saturated liquid that returns to the top of the enriching section and the mass flow of saturated vapor leaving the column (d) From the mass and energy balance of the first plate, the rectifier and the distillate vapor is obtained:

$$R = \frac{\dot{m}_r}{\dot{m}_d} = \frac{h'_d - h_{v,1}}{h_{v,1} - h_r} \quad (3)$$

From a mass and energy balance for the control volume $CV-2$ in Fig. 1b, it yields to:

$$\frac{\dot{m}_{L,m}}{\dot{m}_{V,m+1}} = \frac{x_{V,m+1} - x_w}{x_{L,m} - x_w} = \frac{h_{V,m+1} - h'_w}{h_{L,m} - h'_w} \quad (4)$$

where:

$$h'_w = h_w + \frac{\dot{Q}_G}{\dot{m}_w} \quad (5)$$

The relationship between specific enthalpy and mass fractions in Eq. (4) provides operating lines which intersect at the point (x_s, h'_s) . The projections of points corresponding to the saturated mass fractions of the operation lines of $h - x$ diagram to $x_L - x_V$ diagram provide points of the curve of operation, if these points are connected it is obtained the stripping operation curve. The feed to the column should be done on the plate corresponding to the intersection of the enriching and stripping operation curves. If the feed point is above or below of this point, it would necessary more plates to obtain the desired concentration x_d and x_s , at distillation point and residue point respectively. Joining together the stripping section-generator with the enriching section-rectifier, it is obtained the complete distillation column. Making the overall mass and energy of the distillation column in the control volume $CV-3$, one will obtain:

$$\frac{\dot{m}_d}{\dot{m}_w} = \frac{x_f - x_w}{x_d - x_w} = \frac{h_f - h'_w}{h'_d - h'_f} \quad (6)$$

Eq. (6) gives the overall operating line in the diagram $h - x$, relating the mass fraction and specific enthalpy. If the overall operating line coincides with a line of equilibrium is obtained the “minimum reflux ratio” (R_{min}), under these conditions the number of plates required for the concentration of ammonia vapor desired is very large and the heat flow necessary to be supplied and removed from the generator and rectifier are minimum. When all the vapor flow coming out of the top plate of the enriching section is condensed and returns to the column, and feed to the column and the weak solution output are suspended, the distillation system arrive to the “total reflux” condition, under these situation the number of plates necessities at the columns is minimum and the heat fluxes involved in the generator and rectifier are very large. Kister (1992) indicates that it should be used reflux factors (Eq. 7) between 1.05 to 1.3.

$$f_R = \frac{R}{R_{min}} \quad (7)$$

4. HYDRAULIC AND INTERNAL GEOMETRY DISTILLATION COLUMN

The materials suitable for ammonia/water distillation column are carbon steel, stainless steel or aluminum. When carbon steel is used, corrosion inhibitors should be added. Is shown in Fig. 2 the geometry of the segmented weir sieve tray with some characteristics length.

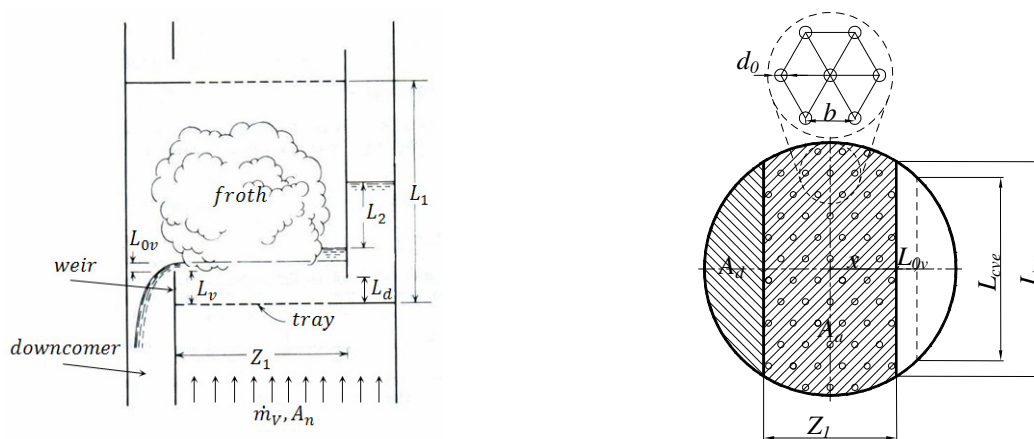


Figure 2. Geometry of the tray (left, adapted from Kister, 1992).

The holes of the plate allow the passage of vapor through them while the downcomer allows the admission of liquid to the plate. There are regimes of flow of liquid and vapor suitable for the distillation column to work correctly (Kister, 1992; Caldas, 2007) outside these regimes exist mixture inefficiencies at the plate like “flooded column” that appears when the liquid or vapor flows are high. When the vapor flow is very small, liquid weeping through the holes of the plate happen.

Another fact that takes place in the column is the vapor pressure drop. It is identified three pressure drops to pass through each tray or plate. The first one when the vapor crosses a dry plate (ΔP_p), another when passing through the liquid (ΔP_L) and last call residual pressure drop (ΔP_R) which is a measure of the difference in pressure drop measured experimentally and calculated which varies with the surface tension of the bubble when it comes off the plate. A detailed study of the internal geometry and the pressure drops was studied by Zavaleta-Aguilar (2010) which will be was in this work.

5. DISTILLATION COLUMN EFFICIENCY

Ideal plates consider the mixing time between liquid and vapor entering the plate is long enough for them to leave the same at thermodynamic equilibrium, but in practice these ideal conditions of equilibrium does not occur. Thus, the mixture of liquid and vapor phases in the plate should consider transport phenomena, thus the number of plates is fixed by the efficiency of the column, according to the following equation:

$$N_r = \frac{N_i}{\eta_c} \quad (8)$$

Where N_r represents the real number plates of the column, N_i the number of plates ideals (calculated by the Ponchon-Savarit method) η_c and efficiency of the column. This efficiency can be evaluated analytically considering the efficiency of point (η_{PV}), the Murphree efficiency (η_{MV}), the Murphree efficiency corrected by entrainment (η_{MVE}). Finally the column efficiency is related to η_{MVE} by Lewis equation, more information on these efficiencies can be found at Locket (1986), Kister (1992) and Perry and Green (1997).

6. RESULTS AND DISCUSSIONS

For an AARC (as shown in Fig. 2a) with a capacity of 5 TR, evaporation temperature of -2°C and condensation temperature of 40°C, the distillation column should have the main variables shown in Tab. 1, (Ortigosa, 2008).

Table 1. Input variables for mass and energy balance of distillation column (data from Ortigosa, 2008).

Position in column	Mass flow (kg/s)	Mass fraction (-)	Temperature (°C)	Pressure (bar)	Quality (-)
Distillated vapor (<i>d</i>)	0.015	0.999	-	15.56	1
Feed (Strong solution) (<i>f</i>)	-	0.4517	98.14	15.56	-
Weak solution (<i>w</i>)	-	0.152	-	15.56	0

The reflux factor is assumed to be 1.1. With the input values provided, the program developed on the EES platform provides the results as shown graphically in Fig. 3.

The EES program developed allows one to know the values of mass flow rate and thermodynamic properties at the entrances and exits of each plate. It is shown in Fig. 3a the location of the strong solution entry in the column above the plate 2. The ideal number of plates for achieving the purification of ammonia vapor of 99.9% is 4. A schematic picture of the distillation column is shown in Fig. 3b, it can be seen that the heat flow required to be supplied to the generator is 27.5 kW, and since the cooling capacity of the cycle is 5 TR, the COP corresponds to 0.64. The heat flow that must be removed from the rectifier corresponds to 4.4 kW. In Fig. 3c it can be noted the temperature variation of the flow along the distillation column, vapor increase its temperature when as it rises and the liquid decreases its temperature as it descends, this behavior is typical of countercurrent flow. The entry of strong solution in the column does not affect the temperature profile since its temperature is close to temperatures for the liquid and vapor at this section. The changes of mass fractions of vapor and liquid along the length of the distillation column are shown in Fig. 4a. In that figure can be observed the increase of the vapor mass fraction when it rises. The mass fraction variation in the stripping section is 51% and at the enriching section is 1.5% and in the rectifier is 2.1%, these last two parts, get a high grade of refined purity for the ammonia vapor. Liquid mass flow decreases highly its concentration at the enriching section although in this section has only of one plate, for the others plates at the stripping section variation is less. It can be demonstrated that vapor mass flow increase upwards by 31% since it leaves from the generator until reach the top of the first plate. The increase in this flow is intensified at the point of feed because of the large amount of ammonia. The variation of the liquid mass flow increases greatly in the second plate because of the feed at the column, already in other plates, its flow rate decreases slightly on the downside. When the reflux ratio is equal to the minimum reflux ratio, the number of plates to suit the desired purification is the largest possible, as it is apparent in Fig. 4b, which shows that this condition the number of ideal plates (N_i) required is 8. It can be see that the number of plates is very sensitive when the reflux factor can be between 1 and 1.06. To higher the reflux factor, the number of plates shown is of little sensitivity. The stripping section will always have a larger number of plates (N_{str}) that the enrichment section (N_{enr}). For values of reflux factor greater than 1.9 the plates in the enrichment section are no longer needed. The flow of heat that must be supplied to the generator is greater values for higher reflux factor, since more liquid returns to column, so the COP will be lower.

To calculate internal geometry of the column, column efficiency and number of real plates, the variables input necessary are presented in Tab. 2.

Table 2. Input variables to calculate the geometry column.

Variable	Value		Variable	Value
	Vapor	Liquid		
Mass flow (kg/s)	0.0126	0.04	Flooding factor (-)	0.80
Mass fraction (-)	0.6306	0.3025	Weir length – column diameter factor (-)	0.85
Temperature (°C)	160.25	122.75	Hole diameter (m)	0.003
Ideal plates (-)	4		Tray thickness (m)	0.002
Froth factor (-)	0.83		Weir height (m)	0.01
			Relative Roughness (-)	0

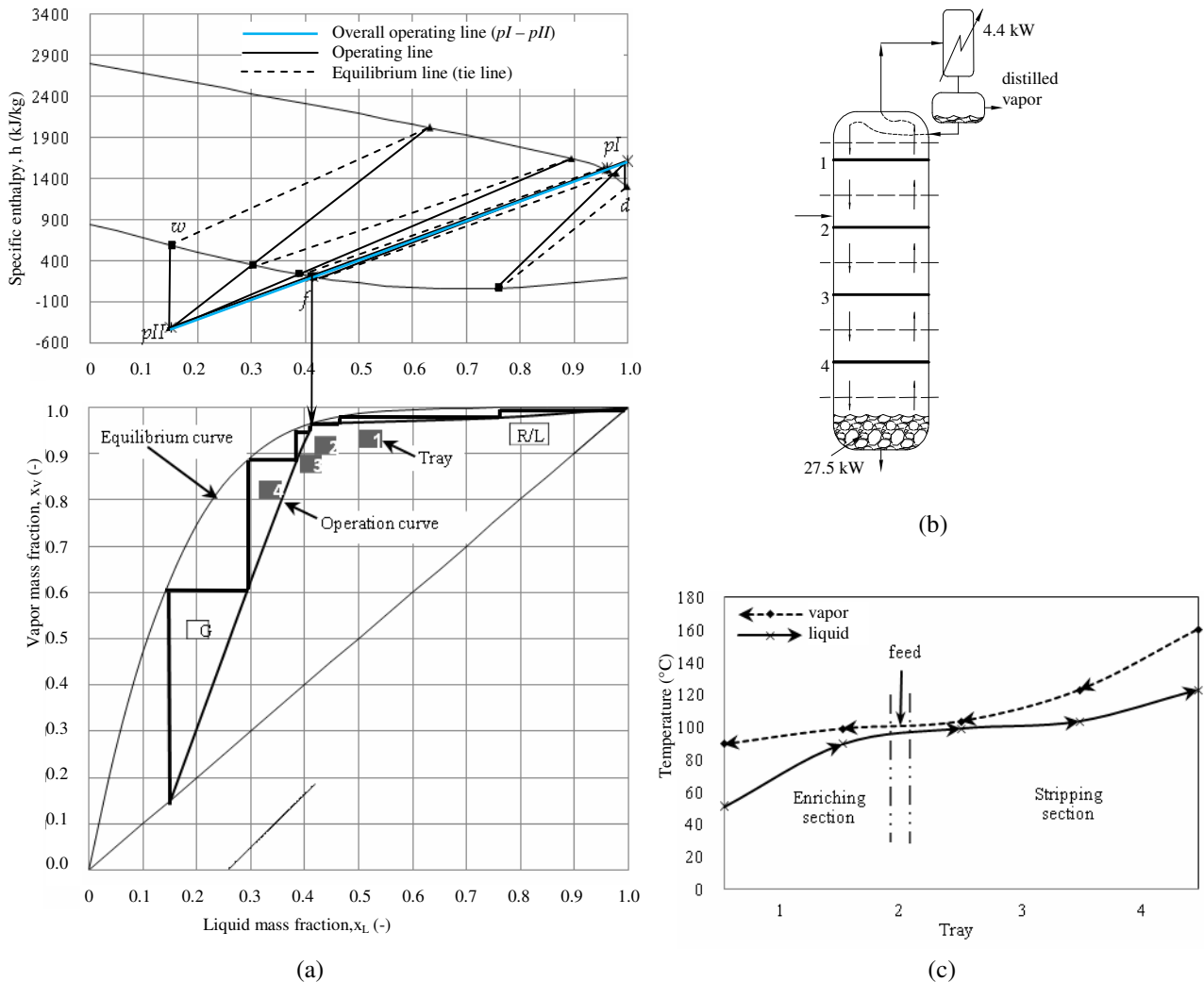


Figure 3. (a) $h - x$ and $x_V - x_L$ diagram for the distillation process; (b) distillation column diagram; (c) Temperature variation of vapor and liquid flows in the distillation column.

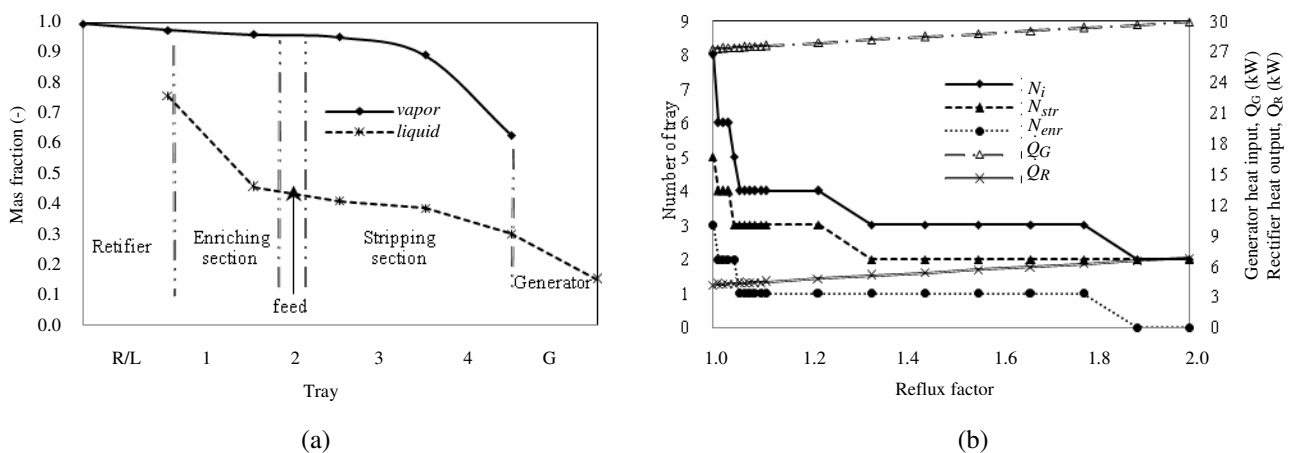
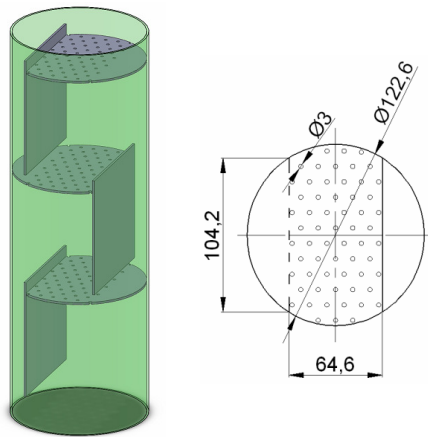


Figure 4. (a) Variation of vapor and liquid mass fraction in the column, (b) Variation of the number of plates and heat fluxes with the reflux factor.

The calculations were made for the bottom plate of the column, the values of mass flow, mass fraction, temperature and ideal number of plates were obtained from the mass and energy balances of the column. The values of other variables represent typical values used in distillation columns. The non-linear set of equations formulated in the EES program have to converge to meet the condition that the distance between plates is at least twice the level of liquid in the downcomer, this to avoid problems caused by entrainment of liquid in the downcomer. Then they are shown the results of the simulation, which are summarized in Fig. 5.



Variable	Value
Column diameter (m)	0.1226
Tray spacing (m)	0.1
Column height (m)	0.8
Real tray number (-)	8
Weir length (m)	0.1042
Liquid flow path (m)	0.0646
Hole number (-)	61
Center hole pitch (m)	0.012
Column efficiency (-)	0.5
Vapor velocity after plate (m/s)	0.16
Hole vapor velocity (m/s)	3.63
Weeping vapor velocity (m/s)	2.22
Vapor pressure drop at plate (Pa)	265.3

Figure 5. Geometry of the distillation column and the results of the EES program.

The same calculation was carried out for the first plate, resulting in a column diameter of 0.1204 m. This represents a difference of 1.8% compared with the same calculation done with the last plate. Kister (1992) recommends that for differences greater than 20% practice should be to use different column diameters. The distance between plates is an indication of a compactable column since if it is smaller, the column height is lower, which is desirable in small absorption refrigeration appliances. A variable that greatly influences this distance is the height of weir, and when it changes it was noted that other variables also change their behavior. This fact can be shown in Fig. 6. The distance between plates takes for a minimum height of the weir between 4 mm and 8 mm. For larger values, the distance between plates always increases. The height of the column has the same behavior as the distance between plates. In this figure we can see that the diameter of the column reaches maximum values for heights of weir of about 6 mm, to values greater than this, the diameter of the column decreases, the same behavior has the length of weir. The graphs show that a compact geometry can be achieved when the height of the weir is between 4 mm and 8 mm. It should take into account the variation of the geometry of the column with the height of the weir, is strongly linked to the velocity of flooding, which depends on the flooding constant. This constant was correlated by Treybal (1981), from the diagram Fair (1961), which was tested in large distillation columns, therefore, for increased reliability should consider the results after the reversal of behavior, i.e., heights of weir greater than 8 mm.

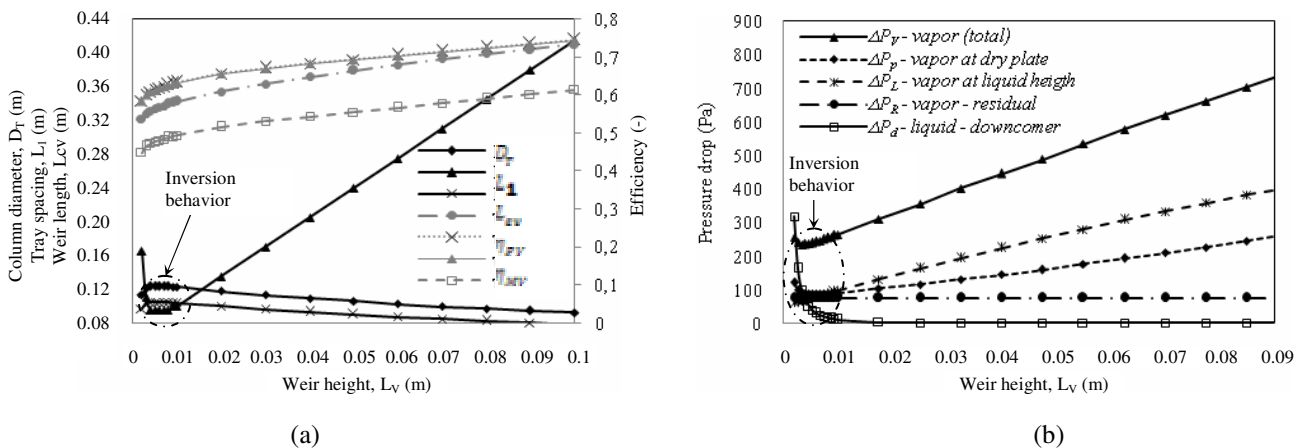


Figure 6. (a) Changes the size and the efficiency of the column according to the height of the weir; (b) Variation of pressure drops according to the height of the weir.

In Fig. 6 one can also see the variation of: point efficiency, Murphree (plate) efficiency, Murphree corrected by entrainment efficiency and column efficiency. The point efficiency is lower than plate efficiency. One can notice that the entrainment does not influence appreciably the plate efficiency. The column efficiency results much less than that of Murphree's corrected by the entrainment efficiency, this is due to the fact that the column efficiency is strongly linked to liquid flow and when this is high compared to the vapor flow, the column efficiency decreases.

The plate hole diameter as shown in Fig. 7a does not influence significantly the diameter of the column, the length of weir and liquid flow path. Now, the distance between plates (L_1) become sensitive to hole diameters between 1 mm and 4 mm. This sensitivity is due to the fact that the distance between plates is related to the total pressure drop of the liquid and vapor, the latter increases like the residual pressure drop when the hole diameter is small, as shown in Fig. 7b. Therefore we recommend using hole diameters larger than 4 mm to achieve pressure drops and distances between plates smaller.

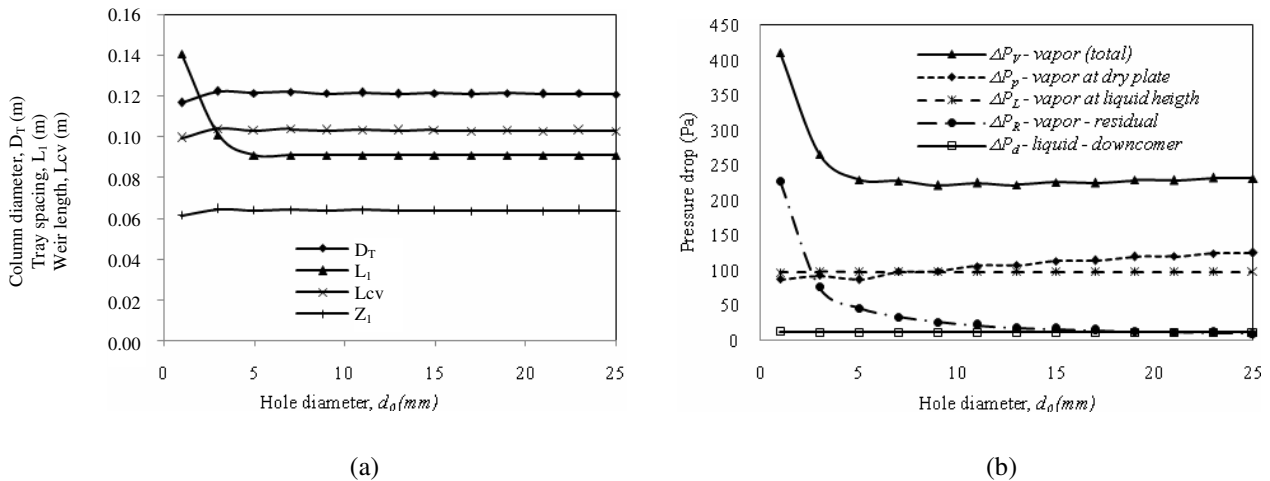


Figure 7. Change in size (a) and the pressure drops (b) with the diameter of hole.

Considering the input variables from Tab. 2 and changing only the vapor flow one can see its influence on the geometry of the column, as observed in Fig. 8a. Proceeds from increase in volume flow of steam, the diameter of the column tends to increase. The column efficiency increases for higher flow rates of vapor, as shown in Fig. 8a, since the velocity of vapor increases, also increasing its turbulence and its ability to mix with the liquid. The distance between plates does not vary significantly since the height of the weir is constant and the sum of pressure drops of the liquid and vapor remains almost constant, as can be seen in Fig. 8b. With the increasing velocity of vapor, its pressure drop when passing by the dry plate increases. The height of the weir is constant, so the pressure drop of vapor passing through the liquid remains almost constant. The pressure drop of the liquid under the downcomer is slightly higher for lower flow rates of vapor since the column diameter is smaller, as well as the passage area of the liquid under the downcomer.

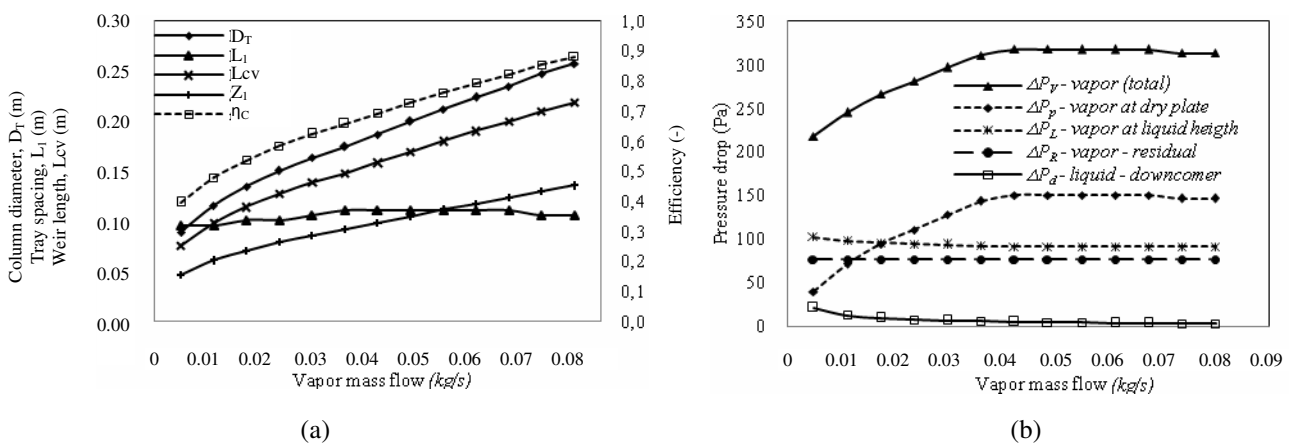


Figure 8. (a) Variation of size and efficiency of the column with the mass flow of steam, (b) Variation of pressure drop with mass flow of steam.

As for the liquid flow rate, when it increases the diameter of the column must be greater, as shown in Fig. 9a, this is due to the fact that the velocity of flooding decreases with increasing the liquid flow, and to maintain the same volumetric flow of vapor, the diameter of the column must increase, L_{CV} and Z_l vary proportionately. The column efficiency decreases with increasing liquid flow rate, as shown in Fig. 9a, because the residence time of liquid on the plate decreases. Since the height of the weir is constant, the distance between plates depends only on the height of the liquid in the downcomer, which is linked to the sum of pressure drops of vapor and liquid, which remains almost constant as shown in Fig. 9b.

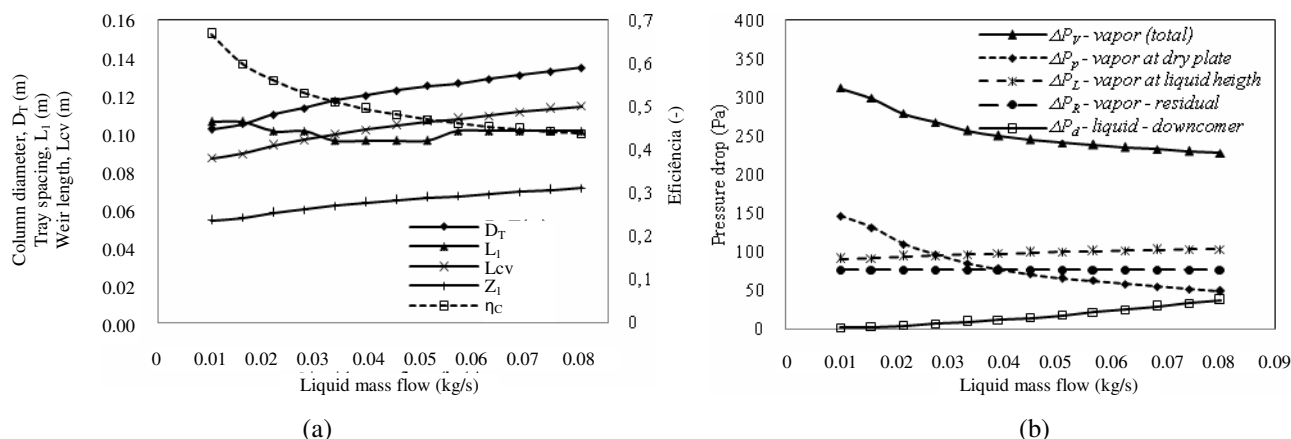


Figure 9. (a) Variation of size and efficiency of the column with the mass flow of liquid, (b) Variation of pressure drop with mass flow rate of liquid.

Since the velocity of vapor decreases, the pressure drop in vapor to pass through dry plate also decreases. The pressure drop of the liquid under the downcomer increases because of increased mass flow of liquid.

7. CONCLUSIONS

In this work, it was presented an analysis of a distillation column with segmented weir sieve-tray of a 5 RT ammonia/water absorption refrigeration cycle. The simulations using the mathematical models were implemented in the program EES (Engineering Equation Solver). The method of Ponchon-Savarit, used to make the balance of mass and energy in the distillation column, appears appropriate as it provides accurate results. The stripping section provides a considerable increase in vapor concentration (51%), the enrichment section increases the concentration of vapor in 1.5% and the rectifier in 2.2%. The last two make a more refined work on the purification process and should not be ignored. The factor of reflux happens to be an important economic parameter in the design of distillation column because the number of plates in the column and the flow heat involved in the generator and rectifier are significantly linked to it, much more for values near to 1. The study allowed calculating the geometry of the plate and the column. The distance between plates is sensitively linked to the height of the weir. The height of the column depends directly on the distance between plates, this second one is a measure of the compaction of the column. The height of the weir influences directly the diameter of the column, the length of the weir, column efficiency, among others, and results are optimal for values between 4 mm and 8 mm, although for greater reliability it would to be used values greater than 8 mm. The diameter of the column is sensible to increase the vapor flow, and to a lesser extent to increase the liquid flow. For hole diameters larger than 4 mm, the geometry of the column shown callous, including pressure drop.

8. ACKNOWLEDGEMENTS

We present our thanks to CNPq for financial support through scholarships.

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