Replacement of Trays by Packing To Increase the Absorption Capacity of Acetone during Cellulose Acetate Spinning

Roberto Nasser, Jr. and Maria Elena Santos Taqueda*

Chemical Engineering Department, Escola Politécnica da Universidade de São Paulo, Avenida Prof. Luciano Gualberto, travessa 3, 380 - Cidade Universitária, CEP: 05508-900, São Paulo, Brazil

All textile uses of cellulose acetate involve acetone recovery, which, because of safety issues, results in large installations, in order to work with dilute streams. This compromises the efficiency of all of the involved unit operations, in this case, acetone absorption in cold water, acetone distillation, and water chilling, making them more expensive. The present article proposes the improvement of the absorption of acetone in water, traditionally performed with sieve trays, by using structured packing instead. The advantageous implementation was enabled through the utilization of a calculation methodology based on concepts of thermodynamic equilibrium of the binary acetone/water system and empirical relations that allow the evaluation of the hydrodynamics of the proposed modification.

1. Introduction

The several textile uses of cellulose acetate all have in common an extremely viscous collodium, resulting from a homogeneous high-solid-content solution in acetone, which must be recovered after spinning, for environmental and economic reasons.^{1,2}

The spinning occurs by extrusion of the collodium through a multiple-hole spinneret, which can vary from dozens to several hundred holes and can also vary in shape, depending on the processed textile product. The filaments formed in each spin cell flow downward, usually pulled by a common feed roll. Depending on the product, the filaments are put together, forming a yarn, similarly to a spinning machine that is constituted by a set of cells, as described. Each cell is a 1–10-m-long pipe with the spinneret installed at the upper portion and the yarn leaving by the bottom, close to the feed roll. Depending on the product, heating can be required, which is achieved using jacket piping with steam, condensate, or both.

The spinning cells are at slightly lower pressure, as they are aspirated by centrifugal blowers. This difference in pressure allows for the feeding of air from the ambient by the upper portion of the cell, close to the spinneret, flowing in the same direction as the filament. The feed flow rate of air is regulated by an orifice placed at the exit of the spinning cell, with a diameter determined by the filament's size, that is, by the mass flow rate of cellulose acetate fed to the cell, usually resulting in a laminar flux, in order not to disturb the formation of the filaments, avoiding them sticking together.

The acetone present in the collodium evaporates, initially, by flash (8–10% of the acetone content of the collodium), because of the difference in pressure. Then, the acetone evaporates gradually along the length of the heated cell, in a process involving radial diffusion within the filament, allowing for the migration of the acetone toward the surface. The filament deforms during formation, decreasing in diameter and thus increasing in velocity, making the flux of entrained air turbulent. This increases the drag and the heat transfer, resulting in the gradual evaporation of the acetone present at the surface.³ A typical representation of a single filament, but that actually applies to all filaments, is given at Figure 1.

A conclusion from the above description is that the mass flow rate of evaporated acetone during spinning depends on several factors such as the spinning velocity, size of the produced filament, and operating temperature, in addition to the pressure. The acetone concentration in the gas mixture leaving each spinning cell varies between 120 and 180 g/Nm³, which is above the lower explosion limit (53 g/Nm³ at 90 °C). Therefore, to avoid risks, it is necessary to dilute the acetone by feeding air to the spinning machine collector, guaranteeing safety of the installation but making acetone recovery more expensive. All acetone vapor obtained during spinning, as well as from subsequent sections, needs to be collected and recycled, resulting in high operating costs, which explains the trend of increasing the solid content by adding small amounts of starch acetate into the collodium.⁴

Traditionally, acetone is absorbed in cold water using columns provided with sieve trays.⁵ The stream with acetone from the spinning is initially cooled in radiators, using cooling tower water. The obtained aqueous solution has a low acetone content, because of the intrinsic characteristics of the unit operation of absorption, consuming significant amounts of energy during the distillation step. Usually, the sump distillation water is recycled to the process, after an initial cooling by an economizer in the distillation, heating of the feed, and cooling to the required temperature, which is performed by a series of electricity-driven chilling machines.

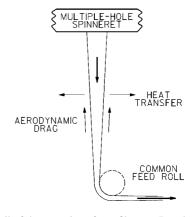


Figure 1. Detail of the operation of one filament. Based on ref 3.

^{*} To whom correspondence should be addressed. Fax: 55 11 3031 3020. Tel.: 55 11 3091 2252. E-mail: mtaqueda@usp.br.

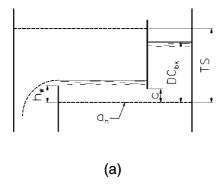


Figure 2. (a) Single-pass sieve tray and (b) effective weir length.

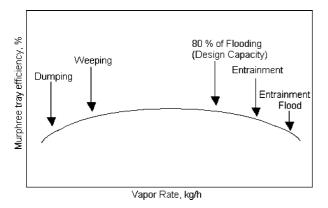


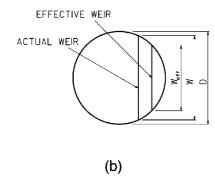
Figure 3. Tray performance by Murphree efficiency's determination. Source:

2. Justification

The sieve trays provide a low efficiency for the absorption operations, as well as reduced operating flexibility. The Murphree efficiency is determined by empirical expressions that analyze the performance of the sieve trays in relation to several possible phenomena, depending on the gas and liquid streams, their flow rates, operating conditions, and physical properties. The geometry of the trays also plays a role, including the internal column diameter (D); the tray spacing (T_S) ; the number of passes of the liquid over the tray; the downcomer area; the active area $(A_{\rm A})$, which is area of the column minus the downcomer area; the hole percentage (a_h) , which is the total hole area in relation to the active area; the clearance between the bottom edge of the downcomer and the trays (c); the weir length (W and W_{eff} , for bent downcomers); the weir height $(h_{\rm w})$; the liquid height in the downcomer (DC_{bk}); and so on. Figure 2 illustrates some of these parameters.

Figure 3 shows the performance diagnosis of trays by determining the Murphree efficiency.

To achieve reasonable operating absorption efficiency, typical calculation recommendations⁸ are to design sieve trays for 80% flooding, providing the maximum Murphree efficiency, assuming that the operation of absorption columns with trays is governed by the liquid stream. Therefore, the required condition to guarantee turbulence over the trays and efficient mass and energy exchange between the liquid and gas streams is to have enough liquid over the tray to provide hydrodynamic equilibrium, considered as a determined gas stream. For the gas stream, this means the imposition of a static pressure drop, due to the liquid height over the trays, and a dynamic pressure drop, due to the passage of gas through the holes of the trays, as well as the movement of the liquid over the trays, in the downcomers, and through the clearance between the downcomers and the trays.



For acetone recovery of the gas stream obtained during cellulose acetate spinning, the flow rates are high, because of the low acetone content. Consequently, the use of sieve trays implies excessive energy consumption, making the process even more expensive.

Moreover, as described above, because of their limiting characteristics, sieve tray absorption columns, for the studied operation, constitute a bottleneck. In contrast, internals, which present a lower pressure drop, are a solution for the issue of increasing the volumetric capacity.

Structured packing consists of thin metallic corrugated strips placed vertically in the upward flux of the gas stream. The strips are continuously grooved and discontinuously perforated, being welded at the edges, resulting in the reasonably rigid spatial structure of a beehive. They are supplied in layers of about 190mm height, split in circular segments to allow assembly at the column. Each layer is assembled with a gap of 45° in relation to the previous layer.9

The distribution of liquid, fed at the top of the column, is guaranteed by a high-performance distributor tray, provided with uniformly distributed holes, above the packing surface, through which the liquid flows, equally fed over the tray by branches leaving the main feed pipe. The gas stream flows from the distributor tray through the risers, which have a large free area, guaranteeing a minimal pressure drop. The liquid fed over the packing bed forms a very thin and continuous skin over the grooved surface of the strips, flowing by gravity, thanks to the suitable bend of the grooves. Upon reaching the holes, the liquid changes direction axially. When the liquid reaches the bottom of a layer, there is a new change of direction, because of the assembly gap. These direction changes provide the required turbulence to the process, but without causing a pressure drop for the gas stream, which governs the process using this sort of internal system, making it suitable for situations where high gas flow rates are involved, as well as for its remarkable operating flexibility.⁹

It is therefore justifiable to study the replacement of sieve trays by structured packing for the described use in the present work.

3. Methodology

The proposed method consists of specifying the absorption of the acetone from the stream obtained during spinning, in water, from a column provided with sieve trays and a second equipped with structured packing. The inner diameter and height of the trays were both kept constant, so that the performances could be compared, mainly in terms of flow rate and pressure drop.

To do so, it is necessary to establish the local conditions¹⁰ of the original situation, setting a coherent simulation with data

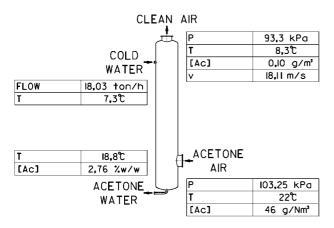


Figure 4. Schematic representation of the local conditions.

taken from the normal operation of an absorption column provided with sieve trays. Local conditions mean the modeling by any means of scientific calculations that reliably reproduce the studied operating situation.

The establishment of the local conditions consists of the steps described in the following sections:

a. Performance of Possible Measurements. The studied absorption column has available only the measurement of the volumetric flow rate (m³/h) of the feed of cold water, a stream for which it is also important to measure the feed temperature (°C).

For the other feed stream of air containing acetone from the spinning diluted at the machines' collectors, only the acetone concentration (g/Nm³), temperature (°C), and pressure (mmwc) are measured, after the stream has been chilled in the radiator

For the exiting liquid stream, i.e., the aqueous acetone solution, the acetone mass concentration (wt %) and temperature (°C) are measured.

Finally, for the exiting gas stream, i.e., the washed air, the acetone concentration (g/m³), temperature (°C), local barometric pressure (mm Hg absolute), and velocity of air leaving the outlet piping (m/s) are measured.

Figure 4 indicates all of the measurements performed.

b. Establishment of a Mass Balance. The measurements of the acetone air and cold water streams indicated in Figure 4, in addition to those for the pressure and velocity of the clean air stream, provide the input data for the mass balance, which is started by the exit gas stream, from the velocity measured using an anemometer, which also measures the temperature, taking several readings for both. As the diameter of the outlet nozzle is known, it is possible to determine the volumetric flow rate. A flame ionization detector, compared to accurate standards, was used to measure the acetone concentration. Because of the negligible acetone content, the water concentration and density of this stream can be obtained from a standard chart for the barometric pressure and temperature. By subtracting the acetone and water mass flow rates, the mass flow rate of air at the exit stream can then be calculated.

For the feed stream, it is assumed that the air mass flow exiting by the top is identical to the feed, which is not far from reality, considering the extremely low solubility of air in water.

Through partial and overall mass balances of the streams, considering the ideal gas behavior to be valid for both the feed and outlet gas streams, it is possible to establish the material balance, applying an iterative method with corrections, as the measurement of the velocity of air leaving the column is not sufficiently reliable. On the other hand, the flow rate, temperature, and density measurements for the cold water stream, as well as the determinations of the acetone concentration, temperature, and density of the bottom stream, are reliable, helping to establish the balance. The iterative method compares the mass data obtained from the velocity with those obtained from the acetone concentration. At every iteration, the ideal velocity of the gas exit stream is obtained; this value is again reinserted into the spreadsheet, and all variables are recalculated. The difference between values obtained from the velocity and from the concentration constitutes the error, which is minimized by the mass balance.

c. Thermodynamic Simulation. The results of the overall mass balance are used for the modeling of the absorption operation, using the data for the inlet streams, the acetone air from spinning after it has been cooled at the radiator, and the cold water. For the first, the mass flow rate, composition, temperature, and pressure are provided, and for the second, the volumetric flow rate and temperature are provided. The outlet pressure is also known, in this case the local barometric pressure.

The acetone concentrations in the outlet streams are obtained from the manual adjustment of the number of theoretical trays $(N_{\rm T})$, in such a way that the results expressed for the outlet streams, in addition to the temperature and flow rate, are sufficiently close to the measured values.

The number of theoretical trays can be given or calculated, determining the Murphree efficiency, or it can be both given or calculated, by choosing an initial number, performing the first check through the simulation, and obtaining a complete set of hydraulic data for each theoretical tray, with which is possible to improve the accuracy of the determination of the Murphree efficiency. The local conditions of the original situation are achieved when the results of the simulation obtained by the established model match the real operating conditions obtained from the measurements, according to the detailed method.

A hydrodynamic counterpart is performed using the rating mode of the simulator, providing the geometric characteristics of the trays and obtaining as a result, the tray's performance in terms of flooding over the tray and at the downcomer, pressure drop per tray, and so on. To confirm the rating obtained from the hydraulic data available for every tray and for both phases, a hydrodynamic rating of the trays can be performed using other methods issued by reference centers⁸ or using available software from different suppliers.

To perform the thermodynamic simulation, the consistency of the vapor-liquid equilibrium must be achieved. Intermolecular forces of nonspherical molecules depend not only on the distance between their centers, but also on their relative orientation, which is shown, for instance, by their boiling points in relation to their molecular weights. In addition to these physical forces, there are chemical forces that lead to the formation of new molecular species, frequently changing the thermodynamic properties of the mixtures, resulting, in the case of vapor-liquid equilibrium, in deviations from ideality caused by changes in the volatilities of the original components with consequent impacts on their fugacities. Hydrogen bonds constitute the most common effect of chemical interactions in the thermodynamics of the solutions, because, even though they are weaker than covalent bonds, they reduce the distance between the centers of the bonded molecules, increasing the polarity and frequently persisting in the vapor form.¹¹

Acetone and water are known for showing a nonideal vapor-liquid equilibrium, explained by their molecular structures: Water has a high polarity, because of the angle between the hydrogen and oxygen bonds in addition to the high electronegativity of the oxygen, resulting in the occurrence of the hydrogen bonds, which explains the high boiling point of the water despite its low molecular weight. Acetone has an oxygen atom with a double bond to a carbon atom, which does not allow for the formation of hydrogen bonds, and exhibits a low polarity, resulting in a relatively low boiling point. In mixtures, the acetone molecules break the hydrogen bonds between the water molecules, forming new hydrogen bonds between their molecules and those of water, resulting in vapor-liquid equilibrium behavior with a positive deviation from ideality, characterized, for pressures close to atmospheric, by behavior according to Henry's law for the most volatile compound, acetone. For the present study, this is clear in the region of low acetone content, where the acetone behaves as any other dissolved gas. Consequently, every component at the liquid phase interferes in the behavior of the other, and specifically, the presence of the components of air in the absorption system interferes with the vapor-liquid equilibri-

The modeling of vapor-liquid equilibrium for systems such as the one studied here requires skill in dealing with the deviations from ideality in both phases.

The nonideality of the liquid phase of mixtures is mathematically determined by the analysis of the fugacities expressing their excess functions, which relate the properties of the real solutions to those of the ideal solutions through the determination of the activity coefficients, which are used in the equation for the Gibbs energy, the accuracy of which depends on the composition and the variability of the coefficients with temperature. However, even if the data are highly accurate, the results are only approximate because, without additional information, equations with two adjustable parameters are very limited, as is the case for equations such as van Laar, Margules, Wilson, and UNIQUAC. To better describe the nonideality of the liquid phase of mixtures, an expression with more than the two binary parameters is required for the calculation of the Gibbs energy. This is the case for the NRTL equation, which best fits nonideal liquid mixtures, through the adequacy of the nonrandomness parameter, which takes into account only the nature of the system, providing the required flexibility to represent the excess forms of the Gibbs energy, constituting the most simple equation with the best theoretical basis, with very accurate results, applicable for binary, ternary, and multiple systems.11,12

The nonideality of the vapor phase of mixtures is corrected by the determination of the partial fugacity of the components, which expresses the dependency of the molecular interactions through the virial equation of state, which consists of an exponential series of the molar densities where the virial coefficients depend on the molecular interactions. The equation is usually truncated at the second virial coefficient as the data for it are much more plentiful and accurate. Therefore, the corrections for the nonideality of the vapor phase of a mixture are calculated from empirical correlations of the second virial coefficient. 11 The methods originally used to perform this correction presented the disadvantage of requiring parameters obtained from data or providing results are that too inaccurate to be acceptable. The advantage of the Hayden-O'Connell model is that the prediction of the second virial coefficient uses only the critical properties and the molecular parameters, both derived from the molecular structure, so that it is a much more accurate method. This accuracy is even improved by taking into account several components that have an influence on the molecular interactions, such as those that take place in the free state, metastable equilibrium, and physically and chemically bound states, confirming that the nonideality of the vapor phase of mixtures affects mainly the heavier compound.¹³

There are positive reports about the combined use of the Hayden-O'Connell equation with the NRTL equation, where the former is used for the correction of the nonideality of the vapor phase of a mixture, through the adequacy of the second virial coefficient, and the latter is used for the correction of the liquid phase. Such an approach is advantageous for mixtures where the deviation of the vapor phase is even more significant, because of the occurrence of dimerization, therefore much more remarkable than the described complexing for the studied binary system^{14,15} or other references, reporting the combination of the Hayden-O'Connell equation for the vapor phase, with several models for correcting the nonideality of the liquid phase (Margules, van Laar, Wilson, UNIQUAC, and NRTL), concluded by the better performance of the combination of the NRTL and Hayden-O'Connell equations. 16,17 Finally, there is a report about the use of the combination of the NRTL and Hayden-O'Connell equations for process development as a reliable source of data.18

Consequently, to obtain satisfactory results for the situation studied here, the combination of the NRTL and Hayden-O'Connell equations was used to establish the local conditions.

Several commercial simulators are provided with databases containing physical properties of the chemical compounds and models for calculating phase equilibria and reproducing ordinary unit operations. Aspen Plus has proven models for equilibrium staged operations, as well as a comprehensive collection of models for vapor-liquid equilibrium, conjugated to parameters of the binary water-acetone system, taken from the database.

The transposition from the tray configuration to that with packing is then initiated from data extracted from the simulation constituting the local conditions. The several packing suppliers have developed their own correlations, usually empirical, which is the case for Interpacking.9 The height of the packed bed in an absorption column can be calculated by the equation

$$H = \frac{N_{\rm A}}{k_{\rm G} a P_i Y_{\rm lm}} \tag{1}$$

where P_i is the partial pressure of vapor of the absorbed component (kPa), Y_{lm} is the average logarithmic molar fraction, and $k_{\rm G}a$ is the mass transport coefficient [kg mol/(kPa m³ $Y_{\rm lm}$)]. $Y_{\rm lm}$ is expressed as

$$Y_{\rm lm} = \frac{(Y_{\rm i} - Y_{\rm o})}{\ln(Y_{\rm i}/Y_{\rm o})} \tag{2}$$

where Y_i is the inlet molar fraction of the absorbed vapor, Y_0 is the outlet molar fraction of the absorbed vapor, and k_Ga is empirically given by

$$k_{\rm G}a = C_1 C_2 (L')^{0.17} (F_{\rm S})^{C_3} (P_i)^{-0.21}$$
(3)

In eq 3, C_1 is an empirical constant for the studied binary system (acetone/water); C_2 is an empirical constant for the type of packing and its dimensions; C_3 is an empirical constant for the type of process (governed by the liquid or by the gas); L' is the liquid flow rate for the column transversal section $[m^3/(m^2 h)]$; P_i is the partial pressure of vapor of the absorbed component (kPa); and F_S is the kinetic factor of the gas phase (m/s), expressed as

$$F_{\rm S} = v(d_{\rm g})^{0.5} \tag{4}$$

where v is the velocity of the gas phase (m/s) and d_g is the density of the gas phase (kg/m³).

The simulation model for the local conditions supplies all of the required process and hydraulic data to satisfy eqs 1-4 tray by tray. This includes the molar and mass compositions of the liquid and gas streams and the volume and mass flow rates of both streams, as well as their physical properties and operating conditions characterizing the vapor—liquid equilibrium. Using eq 1, it is possible to calculate the height of one mass-transfer unit, or one theoretical tray, designated as HTO_G , as the studied process (acetone absorption in water using packing) is governed by the turbulence of the gas stream and by the partial pressure of the acetone. As the calculation is performed tray by tray, the average value of HTO_G is determined.

Using this value and keeping the number of theoretical trays of the local conditions, the corresponding height of packing bed is obtained, which is much smaller than that occupied by the trays. Also, keeping the same flow rate, pressure, and temperature as in the original simulation for the acetone air feed stream, as well as those for cold water feed stream, the simulation was repeated in rating mode. In this case, the geometrical characteristics of the packing were provided, and the result was the packing performance, expressed as a percentage of the maximum operating capacity (MOC) and the pressure drop as a function of packing height. It is important to explain that, to keep the advantageous features of low pressure drop using packing instead of trays, the usual recommendation is that the percentage of the MOC should not exceed 70%. Both values much lower than this reference value and low pressure drops by packing height indicate low turbulence for the gas stream, compromising the efficiency. Another important parameter of the proposed configuration is the liquid rate (L'), which needs to be at least 10 m³/(m² h), to guarantee that the absorption of acetone in water occurs.

This is exactly what happened. Initially, to achieve an accurate simulation model, the pressure of the clean air stream was corrected considering the low pressure drop, but indicative of low turbulence for the gas stream, as previously mentioned. The obtained low percentage of the MOC indicated that the gas stream flow rate would need to be increased. The calculation for L' also indicated an insufficient water flow rate.

In this way, the second simulation model is established, always referred to the rating mode, increasing the feed flow rate of the stream generated in the spinning, keeping the acetone concentration, and increasing the feed flow rate of cold water in such a way that the acetone concentration at the top of the column top remained constant. The gas stream is increased so as to obtain 100% of the MOC, in the rating mode, as already described, thus resulting in a greater pressure drop. This step is concluded by the correction of the pressure of the gas outlet stream. From this second model, the calculation of the height of one mass-transfer unit, HTO_G, is repeated, giving a greater value because of the excessive pressure drop. Even so, the structured packing bed height is less than half of the height occupied by the original trays. It is important to observe that L'is much higher than the recommended value. It is also important to observe that, because of the increase of the gas feed stream, the pressure drop in the radiator cooler increases considerably.

With the conservative results of the second model, the number of possible theoretical trays is then calculated, considering that the height of the structured packing bed is the same as that occupied by the original trays, always considering the same column diameter. The conclusion is that the number of theoretical trays is doubled. Considering this value, the third simulation model is established, always in the rating mode, increasing the feed flow rate of the gas stream even more, in order to achieve 100% of the MOC. As the pressure drop at the packing bed is the maximum of the proposed configuration, this step is concluded by correcting the pressure of the gas outlet stream. The same procedure as already described is followed for the calculation of the height of one mass-transfer unit, HTO_G , this time confirming the previous value and guaranteeing the accuracy of the method, although it should be noted that, with twice as many theoretical trays, the calculation method is even more accurate. Also note that the remarks related to L' and the excessive pressure drop at the radiator cooler are still valid.

Keeping the value for the height of one mass-transfer unit, $\rm HTO_G$, calculated and confirmed through the second and third models, the feed flow rate of the gas stream is reduced in such a way that 70% of the MOC is achieved. The pressure of the outlet gas stream is corrected, having in mind that the pressure drop is smaller. In the same way as performed for the previous models, this fourth model follows the described calculation procedure, which, although resulting in a different value than the previous calculations, does not allow the number of theoretical trays to increase; that is, the difference is less than one entire theoretical tray, once again confirming the accuracy of the calculation method. The obtained value of L' is rather close to the recommended value, but the pressure drop in the cooling radiator continues to be excessive.

Keeping the value for the height of one mass-transfer unit, HTO_G , the fourth model is repeated, simulating the elimination of the cooling radiator, because of its excessive pressure drop, adjusting the feed flow rate of the gas stream in such a way that 70% of the MOC is preserved. As in all previous models, the outlet gas stream pressure is adequate but much smaller because of the removal of the radiator. Once again, the described calculation procedure is repeated, yielding the same value as obtained from the previous model, which is then adopted as the final value. Because of the increase of the temperature of the gas feed stream, the L^\prime value increases slightly but continues to be close to the recommended value.

It is important to conclude this section by indicating that the HTO_G values calculated by the described methodology were compared to values given or calculated for the absorption of acetone in water, indicated in references traditionally used in the industry, $^{19-21}$ and they were found to be satisfactory.

4. Discussion of the Methodology's Validation

As detailed at the beginning of the description of the methodology, the effectiveness of the proposed method was tested by a comparison between a column with structured packing specified from a column equipped with sieve trays, keeping constant both the internal diameter and height occupied by the trays, comparing their performances mainly in terms of flow rate and pressure drop. Table 1 presents the complete comparison, not only restricted to these control parameters, for all of the described steps of development of the proposed methodology.

The majority of the described characteristics of the methodology is presented in Table 1, as the number of theoretical trays, rating, operating conditions, and acetone concentration in the involved streams. The liquid flow rate (L'), also referred to in the description of the methodology, is an important parameter for evaluating the column's performance, as explained in Table 1. Another parameter included in Table 1 is the kinetic energy factor (F_S) , which is determined in the inlet and outlet nozzles of the gas streams and guides their adequate sizing, as they are

Table 1. Validation of the Froposed Methodology	posed intelliodology						
simulation description of internals characteristic dimension	ation of internals c dimension	original local conditions 30 2-pass sieve trays 260 mm TS	original packing structured packing ^a 2926 mm BH	PMC structured packing ^a 3577 mm BH	PMC structured packing ^a 7785 mm BH	POC structured packing ^a 7785 mm BH	POC without cooler structured packing" 7785 mm BH
			Process Data				
feed streams	•	expt^b	$modeling^c$	confirmed modeling c	$modeling^c$	$modeling^c$	$\operatorname{modeling}^d$
to column	volumetric flow rate (m^3/h)	11590	<i>TTT</i> 21	37191	38808	28462	28919
	[Ac] (g/Nm ³)	64.98	58.94	62.22	64.06	59.65	56.10
	temperature (°C)	31	31	31	31	31	50
	pressure (kPa)	103.47	93.86	101.02	102.02	94.99	94.89
to gas cooler (fed at 50 °C)	volumetric flow rate (m^3/h)	11955	13125	36055	40429	28749	I
	pressure (kPa)	106.58	80.76	107.85	109.24	99.92	I
cold water (fed at 10 °C)	flow rate (m^3/h)	18.63	19.46	60.42	56.34	39.80	40.72
		Main (Main Characteristics of Outlet Streams	t Streams			
qot	$[Ac]_{clean air} (g/m^3)$	0.24	0.24	0.24	0.24	0.24	0.24
bottom	[Ac]acetone/water (% w/w)	3.79	3.64	3.67	4.12	3.99	3.74
		Th	Thermodynamic Characteristics	istics			
no. of theoretical trays	etical trays	7	7	7	15	15	15
		H	Hydrodynamic Characteristics	istics			
rating: sieve trays (% flooding) - packing (% MOC)	ling) - packing (% MOC)	70.65	32.04	100	100	70	70
pressure drop through column internals (kPa)	column internals (kPa)	06.6	0.29	6.79	7.78	1.42	1.32
liquid flow rate $[m^3/(m^2 h)]$	$e^{e} [m^{3}/(m^{2} h)]$	ı	5.75	17.82	16.63	11.75	12.02
gas kinetic factor at inlet nozzle ^f (m/s)	t inlet nozzle ^f (m/s)	17.96	18.86	61.63	59.91	18.20	17.93
gas kinetic factor at outlet nozzle ^f (m/s)	outlet nozzle ^f (m/s)	17.13	17.13	56.02	56.60	16.65	15.90
total pressure drop through system (kPa)	rrough system (kPa)	13.46	4.03	16.69	18.09	6.77	1.75

Table 1. Validation of the Proposed Methodology

^a Europack 250Y from Interpacking. ^{9 b} Experimental data or results from geometric data of the original sieve-tray configuration. ^c Results from modeling. ^d Results from modeling confirmed at the implemented structured packing column. ^e For absorption, >10. ^f For absorption, <20.

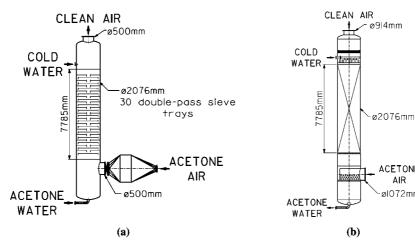


Figure 5. (a) Sieve tray column with cooling radiator and (b) packing column.

Table 2 Summary of Savings

description	% saving (per item)	explanation
increase in production capacity	4	increase in volume capacity of acetone air absorption
reduction in electric power consumption for moving the acetone air generated at spinning toward the absorption columns	34	reduction in pressure drop allows replacement of three blowers of 15 kPa pressure elevation by one of 5 kPa; less pressure elevation decreases noise, improving comfort
reduction of acetone losses	35	increase in process efficiency and improvement of aspiration, due to the implementation of the proposal; lower VOC emissions
reduction in steam consumption at acetone distillation and electric power consumed at the chilling of recycled water to absorption	10	efficiency improvement increases acetone concentration of the resulting absorption's acetone/water mixture, indicating that the heating is direct, by injection of live steam
reduction in maintenance costs	22	replacement of four old columns, eliminating the corresponding cooling radiators, in addition to the use of blowers of lower pressure elevation, requiring lower-power electric motors

required to increase, as is the interconnecting piping. This makes the obtained reduction of the pressure drop by adopting the proposal of replacing trays by structured packing effective throughout the overall installation.

Although Table 1 reproduces the description of the proposed methodology, allowing it to be visualized, the conclusive test is to compare the first and last columns of the table, namely, the column referring to the local conditions of the original configuration of the absorption column provided with sieve trays and the column referring to the optimized proposed condition, provided with structured packing and without the feed cooling radiator. Figure 5 schematically presents this comparison.

As the objective of the study was to solve the installation's bottleneck, constituted by a lack of absorbed volume, by comparing the original volume flow rate with that of the proposed method, it is possible to see that the proposal results in an increase of approximately 150%, with an 85% reduction in the pressure drop, meaning a remarkable reduction in energy consumption. Table 2 summarizes the percent savings in terms of the proportional costs.

ACETONE

øI072mm

The remarkable previewed savings obtained by using the described methodology justify the investment's authorization, thanks to its quick amortization, confirmed by the successful implementation of the proposal.

5. Conclusion

The proposal of replacing sieve trays by structured packing for the described application was found to be valid, and the described methodology proved to be effective in allowing the successful implementation of the proposal.

Acknowledgment

Rhodia and the Chemical Engineering Department of the University of São Paulo's Polytechnic School are acknowledged for supporting the development of the research project of R.N.'s doctoral degree.

Nomenclature

 $A_{\rm A}=$ active area

 $a_{\rm h} = {\rm hole\ percent}$

c = clearance between downcomer and tray

 C_1 = empirical constant for the studied binary system (acetone/

 C_2 = empirical constant for the type of packing and its dimensions

 C_3 = empirical constant for the type of process (governed by the liquid or by the gas)

 $DC_{bk} = downcomer backup$

 $d_{\rm g} = {\rm density} \ {\rm of the gas \ phase} \ ({\rm kg/m^3})$

 $F_{\rm S}$ = kinetic factor of the gas phase (m/s)

 $h_{\rm w} = {\rm weir \ height}$

H = packing bed height (m)

 $k_{\rm G}a = {\rm mass\text{-}transport\ coefficient\ [kg\ mol/(kPa\ m^3\ Y_{\rm lm})]}$

 $L' = \text{liquid flow rate for column transversal section } [\text{m}^3/(\text{m}^2 \text{ h})]$

 $N_{\rm A} = \text{molar flux [kg mol/(m}^2 \text{ h)]}$

 $N_{\rm T}$ = number of theoretical trays

 P_i = partial pressure of vapor of the absorbed component (kPa)

 $T_{\rm S} = {\rm tray \ spacing}$

v = velocity of the gas phase (m/s)

W = weir length

 $W_{\rm eff} = {\rm effective \ weir \ length}$

 Y_i = inlet molar fraction of the absorbed vapor

 $Y_{\rm lm}$ = average logarithmic molar fraction

 Y_0 = outlet molar fraction of the absorbed vapor

BH = bed height

MOC = maximum operating capacity

PMC = packing maximum capacity

POC = packing optimal capacity

VOC = volatile organic compound

Literature Cited

- (1) Ullmann's Encyclopedia of Industrial Chemistry, 5th ed.; VCH Verlagsgesellschaft: Weinhein, Germany, 1994; Vol. 5A.
- (2) Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed.; John Wiley & Sons: New York, 1984; Vol. 5.
- (3) Miller, C. Effect of Filament Drawdown on Aerodynamic and Heat Transfer in Fiber Spinning. *AIChE J.* **2004**, *50* (5), 898.
- (4) Lepeniotis, S.; Feuer, B.; Bronk, J. Phase Systems of Starch Acetate and Cellulose Acetate in Acetone: Water. *Chemom. Intell. Lab. Syst.* **1998**, 44, 293.
- (5) Henley, E. J.; Seader, J. D. Equilibrium-Stage Separation Operations in Chemical Engineering; Wiley: New York, 1981.
- (6) Treybal, R. E. *Mass-Transfer Operations*; 3rd ed.; McGraw-Hill: New York, 1980.
- (7) Humphrey, J.; Keller, G. Separation Process Technology; McGraw-Hill: New York, 1997.
 - (8) Sieve Tray Design; Fractionation Research Inc.: Stillwater, OK, 1966.
- (9) Riemer, H. *Interpacking's Electronic Brochure*; Interpacking: São Paulo, Brazil, 2007; www.interpacking.com.br.
- (10) Bird, R. B.; Stewart, W. E.; Lightfoot, E. N. *Transport Phenomena*; John Wiley & Sons: New York, 2002.
- (11) Prausnitz, J. M.; Lichtenhaler, R. N.; Azevedo, E. G. *Molecular Thermodynamics of Fluid Phase Equilibrium*; Prentice-Hall: New York, 1999.

- (12) Renon, H.; Prausnitz, J. M. Local Compositions in Thermodynamic Excess Functions for Liquid Mixtures. *AIChE J.* **1968**, *14* (1), 135.
- (13) Hayden, J. G.; O'Connell, J. P. A Generalized Method for Predicting Second Virial Coefficients. *Ind. Eng. Chem. Process Des. Dev.* **1975**, *14* (3), 209.
- (14) Zhicai, Y.; Xianbao, C.; Jing, G. Esterification—Distillation of Butanol and Acetic Acid Method for Predicting Second Virial Coefficients. *Chem. Eng. Sci.* **1998**, *53* (11), 2081.
- (15) Bernatová, S.; Aim, K.; Wichterle, I. Isothermal vapour-liquid equilibrium with chemical reaction in the quaternary water + methanol + acetic acid + methyl acetate system, and five binary subsystems. *Fluid Phase Equilib.* **2006**, *247*, 96.
- (16) Yu, Y.-X.; He, M.-Y.; Gao, G.-H.; Li, Z.-C. Boiling Point for five binary systems of sulfolane with aromatic hydrocarbons at 101.33 kPa. *Fluid Phase Equilib.* **2001**, *190*, 61.
- (17) Chang, W.; Wan, H.; Guan, G.; Yao, H. Isobaric vapor—liquid equilibria for water + acetic acid + (*N*-methyl pyrrolidone or *N*-methyl acetamide). *Fluid Phase Equilib.* **2006**, 242, 204.
- (18) Wu, Y.-Y.; Zhu, J.-W.; Chen, K.; Wu, B.; Shen, Y.-L. Vapor—liquid equilibria for the binary mixtures of 2,3-butanediol with *n*-butanol, *n*-butyl acetate, and ethyl acetate at 101.3 kPa. *Fluid Phase Equilib.* **2007**, 262. 169.
- (19) Leva, M. *Tower Packing and Packed Tower Design*; The United States Stoneware Company: Akron, OH, 1953.
- (20) Vital, T. J.; Grossel, S. S.; Olsen, P. I. Estimating Separation Efficiency, Part 3—Packed Columns. *Hydrocarbon Process.* **1984**, *12*, 75.
- (21) Green, D. W. Perry's Chemical Engineers' Handbook; McGraw-Hill: New York, 2007.

Received for review April 23, 2008 Revised manuscript received August 6, 2008 Accepted August 12, 2008

IE800612E