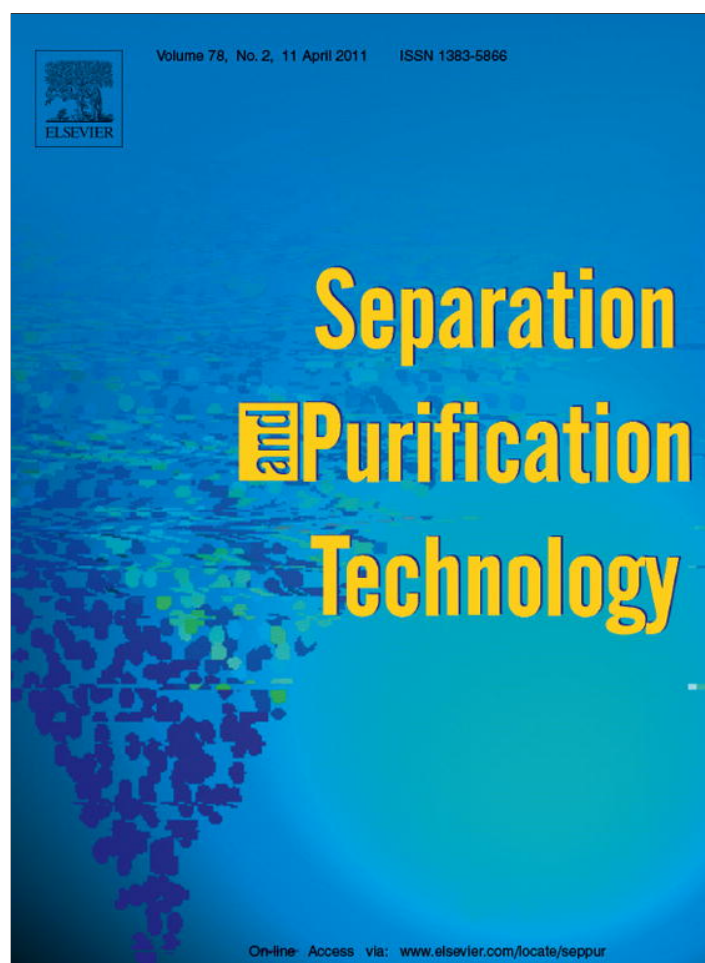


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Feasibility analysis of isopropanol recovery by hybrid distillation/pervaporation process with the aid of conceptual models

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ABSTRACT

In this contribution, main results of a techno-economic feasibility study to recover spent isopropyl alcohol (IPA) from a pre-treated waste stream composed by IPA (95.64 wt.%) and water (4.36 wt.%) are presented. Based on conceptual models for the unit operations, a quasi-optimal design for a hybrid process combining pervaporation and distillation is found under process specifications given by a pharmaceutical company. The proposed procedure allows a separated design of each unit with the aid of conceptual models. While distillation is evaluated from pinch theory, the conceptual model for pervaporation considers that the maximum driving force (i.e., no liquid temperature drop) is maintained across the membrane unit.

A brief performance comparison for different membranes is also performed as part of the assessment to the company. For this purpose, the pervaporation separation index (PSI index) defined as the product of the permeate mass flux and the separation factor was used for membranes for which either literature data or membrane supplier brochures were available. In the case of the membrane PERVAP 2216 from Sulzer, several pervaporation experiments at 80 °C and permeate pressure of 1.52 kPa were carried out. The PSI index was then redefined as the overall separation factor times the inverse of the minimum membrane area required to perform a given separation.

The results obtained emphasize the usefulness of conceptual modeling in all steps of process design.

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1. Introduction

Organic solvents are widely used in pharmaceutical companies for carrying out the process reactions and crystallizing the product. Solvent recovery is mandatory in order to fulfill environmental regulations while minimizing raw material costs.

Among other alternatives like azeotropic distillation [1] and extractive distillation [2], hybrid processes comprising distillation and membrane separation [2] are emerging as suitable choices, mostly due to the independence presented by the separation performance of membrane technologies with the phase equilibrium. Hence, the hybrid process is able to overcome azeotropic compositions of azeotrope forming waste streams while reducing the energy demand of the distillation task [3]. Moreover, the hybrid process distillation/pervaporation does not only present best economical figures when compared with the alternatives distillation plus extractive distillation [2] and azeotropic distillation [4] but also avoids the need of an entrainer to break the azeotrope.

While feasibility of pervaporation in removing water from isopropyl (IPA) alcohol in aqueous mixtures has been subject of many thorough investigations (see Refs. [5–7] for hydrophilic membranes based on polyvinyl alcohol and the paper of Urriaga et al. [8] for an exhaustive list of relevant contributions in this field), only a limited number of research studies have been carried out to demonstrate the economical viability of the hybrid process [2,4].

In this contribution, main results of a techno-economic feasibility study to recover spent isopropyl alcohol (IPA) from a pre-treated waste stream composed by IPA (95.64 wt.%) and water (4.36 wt.%) are presented. Main process specifications given by the pharmaceutical company were: (i) plant capacity of 1300 m³/year, (ii) IPA purity in product stream above 99.7 wt.%; (iii) IPA content in the waste stream below 0.00417 wt.% (COD 100 mg/l), and (iv) production scheduling: monthly continuous runs of 20 consecutive days.

Due to the low water content in the process feed (pre-treated waste stream), a two steps process was selected to recover the spent solvent. A first step consisting on pervaporation with a hydrophilic membrane to achieve a retentate stream rich in alcohol followed by a distillation step to recover IPA losses in the permeate stream.

In order to generate different designs, a mass balance through the whole process is performed first to calculate both retentate and column bottom flow rates. Then, mass balances for five feasible

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alternatives are calculated by selecting different values for the mole fraction of the feed to the pervaporation sector (the pre-treated waste stream fed to the process plus the recycle from the column top), which was selected as the optimization variable to cover the degree of freedom left for specification.

The proposed procedure allows a separated design of each unit with the aid of conceptual models. While distillation is evaluated from pinch theory [9], which leads first to the calculation of the minimum energy demand and then to the estimation of the number of stages via the well-known McCabe–Thiele method, the membrane unit performance is obtained integrating the rigorous mass transfer model for the commercial membrane CMC-CF-23 from Celfa [8]. However, as suggested in [3], the model integration is done by considering the maximum driving force (i.e., no liquid temperature drop) at each volume element to obtain the minimum membrane area needed for separation. Actual membrane area is approximated by multiplying the minimum membrane area by a fixed factor of 1.25.

As a result, a quasi-optimum design taking into account both operation and investment costs is found. In addition, a feasible design for both the membrane unit (i.e., number of modules and, area and temperature drop per module) and the distillation column (i.e., reflux ratio, column diameter and packing height) is shown.

Finally, a brief performance comparison for different membranes is also performed as part of the assessment to the company. To do this, the pervaporation separation index (PSI index) defined as the product of permeate mass flux and separation factor was used for membranes for which either literature data or membrane supplier brochures were available. In the case of the membrane PERVAP 2216 from Sulzer, several pervaporation experiments at 80 °C and permeate pressure of 1.52 kPa were carried out. The PSI index was then redefined as the overall separation factor times the inverse of the minimum membrane area required to perform a given separation. Thus, the concept of maximum driving force developed by Bausa and Marquardt [3] for the design of a pervaporation process is used to allow a proper comparison of the performance of different polymeric membranes.

While the feasibility analysis of the recovery process is the main objective of this contribution, usefulness of the conceptual modeling approach in every step of the process design is also emphasized along the paper.

2. Process description and scheduling

The fresh feed is pre-treated in an evaporator-crystallizer [10] in order to recover a crystalline medicinal product by separating it from the IPA-rich stream. This train operates continuously for IPA, with intermittent discharge of solids. As a result of this operation a pre-treated stream F composed by IPA (95.64 wt.%) and water (4.36 wt.%) is obtained.

The pre-treated waste stream F is then fed to the pervaporation sector to achieve a retentate stream R with an IPA content of 99.7 wt.%. The condensed permeate stream P is diverted to a distillation column that separates it into a water-rich bottom W with traces of alcohol (COD 100 mg/l) and an IPA-rich distillate D , which is recycled to the membrane unit as shown in Fig. 1.

The production schedule suggested by the company of monthly continuous runs of 20 consecutive days gives rise first to a ten-day accumulation period of the pre-treated waste and then to a continuous operation of the pervaporation unit during the following twenty days. As a result, the capacity of the pervaporation unit must be ca. 6000 l/day to process all the waste generated in a month. Due to the low permeate flow rate, the production schedule for the distillation section is to continuously process the entire amount

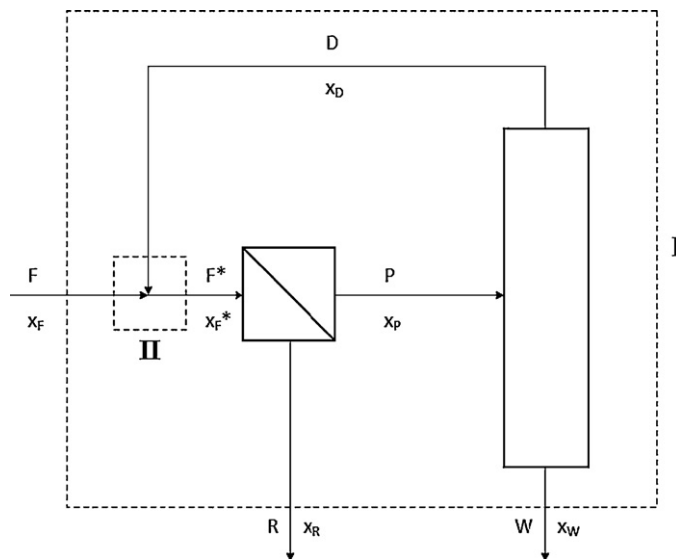


Fig. 1. Schematic representation of the hybrid process. The retentate R and bottom W flow rates are calculated by a material balance for the whole process (Envelope I). The composition x_F^* is selected as the optimization variable.

produced at the permeate side during a month in one single day. In this way, the column diameter will be above 4 in., the minimum value suggested by a local contractor.

In this paper we will focus our attention in the main recovery process formed by the pervaporation unit and the distillation column.

3. Generating possible designs

In order to generate different designs, a mass balance through the whole process (Envelope I in Fig. 1) is performed to calculate both the retentate flow rate R and the column bottom flow rate W from known or specified values of the waste feed flow rate F (3.61 kmol/h) and the composition of feed x_F (86.8 mole%), retentate x_R (99 mole%), and bottom product x_W (0.001250 mole%).

A degree of freedom analysis [3] shows that one degree of freedom remains unspecified. We select the composition x_F^* of the feed to the membrane sector (the pre-treated waste stream fed to the process plus the recycle from the column top) as the degree of freedom to generate possible alternatives. Table 1 shows the mass balances corresponding to six possible designs calculated from different values of the feed composition to the pervaporation unit. Calculation details are given in the following sections. The composition for the first design equals the composition of the pre-treated waste stream in order to consider an alternative without distillation. For the remaining alternatives the feed composition will be always below the composition of the pre-treated feed as the distillate composition is limited by the composition of the azeotrope IPA–water (69.75 mole%).

Table 1

Mass balances for six different designs. Feed $F=3.610$ kmol/h, retentate $R=3.165$ kmol/h, and waste water stream $W=0.445$ kmol/h.

Design	F^* [kmol/h]	x_F^*	P [kmol/h]	x_P	D [kmol/h]	x_D
0	3.610	0.868	0.528	0.1360	0.000	0.0000
1	3.730	0.860	0.565	0.1309	0.119	0.6183
2	3.753	0.855	0.588	0.1278	0.143	0.5263
3	3.777	0.850	0.611	0.1249	0.166	0.4593
4	3.824	0.840	0.659	0.1195	0.214	0.3679
5	3.923	0.820	0.758	0.1100	0.313	0.2664

4. Conceptual model for the pervaporation unit

In the typical plate and frame arrangement of a staged pervaporation process a heat exchanger is placed either after a constant temperature drop of the liquid mixture or a constant membrane area. The decrease in the temperature, which results in a decrease of the driving force for the permeation process, is due to the change of state of the permeating components which take their vaporization heat from the retentate liquid. An additional drop in the driving force for the separation is caused by a concentration decrease along the module of the preferentially permeating component in the liquid mixture [11].

Bausa and Marquardt [3] introduced the concept of minimum membrane area, a limiting design requiring an infinite number of heat exchangers for the membrane unit in order to simplify the design process. In this case, the membrane model is integrated by considering the maximum driving force (i.e., no liquid temperature drop) at each volume element of the membrane unit until the composition of the product in the retentate achieves the specified value. Actual membrane area is approximated multiplying the minimum membrane area by a fixed factor of 1.25. Note that in order to account for differences in the performance between laboratory and plant scale and considering that the pressure drop across the modules strongly depends on the module design [11], a value for the “Murphree” efficiency should be assumed. In this work, we set this value to one. To counteract this effect the plant should be operated at a temperature greater than the value used in the conceptual design (80 °C).

As the feed flow rate F^* of a given alternative is unknown, integration of the model from known values of the retentate flow rate R and composition x_R must be performed in the following way:

- (i) integrate the mass transfer model [8] for a normalized value of the feed flow rate $f^* = 1$ kmol/h with mole fraction x_f^* , until the retentate composition x_R specified at the design level is achieved;
- (ii) calculate the values of the minimum membrane area A_{\min} , feed flow rate F^* and permeate flow rate P from normalized values of the area a_{\min} and retentate flow rate r obtained in step (i), and the retentate flow rate R calculated from the mass balance around the whole process:

$$A_{\min} = \frac{R}{r} a_{\min} \quad (1)$$

$$P = \frac{R}{r} (1 - r) \quad (2)$$

$$F^* = \frac{R}{r} \quad (3)$$

Hence, a minimum membrane area can be calculated for each value of the optimization variable x_f^* of the design alternatives shown in Table 1. The algorithm corresponding to step (i) is given in detail in Appendix A and it can be applied to calculate either the minimum membrane area (conceptual design) or the required number of modules (process simulation). Step A.6 is skipped when calculating A_{\min} . Another important aspect of the algorithm is given by the mass balance equation in step A.5. In the case of the conceptual model both equation members must be divided by the unknown value of the flow rate F^* giving rise to normalized values of the membrane area and retentate flow rate. In this case, step (ii) must be done for calculating actual values for A_{\min} , P and F^* (Eqs. (1)–(3)).

Fig. 2(a) shows the minimum membrane area versus the alcohol composition in the retentate obtained from integration of the mass transfer model developed in [8] for the membrane CMC-CF-23 from Celfa at $T = 80$ °C and $P_p = 1.52$ kPa. Fig. 2(b) shows the overall permeate flux versus x_R .

5. Conceptual model for the distillation unit

Minimum reflux situation of the distillation unit is characterized by the intersection at the same point on the equilibrium curve of the operating lines starting at product compositions. For a saturated liquid feed, this pinch composition is equal to the feed composition [9]. Actual number of stages N is calculated via the McCabe–Thiele method with $RR = 1.2RR_{\min}$.

Once the mass balance around the membrane unit is computed, the distillate composition x_D and flow rate D are obtained from the mass balance around the mixer located upstream of the pervaporation sector (see Envelope II in Fig. 1). Finally, the performance calculation of the distillation column can be estimated as the water-rich column bottom (W, x_W) is already known either as specification (x_W) or calculated from the overall mass balance around the plant (W).

Fig. 3(a) and (b) shows the typical McCabe–Thiele diagrams for separation specifications corresponding to design alternatives #1 and #3, respectively. Note that, for design #3 the column is actually a stripper. A simple way to decide between a column with both rectifier and a stripper section or a stripper column, which in turn appears as an alternative column configuration, is resorting to the intersection of the q -line, a vertical line beginning at $[x_p, x_p]$ (because the feed is introduced as a boiling liquid), with the equilibrium line in the diagram xy . Whenever the mole fraction $y_{x_p}^*$ of the light species in the vapor phase, that is in equilibrium with the feed x_p , is greater than the mole fraction of the light component in the distillate x_D , either a stripper or a simple column are feasible choices. In the last case, however, the feed to the column must be introduced to the column as a vapor–liquid mixture; i.e., $0 \leq q \leq q_{\max}$ with q_{\max} defined from:

$$m = \frac{x_D - x_p}{x(x_D) - x_p} = \frac{q_{\max}}{q_{\max} - 1} \quad (4)$$

where m is the slope of the q -line defined in terms of the feed composition x_p , the distillate composition x_D , and its liquid in equilibrium $x(x_D)$. In all the cases where a stripper was a feasible choice, we selected this column arrangement.

6. Calculation of each alternative's performance and process economics

As explained in Sections 4 and 5 by selecting the feed to the pervaporation unit as the optimization variable, the proposed procedure allows a separated design of each unit with the aid of conceptual models. While actual membrane area is approximated by multiplying the minimum membrane area by a fixed factor of 1.25, actual number of stages N is calculated via the McCabe–Thiele method [12] with $RR = 1.2RR_{\min}$. Table 2 summarizes the main equipment design and operating variables. While the membrane performance is characterized by both the dew point temperature of the permeate stream and the area required for the separation, the different designs for the distillation column are given in terms of required values for the column diameter, packing height for both rectifying and stripping sections and, condenser and reboiler duties. Note that for the last three designs the columns do not need a rectification section to achieve the desired distillate composition. In all cases, operating and design variables for the column correspond to a distillation unit which is able to process all the amount of permeate produced during a month in one day.

Table 3 summarizes both operating and investment costs calculation for all alternatives studied. To perform the calculations the following aspects must be taken into account: (i) investment costs were annualized by considering an interest rate of 10% and an equipment lifetime of 10 years, (ii) investment cost for the membrane unit was estimated from the actual membrane area with

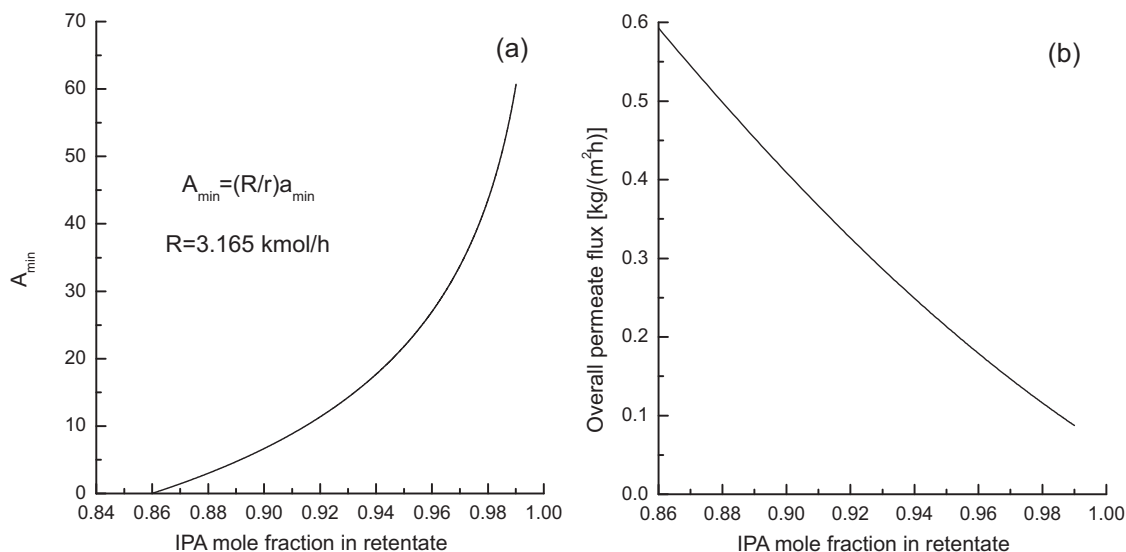


Fig. 2. (a) Minimum membrane area and (b) overall permeate flux versus IPA composition in the retentate. $T = 80^\circ\text{C}$, $P_p = 1.52\text{ kPa}$. Both graphics correspond to design #1. $A_{\min} = 61.122\text{ m}^2$, $A = 76.40\text{ m}^2$.

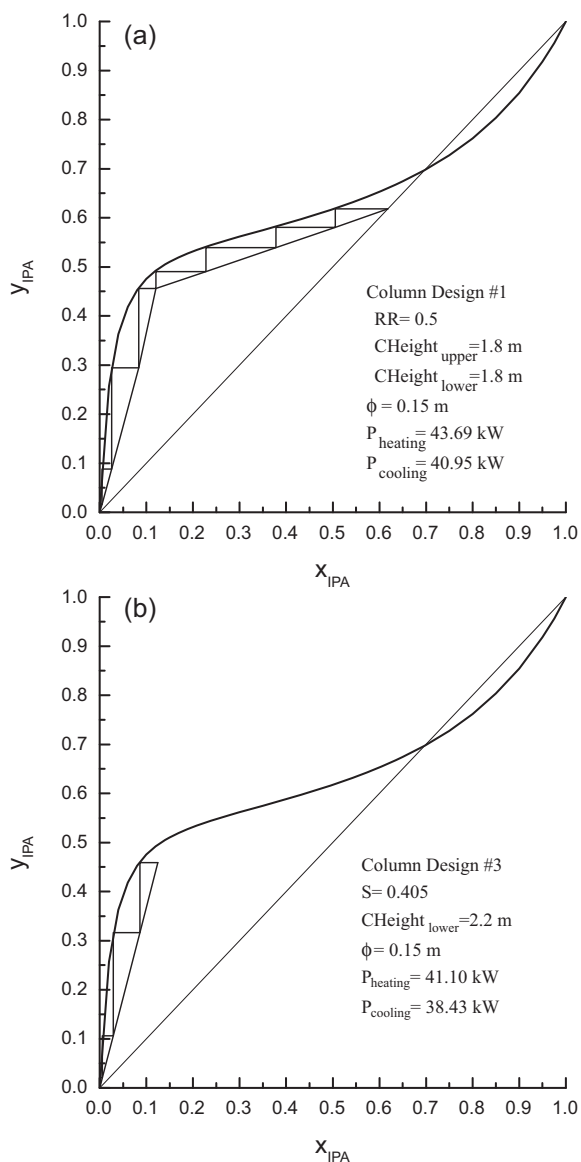


Fig. 3. McCabe–Thiele diagrams for (a) design #1 and (b) design #3.

a value of 3050 US\$/m² [13], (iii) operating cost of the pervaporation unit includes refrigeration to condense the permeate and keep vacuum, reheating between stages to keep the temperature level and the replacement cost of membranes (400 US\$/m², operation lifetime of 2 years), (iv) operating costs of the distillation unit includes the cost of the steam to pre-heat the feed up to its bubble point, the heating steam in the reboiler, and the cooling water in both condenser and product coolers, and (v) other costs include maintenance, insurance, labor and related analytical determinations. Table 3 shows both investment and overall costs per-ton of IPA for all the considered alternatives. The costs per ton of IPA recovered for all the designs are well below the purchase cost of fresh IPA. Therefore, the hybrid technology is appropriate to recover isopropyl alcohol from the pre-treated waste stream.

7. Quasi-optimal design

Even though the alternative #0 seems to be very attractive due to its low cost, this design does not consider the recovery of IPA losses in the permeate stream (23 ton/year) and therefore, we recommended the company to implement design #1 for three main reasons: (i) only few years are necessary to recover the investment cost of the distillation unit taking into account the purchase cost of IPA, (ii) the outsource of the recovery of IPA in the permeate does not guarantee the control on the composition of trace components that could be added in the recovery process using a non-dedicated batch column, and (iii) on-site recycling is one of the preferred alternatives in the waste management hierarchy [14].

Putting away design #0, design #1 presented the lower recovery cost and therefore, it was selected as reference for final recommendations to the company.

It is noteworthy that even when an optimal design could have been found by searching alternatives in the interval $x_r^* = [0.86, 0.868]$, this task was beyond the scope of the study as a result of the deadlines established by the company.

Fig. 4(a) shows the variation of the temperature at the retentate side of the membrane for the quasi-optimal design. Simulation of the operation includes now the energy balance (see Appendix A). Five modules of 15 m² each are necessary to achieve the desired IPA purity in the retentate. As membrane CMC-CF-23 from Celfa enables process temperatures as high as 90 °C, this temperature is recommended in order to counterbalance possible performance

Table 2
Operating and design variables of the membrane unit and the distillation column for each alternative design.

Design	T_{DewP} [°C]	Membrane area [m ²]	Column height _{Upper} [m] ^a	Column height _{Lower} [m] ^a	Column diameter [m] ^a	$P_{heating}$ [kW]	$P_{cooling}$ [kW]
0	11.09	74.8	–	–	–	–	–
1	11.18	76.4	1.8	1.8	0.15	43.69	40.95
2	11.23	77.4	0.8	2.4	0.15	39.47	36.76
3	11.28	78.3	0.0	2.2	0.15	41.10	38.43
4	11.37	80.1	0.0	1.8	0.15	52.40	49.76
5	11.52	83.5	0.0	1.6	0.20	75.64	73.08

^a Information supplied by a local contractor from calculated values of RR and N.

Table 3
Costs of the IPA recovery plant. Cost of fresh IPA = 750 US\$/ton.

Design	Investment Costs [US\$]			Overall costs per ton IPA [US\$/ton]			
	Pervap. unit	Dist. unit	Overall	Pervap. unit	Dist. unit	Others	Overall
0	228,052	–	228,052	53.85	–	22.81	76.66
1	233,028	50,037	283,065	55.94	10.33	24.41	90.68
2	236,013	48,234	284,247	56.74	9.90	24.44	91.08
3	238,887	47,667	286,554	57.51	9.89	24.50	91.90
4	244,389	50,707	295,096	59.00	10.84	24.71	94.55
5	254,526	59,172	313,698	61.79	13.16	25.17	100.12

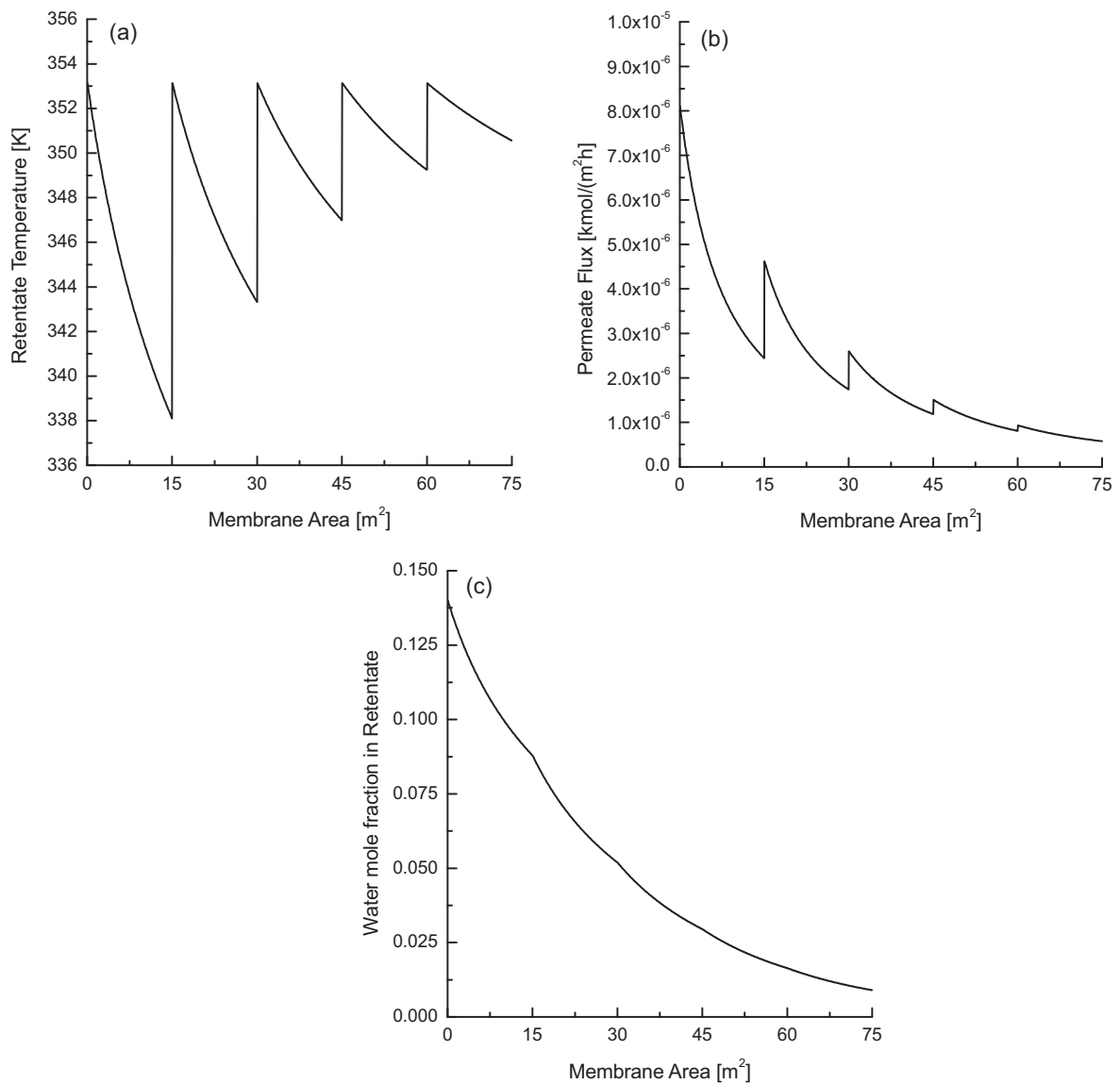


Fig. 4. Variation across the membrane of (a) retentate temperature, (b) permeate flux and, and (c) water mole fraction in the retentate side. Quasi-optimal design.

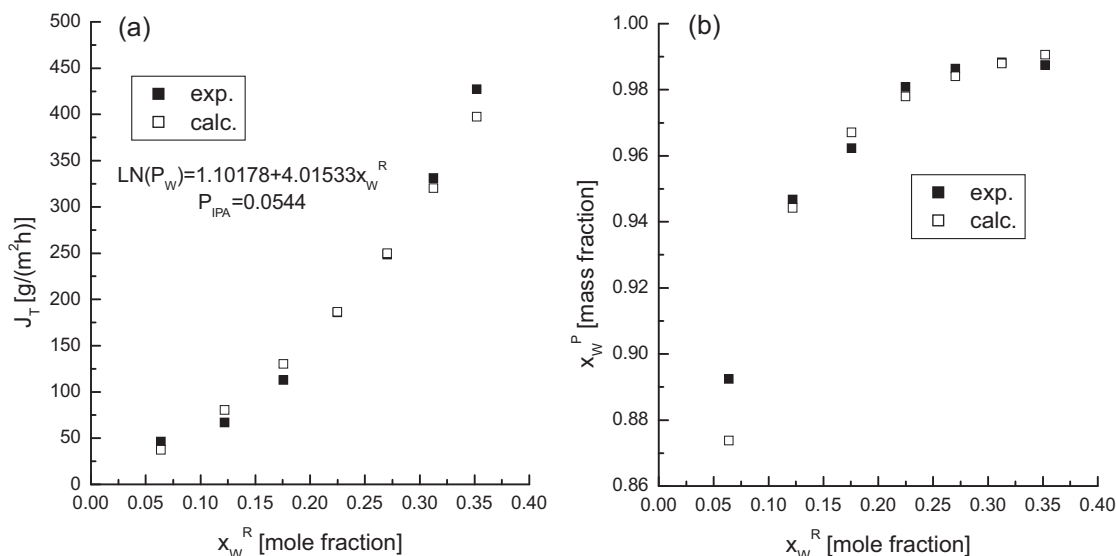


Fig. 5. Results of the pervaporation experiments at 80 °C and 1.52 kPa for seven feed compositions. Fitted values from the permeance model [16] are also included. (a) Overall permeate flux and (b) water mass fraction in permeate versus water mole fraction in retentate.

differences due to process scale-up. A retentate-side operation pressure of 202.6 kPa is suggested to avoid vapor formation along the module. Fig. 4(b) and (c) shows the variation of the permeate flux and water mole fraction in the retentate across the membrane unit, respectively.

A packed distillation column of 3.6 m height and 0.15 m diameter is required to avoid IPA losses in the permeate stream. The distillate composition is around 84.39 wt.% in isopropyl alcohol and the column must operate at a reflux ratio of 0.5.

8. Membrane performance comparison

Bearing in mind that the final design strongly depends on the performance of a given membrane, an assessment in this issue was also performed. For this matter, the PSI index defined as the product of permeate mass flux and separation factor was used. We resorted to literature data (PERVAP 2510 and PERVAP SMS from Sulzer [6], CMC-CF-23 from Celfa [8] and NaA type Zeolite from MITSUI [15]), membrane supplier brochures (CMC-VP-31 from Celfa) and to pervaporation experiments at our laboratory (PERVAP 2216, Sulzer). The search was not exhaustive as the goal was to provide the company with enough elements to judge process feasibility taking into account both economic and technical aspects.

Focusing our attention on the performance of the hydrophilic membrane PERVAP 2216 supplied by Sulzer Chemtech, this membrane has a cross-linked PVA selective layer and a supporting layer of non-woven porous polyester [16]. Main operation constrains for this membrane are the maximum operation temperature (<100 °C) and maximum water composition in feed (<40 wt.%).

To perform the experiments, we used the setup P-28 provided by Celfa [17]. While permeate compositions were analyzed by refractometry, feed tank mixtures of desired compositions were prepared from isopropyl alcohol grade pro-analysis and distilled water. In order to minimize the error in the composition of the feed to the tank, the gear pump (Scherzinger, Series 3000) was emptied as much as possible previously to run each experiment following the stopping operation procedure of the pump.

The analysis of the permeate samples were performed at the Laboratory of Physico-Chemical Essays from SECEGRIN-CONICET

using an Abbe High accuracy ED refractometer (supplied by Bellinghan and Stanley) following the method based on ASTM D1218 and D1747 Standards. A calibration curve for IPA compositions in the range [0, 100%] was also provided by the Laboratory.

Fig. 5(a) and (b) shows both the overall permeate flux and the mass fraction of water in the permeate versus the composition of water in the retentate (mole fraction). Each experiment was performed twice at a temperature of 80 °C and at a permeate pressure of 1.52 kPa. Fig. 5 also shows the fitted values corresponding to a model based on the solution/diffusion model [16]:

$$J_i^{mass} = P_i(x_i^f \gamma_i^f P_i^{sat} - y_i^P P_P) \quad (5)$$

with the permeance P_i , [g/(m²h kPa)] defined as the permeation flux divided by the permeant driving force. The dependence of P_i with the feed water mole fraction is also shown in Fig. 5(a).

By extending the idea developed by Bausa and Marquardt [3] from the operation design to the performance comparison between membranes, the PSI index was then redefined as the overall separation factor S times the inverse of the minimum membrane area A_{min} required to perform a given separation. In this case, we selected design #0 to compare the performance of the membrane CMC-CF-23 from Celfa with that of the membrane PERVAP 2216 from Sulzer.

Table 4 summarizes the results obtained from integration of both the permeance model and the model developed by Urriaga et al. [8]. While the PSI index for the membrane from Celfa was 10.5, the corresponding value for the membrane PERVAP 2216 was 4.02. From the analysis of the results becomes obvious that the higher selectivity of the membrane from Sulzer does not compensate its greater minimum membrane area needed to perform the separation.

Table 4
Membrane performance comparison in terms of a new PSI index definition.

Membrane	CMC-CF-23	PERVAP 2216
A_{min} [m ²]	59.817	349.8
x_{IPA}^R	0.99	0.99
x_{IPA}^P	0.136040	0.065848
S_w	628.73	1404.46
PSI index [1/m ²]	10.51	4.02

9. Results and discussion

According to the results obtained from the models developed for both the pervaporation unit and the distillation column, the adoption of this technology was recommended to the company in order to achieve high purity isopropanol (99.7%, w/w). The studied alternative is feasible from both technological and economical standpoints. Even when the economical analysis has a precision of about $\pm 30\%$ [11], the gap between the estimated cost per ton and the cost per ton of fresh IPA encourages the use of the hybrid technology.

Bearing in mind that the values for the reported design and operation variables are only reference values as they strongly depend on the alternatives offered by technology suppliers, the following variants could be relevant: (i) alternatives based on polymeric membranes that are more efficient in terms of flux, selectivity and/or membrane lifetime, (ii) alternatives based on ceramic membranes and isothermal pervaporation: “integrated direct heating”, and (iii) alternatives based on “vapor permeation”.

Whatever the membrane selected to perform the separation, final recommendations include to operate the plant at a temperature near its maximum feasible operation temperature.

Focusing our attention on the approach selected to carry out the feasibility analysis, two main issues deserve interest:

First, the search of a quasi-optimum design with the aid of conceptual models for each unit operation presented an advantage with respect to rigorous optimization models. While the use of either a distillation column or a stripper comes up naturally from the design of the distillation unit within the conceptual modeling approach, these alternative process configurations are very difficult to be foreseen when implementing a rigorous optimization approach. It is clear from this study, that solving this kind of problems should require either a MINLP [18] or a disjunctive programming approach [19] in order to capture all the possible process configurations.

Second, we found that, at least for polymeric membranes, the PSI index would be more useful if redefined in terms of a given separation as the overall separation factor times the inverse of the minimum membrane area required. The new definition of the PSI index for membrane performance comparison requires a limited number of experiments at a given quasi-optimal temperature (i.e., seven points at 80 °C) instead of a single experimental point. In this way, the performance behavior of a given membrane is related to a specific separation instead of a single experimental point.

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Appendix A. Integration algorithm for conceptual design (conceptual model) and process simulation (model with energy balance)

Step A.1. Calculate components activities $a_{i,353.14}^f = x_i^f \gamma_i^f$

Step A.2. Calculate the water flux [kg/(m²h)] $J_{w,353.14} = A_1[\exp(A_2 a_w^f) - 1]$

Step A.3. Calculate the ratio of partial fluxes q and then the IPA flux [kg/(m²h)]

$$q = \frac{J_{w,353.14}}{J_{IPA,353.14}} = \frac{A_3}{a_{IPA}^f} [\exp(A_4 a_w^f) - 1]$$

Step A.4. Use the Arrhenius-type equation to account for the dependence of water and isopropyl alcohol fluxes [kg/(m²h)] with temperature

$$J_{i,T} = J_{i,T_0} \exp\left(-\frac{E_{a,i}}{RT}\right)$$

with

$$\ln J_{i,T_0} = \ln J_{i,353.14} + \left(\frac{E_{a,i}}{R}\right) \frac{1}{353.14}$$

Step A.5. Calculate the molar fluxes [kmol/(m²h)] $J_{i,T}^{mol} = J_{i,T}/MW_i$ and then solve the mass balance from:

$$d\left[\left(\frac{L}{F^*}\right) x_i\right] = -J_{i,T}^{mol} \left(\frac{dA}{F^*}\right) \quad (\text{conceptual design})$$

$$d[Lx_i] = -J_{i,T}^{mol} dA \quad (\text{process simulation})$$

with $r=L/F^*$ and $a=A/F^*$.

Step A.6. (only for process simulation) Solve the energy balance from:

$$Lc_p d(T) = -\Delta H_{vap} J_T^{mol} d(A)$$

Step A.7. Update values for the retentate flow rate, retentate mole fraction for each component and temperature ($T=353.14$ K for conceptual design) and go to step A.1 either until the retentate composition x_R specified at the design level (conceptual design) or the module area (process simulation) are achieved.

Note that in the case of process simulation, several membrane modules can be connected to achieve the desired final retentate composition. Parameters needed to run the model can be found elsewhere [8].

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