

Selection of Optimal Operating Conditions based on Minimum Energy Consumption for an Acrylonitrile Recovery Unit

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Abstract

The selection of the optimal operating conditions for an industrial acrylonitrile recovery unit was conducted by the systematic application of the Response Surface Methodology (RSM), based on the minimum energy consumption and products specifications as process constraints. The system is a very complex extractive distillation due to the limited reciprocal solubility of acrylonitrile and water (solvent) and the narrow range of temperature difference between the normal boiling point of acetonitrile (byproduct) and acrylonitrile, that is only 4 °C. Adjustment of vapor-liquid (VLE) and vapor-liquid-liquid equilibria (VLLE) binary parameters for Redlich-Kwong equation of state and NRTL model for the quaternary system acrylonitrile (ACN), acetonitrile, water and hydrocyanic acid (HCN) was conducted. Unit models and plant simulation were validated against operating data and information. A sensitivity analyses was carried out in order to identify the set of parameters which strongly affect the trajectory of the reboiler duty while keeping products specifications. It was found that solvent-feed ratio, and solvent and feed temperatures are these variables. Their operating ranges and role in the operational flexibility were also established. By applying the response surface methodology (RSM) and statistical analyses techniques, it was possible to determine the optimal operating point and the multifunctional relationship among the three parameters and the reboiler duty. The results suggest that energy savings up to 10% are possible by systematically adjusting operating conditions. In general, the study shows that an efficient energy management can ensure greater environmental sustainability even for old industrial facilities.

Keywords: Acrylonitrile, extractive distillation, optimal operating conditions

1. Introduction

Chemical process industries in general and acrylonitrile units in particular require large amount of energy for their operation. Therefore, the advantages of operating at optimal conditions based on minimum energy consumption are twofold: reduction in operating costs and protection of the environment.

Acrylonitrile (ACN) is a product used in a variety of applications, ranging from water treatment to the synthesis of complex petrochemicals such as thermoplastics (ABS, SAN), textiles, rubbers and especially acrylic fibers. The ammoxidation process developed by Sohio in late 50s reacts propylene, ammonia and air to produce acrylonitrile [1] and a wide variety of compounds, such as hydrocyanic acid, acrolein, water and large amounts of acetonitrile. Currently, there are alternative routes, such as those using propane [2] or glycerol from biomass [3]. However, the original Sohio process, and its modifications for improving efficiency and reaction conversion, are still the main routes for acrylonitrile production, used nowadays to synthesize 90% of the 4 million tons produced worldwide each year [4].

The effluent from the Sohio process reactor is a complex mixture of nitrogen compounds and water. Besides the limited reciprocal solubility of acrylonitrile and water, the temperature difference between the normal boiling point of acetonitrile and acrylonitrile is only 4 °C. Therefore, decantation and extractive distillation are indicated as good choices for the purification of acrylonitrile. Water is present in almost all steps of the acrylonitrile production and is a good separation agent for the acetonitrile-acrylonitrile binary system. However, it forms azeotropes with almost all nitrogen compounds present in the system making further separations more complex. At 1 atm the acrylonitrile-water system presents a minimum boiling point azeotrope at 71 °C and 88% of acrylonitrile mass fraction. Acetonitrile-water binary also presents a minimum boiling point azeotrope at 76 °C and 72.6% of acetonitrile mass fraction at 1 atm [5]. Hydrocyanic acid and water also form an azeotropic mixture.

The application of modelling and simulation for representing an extractive distillation is a well established technique. In relation to the simulation of an acrylonitrile recovery unit there is the work by Dimian and Bildea (2008) [6] which used a process configuration different from the one studied in this work and did not consider separation efficiency and pressure drop along the column. Furthermore, the authors used feed conditions and thermodynamic models different from the ones presented here and did not compared the results with real plant data in order to replicate plant behavior.

For optimizing a process where many factors and interactions affect the desired result, response surface methodology (RSM) has proved to be an effective tool [7] and it has been successfully applied to many modelling and optimization problems [8]. Essentially, RSM is a set of mathematical and statistical methods for designing experiments, building models, evaluating the effects of variables, and searching optimum conditions of variables to predict targeted responses [9].

Few research work related to the optimization of operating conditions of industrial facilities have been reported and none focusing on acrylonitrile purification units. Therefore, this work aims at applying the Response Surface Methodology (RSM) for the

selection of optimal operating conditions for a modified Sohio acrylonitrile recovery unit based on the minimum energy consumption and products specifications as process restrictions. Thermodynamic models for representing the VLLE are chosen and binary interaction parameters are estimated. The modeling and simulation consider pressure drop along the column, the efficiency of stages and uses a rigorous model approach based on the AspenPlus RadFrac. The validation is conducted against real plant data and information. A sensitivity analyses is carried out in order to identify variables that mainly influence the plant energy consumption. Finally, the RSM analysis is applied to determine the optimal operating condition.

2. Modeling the Acrylonitrile Recovery System

The analyzed acrylonitrile recovery system shown in Figure 1 is based on an existing unit and is a modification of the Sohio process. It consists of two columns: an extractive distillation column (T101) and a distillation column (T102).

The extractive distillation column is fed by a complex mixture (stream 12) effluent from the reactor/absorption process. This is mainly composed of acrylonitrile, acetonitrile, water and hydrocyanic acid (HCN), and contains traces of organic impurities such as acrolein. It is formed by the mixture of streams 1, 3 and 4, effluent from the reactor/absorption system and from the acetonitrile and acrylonitrile purification unities, respectively. Stream 9 is an extra feed rich in acrylonitrile. Water is the extractive separation agent (stream 5) that changes the relative volatilities of the components and preferentially dissolves acetonitrile. Part of this aqueous phase is taken off as the side stream 15 and fed to the column 2 for the recovering of acetonitrile, a valuable byproduct. At the bottom, streams 11 and 16 are nearly pure water reused in the process, being part recycled as the extractive agent (stream 5). From the top of the column 1 the vapor phase is completely condensed forming two liquid phases: one rich in acrylonitrile (stream 7) and the other rich in water (stream 2), which is used as the tower reflux.

The distillation column (T102) is fed by stream 15 that is separated into a lighter mixture rich in acetonitrile and water (close to the azeotropic composition) and containing some acrylonitrile and HCN (stream 6), and a heavier aqueous solution at the bottom, considered as pure water (streams 18 e 8), which returns to the T101. Client requirements in terms of maximum content of acrylonitrile in the acetonitrile stream (6) impose a very low acrylonitrile concentration in stream 15, since the original design of column 2 was not prepared to attend the recent purity standards.

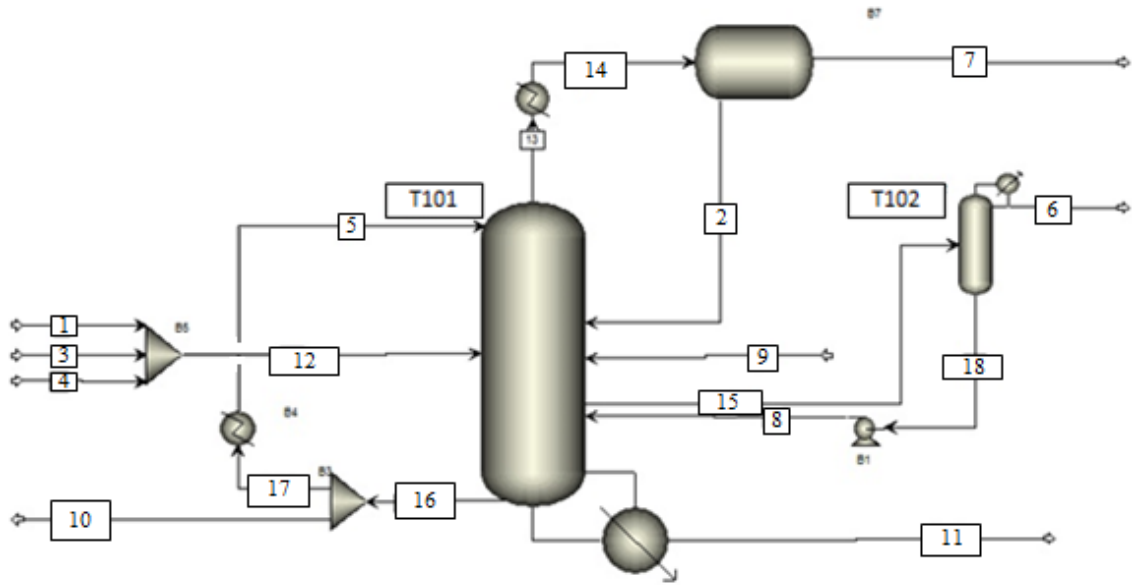


Figure 1. Acrylonitrile recovery system (adapted from an existing unit)

2.1. Thermodynamic Models

After several tests, the Redlich-Kwong equation of state and the NRTL excess Gibbs energy model were selected to compute the vapor-liquid (VLE) and vapor-liquid-liquid equilibrium (VLLE) of the highly non-ideal quaternary system, acrylonitrile (ACN), acetonitrile, water and hydrocyanic acid (HCN), using the gamma/phi approach. Models parameters were regressed based on binary data from literature [10], [11], [12], [13], [14] and [15]. Figure 2 shows the regression results for the highly non-ideal binary system: acetonitrile + water. It can be seen that model predictions (lines) are in good agreement with literature data (points) with mean percentual error of 0,78% and 1,95% for temperature and vapor phase composition, respectively.

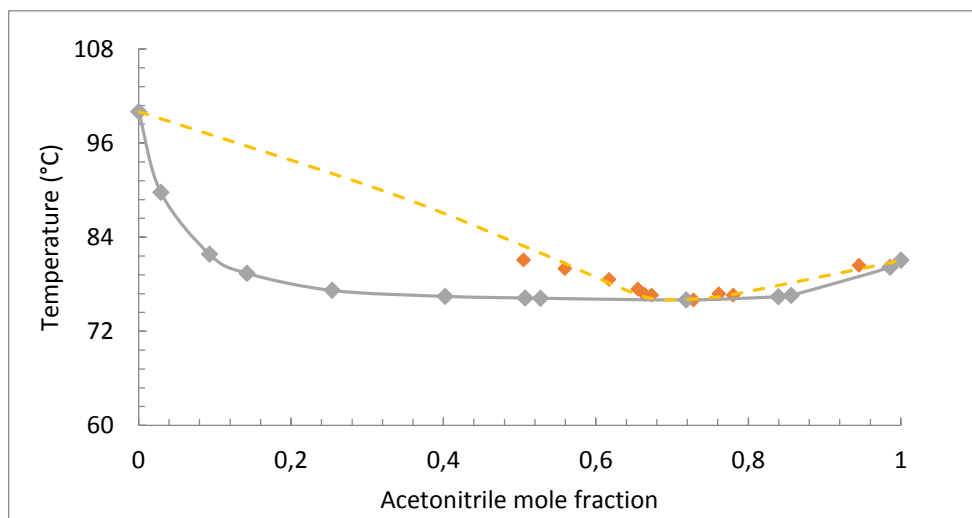


Figure 2. VLE diagram for the binary acetonitrile + water at 1 atm. Experimental data from Blackford and York (1965).

2.2. Modeling the separation system

The acrylonitrile recovery system (Figure 1) was modeled with RadFrac module of Aspen Plus. It uses rigorous methods based on the equilibrium assumption between leaving vapor and liquid flows for each stage and MESH (Material balance equation, Equilibrium phase equations, Summation equations and Heat balance equations) equations. This method is difficult to converge as already reported in literature [16]; Akpa and Umuze, 2013, among others).

Besides ensuring a good thermodynamic modeling it was necessary to consider separation efficiencies for each stage in both towers by using the O'Connell (E_{oc}) correlation (Kister, 1992), shown in Equation (1). It is a way to compute how far the system is from the thermodynamic equilibrium.

$$E_{oc} = 0.492(\mu_L \alpha)^{-0.245} \quad (1)$$

where μ_L is the average viscosity of the liquid phase and α is the relative volatility between the key components, both evaluated at the average arithmetic temperature between the column top and bottom temperatures.

Calculated average efficiencies for both columns were of 43% and 67,6% for tower1 and T102, respectively. The lower efficiency of column 1 is due to the formation of two liquid phases in some stages increasing the non-ideality and the resistance for mass transfer.

2.3. Model Validation

The accuracy of the model equations and adequacy of simulation method were validated by comparing predicted tray temperatures with those from the industrial facility and literature. Process information and specifications are shown in Tables 1 to 4.

Table 1. Extractive distillation column data

| Parameter | Value |
|-----------------------|-------|
| Number of stages | 95 |
| Feed stage | 22 |
| Solvent stage | 1 |
| Removal side stage | 60 |
| Return solvent stage | 60 |
| Reflux stage | 22 |
| Top pressure (bar) | 1.08 |
| Bottom pressure (bar) | 2.26 |
| Condenser | Total |

Table 2. Acetonitrile recuperation column data

| Parameter | Value |
|----------------------------|-------|
| Number of stages | 30 |
| Feed stage | 15 |
| Reflux stage | 1 |
| Reflux ratio | 3 |
| Top pressure (bar) | 1.29 |
| Bottom pressure (bar) | 1.4 |
| Condenser temperature (°C) | 80.2 |
| Condenser | Total |

Table 3. Feed conditions.

| Stream | 1 | 3 | 4 | 9 |
|---------------------------|-------|-------|-------|-------|
| Molar rate (kmol/h) | 10898 | 68 | 632 | 23 |
| Temperature (°C) | 75 | 75 | 75 | 70 |
| Pressure (bar) | 2 | 2 | 2 | 2 |
| Mole fraction composition | | | | |
| Water | 0.972 | 0.948 | 0.983 | 0.310 |
| Acrylonitrile | 0.022 | 0.029 | 0.011 | 0.329 |
| Acetonitrile | 0.001 | 0.000 | 0.002 | 0.153 |
| HCN | 0.005 | 0.023 | 0.004 | 0.207 |

Table 4. Process specifications.

| | |
|--|-------------|
| Acetonitrile mole fraction in stream 7 | 100 ppm |
| Acetonitrile mole fraction in stream 6 | ≥ 0.38 |

Process specifications shown in Table 4 are important product quality constraints since acrylonitrile loses commercial value for acetonitrile composition in stream 7 greater than 100 ppm. Moreover, in order to have acetonitrile within commercial specifications, stream 6 must present an acetonitrile concentration greater than 38% and stream 15 a maximum of 0.1% of acrylonitrile. To accomplish these goals, a distillate flow rate of 418 kmol/h and a solvent/feed mass ratio of about 0.37 are needed in column 1. While a distillate flow rate of 20 kmol/h is necessary in column 2.

Figures 3 and 4 and Table 5 compare simulation results with those obtained from the industrial plant. It can be seen that the temperature profiles are well described in both columns. The low magnitude of the deviations shown in Table 5 reinforces the validity of the proposed model. At the top of the column the errors are larger, but still acceptable, since in a real industrial plant, the separation system is further more complex than the one described in this work. This is due to the presence of other components, such as, acrolein, oxazole, allylic alcohols, among others. There are also injection of products to prevent polymerization of acrylonitrile and of caustic soda to control pH. All these contribute to explain temperature differences.

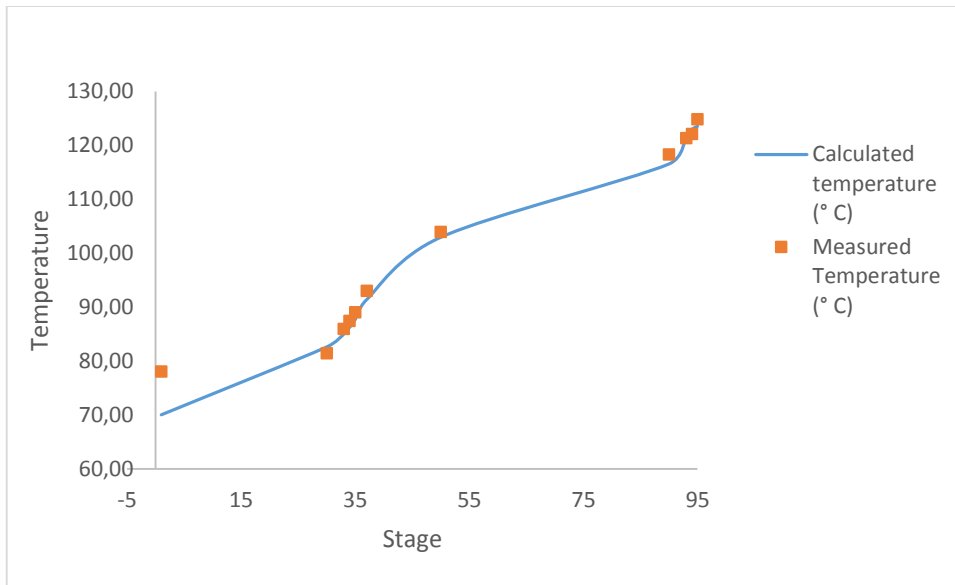


Figure 3. Temperature profile of the extractive distillation column

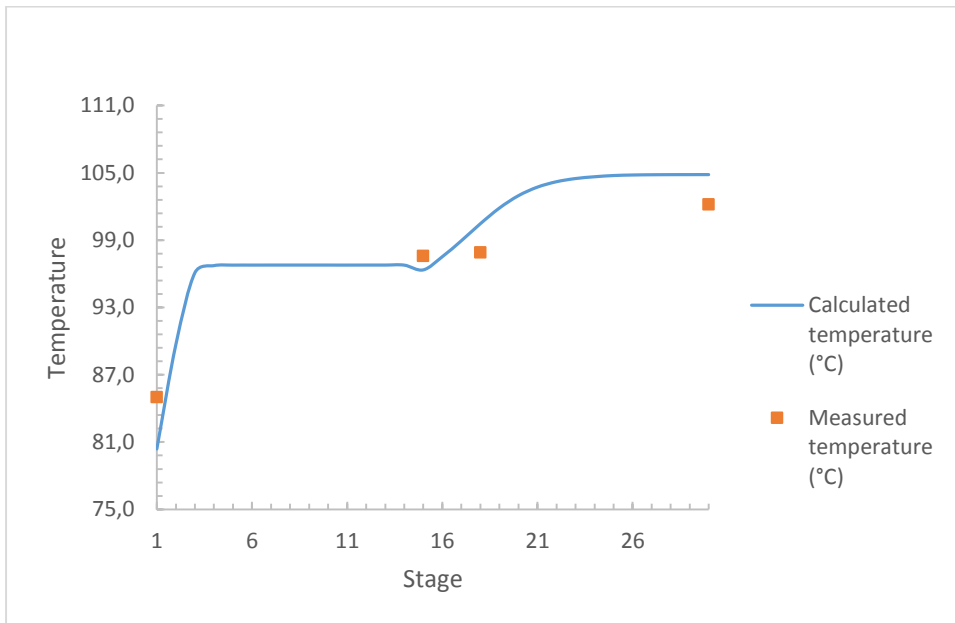


Figure 4. Temperature profile of the acetonitrile recovery column

Table 5. Relative deviations between the calculated and measured temperatures in different stages of the extractive distillation column.

| Stage | Deviation (%) |
|-------|---------------|
| 1 | 10.26 |
| 30 | 1.46 |
| 33 | 1.05 |
| 34 | 1.36 |
| 35 | 1.48 |
| 37 | 1.76 |
| 50 | 0.92 |
| 90 | 1.49 |
| 93 | 0.48 |
| 94 | 0.70 |
| 95 | 1.03 |

3. Sensitivity Analysis

Once the simulation is functioning properly, the sensitivity analysis can be carried out. The direct method has been chosen, where parameters are varied one at a time and effects on system responses are analyzed [17]. Based on operational experience and information from plant digital control, the following parameters were selected as important to adjust products specifications: solvent/feed mass ratio (RSF), feed stage (FS), solvent stage (SS), feed temperature (FT) and solvent temperature (ST). The normal operating point for these variables is: RSF = 0.37, FS = 22, SS = 1, FT = 75 °C and ST= 40 °C.

Figure 5 shows feed stage (FS) and RSF influence on the distillate (stream 7) acetonitrile mole fraction, which specification is a maximum of 0.01%. For RSF greater than 0.4 and feed stage between 22 and 50 a little influence on the distillate composition is observed. However, for RSF values greater than 0.25 and feed stage greater than 42 (nearer the column bottom), acetonitrile tends to be concentrated in the distillate and specification cannot be achieved. The same occurs for RSF equal or smaller than 0.25, since there is not enough solvent to promote the separation. Therefore, RSF must be greater than 0.25 and feed stage between 22 and 42.

Considering that the stream 15 must contain a maximum of 0.1% of acrylonitrile in order to guarantee the specification of stream 6, it was analyzed the behavior of this variable for different RSF and feed stages (FS). Figure 6 shows that for feed stage between 22 and 42 and RSF greater than 0.25 the composition of acrylonitrile on stream 15 is almost unchanged and very small. Specification is not achieved for RSF equal or smaller than 0.25 or feed stage greater than 42.

Figure 7 illustrates the influence of feed stage (FS) and RSF on the reboiler duty. There is a very small variation on heat duty when changing the position of the feed stage. In

fact, what is changing is the concentration profile along the column and the distillate composition. However, a large increase on the reboiler duty is observed when RSF increases. This was expected, since larger amounts of solvent are recovered at the bottom of the tower, causing higher heat rates on the reboiler. Therefore, there is no point in using RSF greater than 0.45.

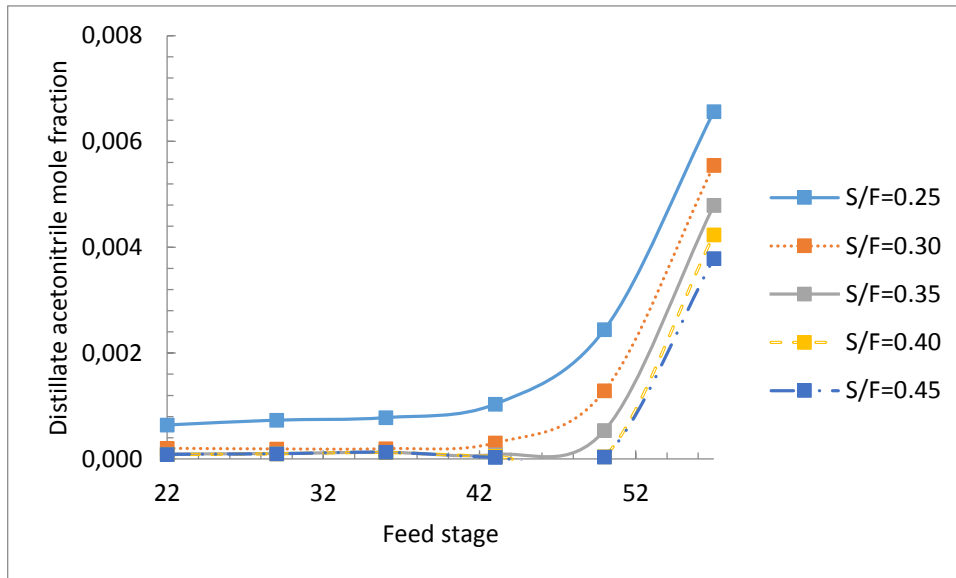


Figure 5. Feed stage and solvent/feed mass ratio (RSF) effects on distillate acetonitrile molar composition

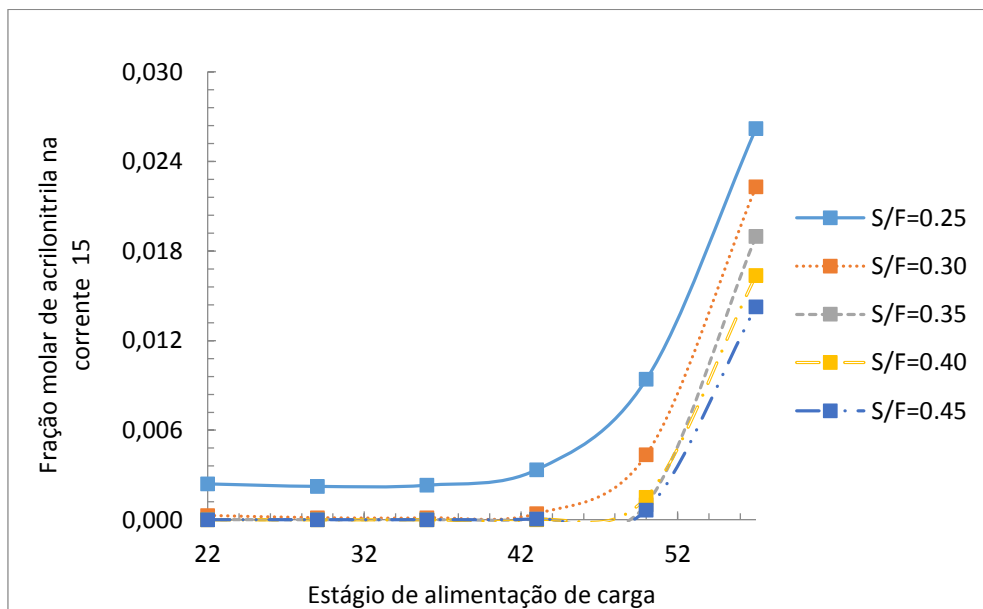


Figure 6. Feed stage and solvent/feed mass ratio (RSF) effects on stream 15 acrylonitrile molar composition

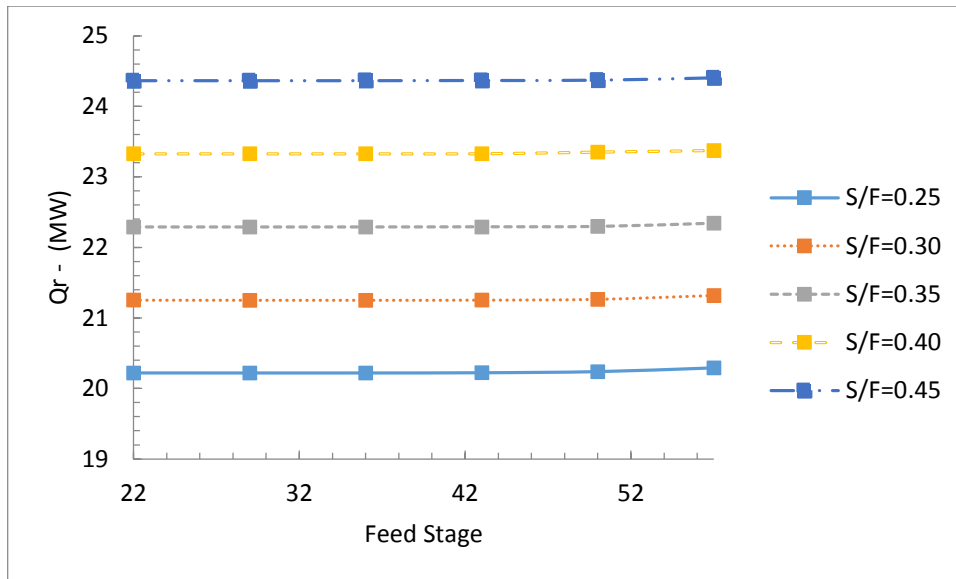


Figure 7. Feed stage and RSF effects on the reboiler duty

The influence of the solvent stage (SS) and RSF on the distillate acetonitrile molar composition is shown in Figure 8. It can be seen that there is a clear trend to increase the acetonitrile composition in the top by moving the solvent feed stage towards the bottom. This is due to the reduction of the amount of solvent in upper stages available to dissolve acetonitrile, thus concentrating it in the vapor phase. For RSF greater than the normal operation point (0.37) and solvent feed stage between 4 and 7 there will initially be a trend to decrease the composition of acetonitrile in the distillate due to the great dilution near the top. Afterwards, the increasing behavior is restored. Specification is only achieved for SS equal to 1 or RSF greater than 0.35 and stages between 4 and 8.

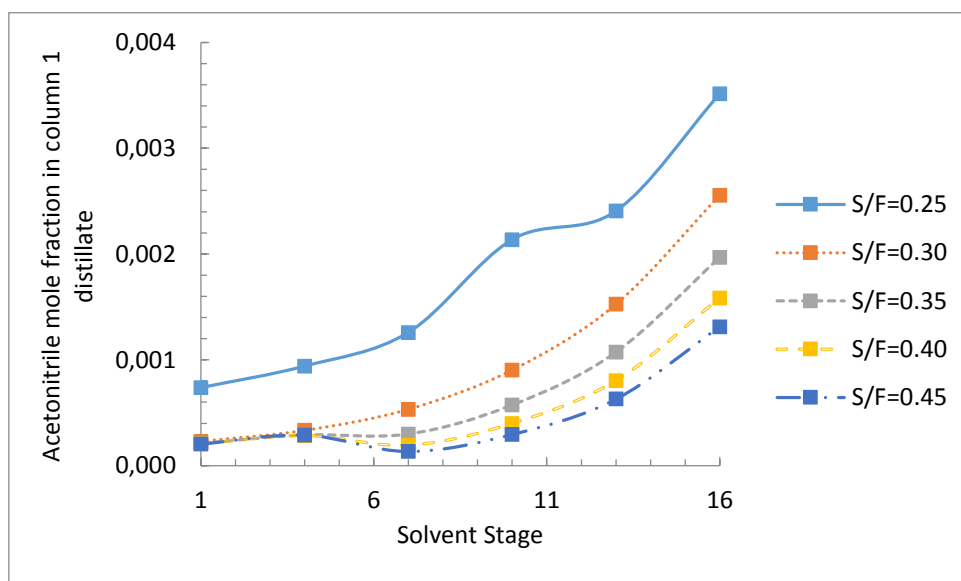


Figure 8. Solvent stage and RSF effects on the distillate acetonitrile molar composition

The composition of acrylonitrile in stage 15 obeys a similar pattern of acetonitrile in the distillate. As shown in Figure 9 there is a clear trend to increase the acrylonitrile composition by moving the solvent feed stage towards the bottom of the column. Moreover, if the solvent is fed below stage 5 the specification in column 2 is not achieved, because the number of stages available to promote the extraction of acrylonitrile and acetonitrile is reduced. The RSF parameter will only affect the composition if it falls below 0.30.

Figure 10 shows solvent stage and RSF influences on the reboiler duty. The behavior is the same of Figure 7. The position of solvent stage does not influence the reboiler duty and the RSF is the main factor affecting this variable.

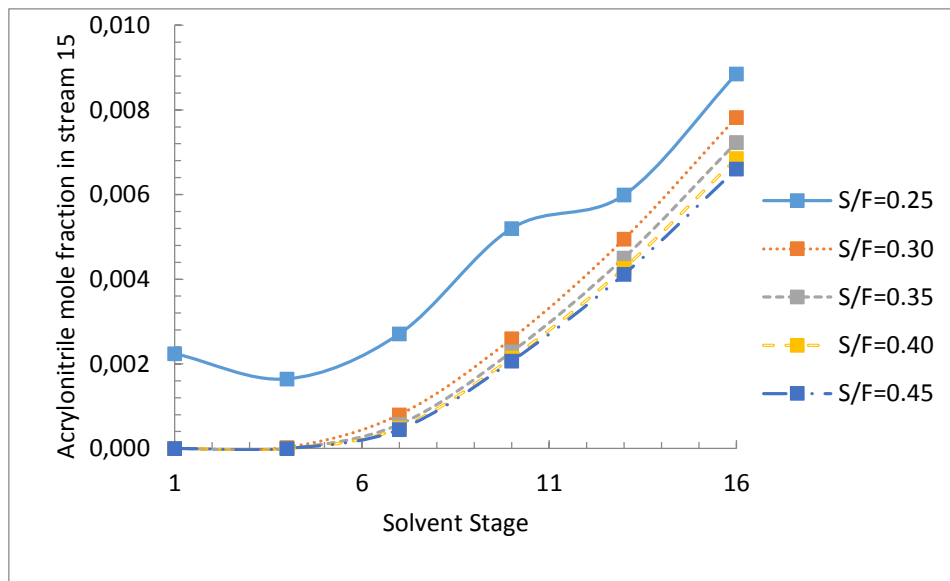


Figure 9. Solvent stage and RSF effects on stream 15 acrylonitrile molar composition

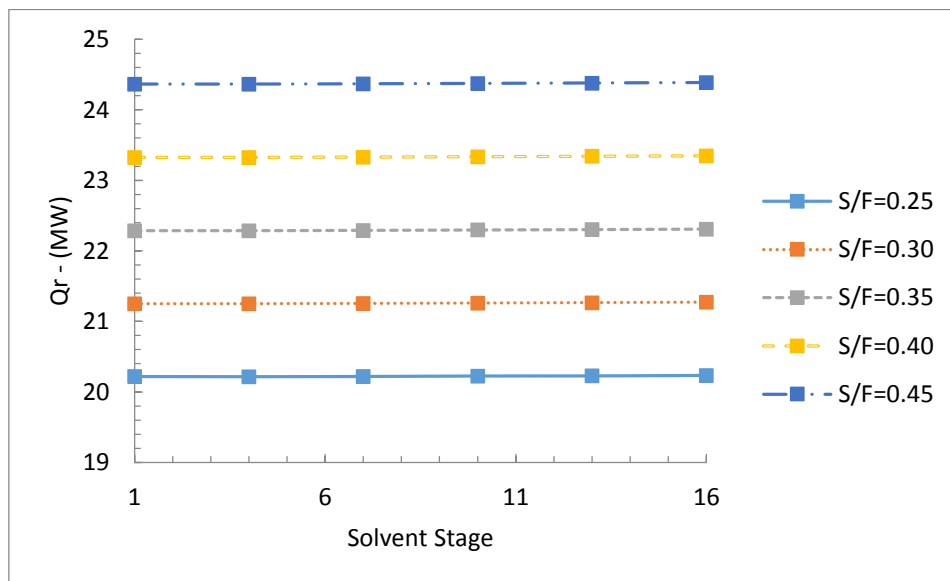


Figure 10. Solvent stage and RSF effects on the reboiler duty

Feed temperature will only affect products specifications for values greater than 85 °C or RSF smaller than 0.30, as shown in Figures 11 and 12. High temperatures will increase the acrylonitrile and acetonitrile solubility in the liquid phase. This pattern guarantees operating flexibility since it allows operating in a large range of temperatures. Otherwise, Figure 13 shows a strong inverse relationship between the reboiler duty and feed temperature.

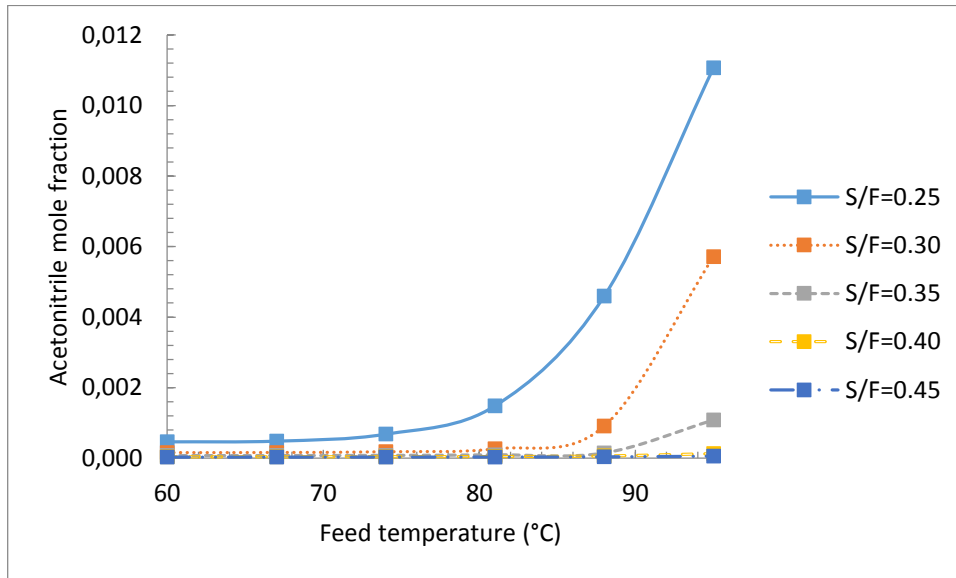


Figure 11. Feed temperature and RSF effects on the distillate acetonitrile molar composition

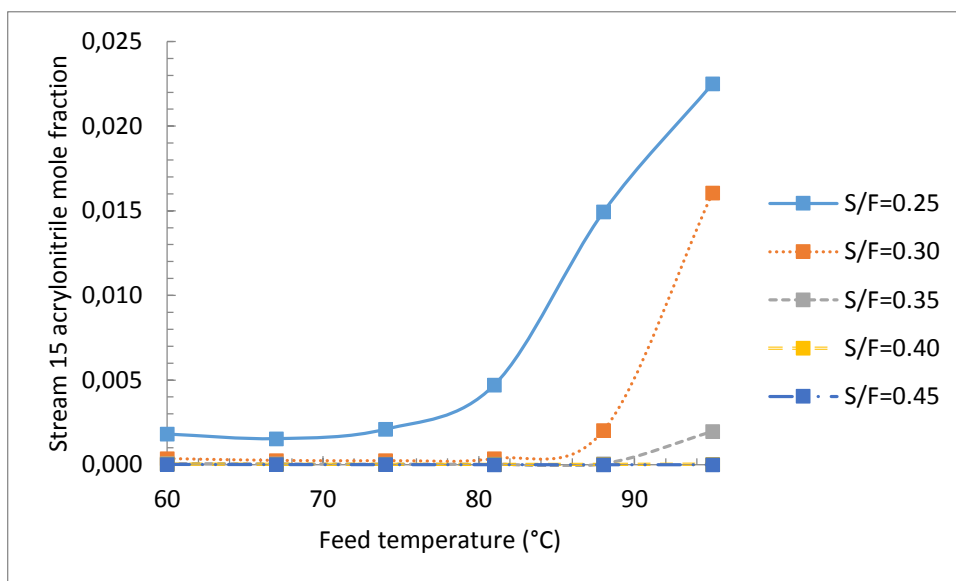


Figure 12. Feed temperature and RSF effects on stream 15 acrylonitrile molar composition

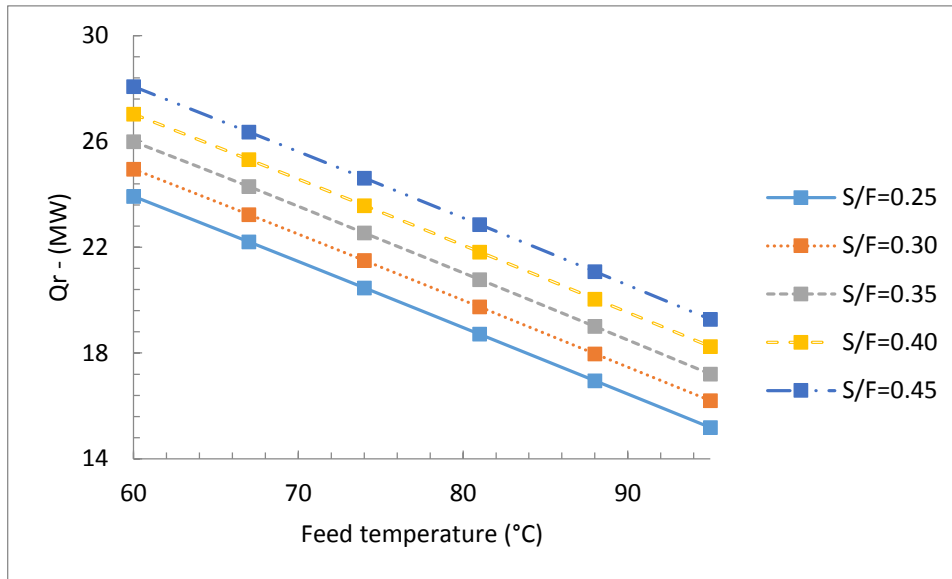


Figure 13. Feed temperature and RSF effects on the reboiler duty

Solvent temperature has a strong influence in the distillate and tray 15 compositions (Figures 14 and 15). For RSF 0.30 or greater and temperatures up to about 56 °C, increasing solvent temperature reduces the acetonitrile mole fraction in the distillate, and then a minimum is attained. This is due to the increased solubility of acetonitrile in liquid phase. Above 60 °C, acetonitrile tends to concentrate in the vapor phase, and it is concluded that independently of RSF, it is not interesting to feed solvent in that temperature range. Aiming at keeping operating flexibility the RSF parameter should be kept above 0,35.

For the acrylonitrile mole fraction in stream 15 (Figure 15), the limit of solvent temperature is about 40 °C. Between 40 and 50 °C the acrylonitrile solubility in the liquid phase increases considerably with temperature and then tends to be constant. The RSF parameter seems to have no effect on this composition.

Regarding heat duty (Figure 16), the effect of solvent temperature is similar to the one of feed temperature i.e, a strong inverse relationship between these parameters.

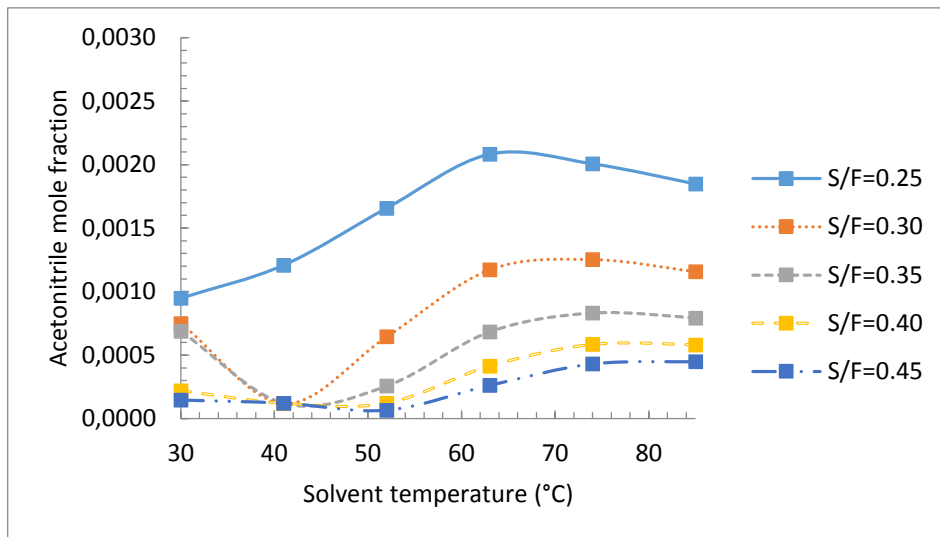


Figure 14. Solvent temperature effect on the distillate acetonitrile molar composition

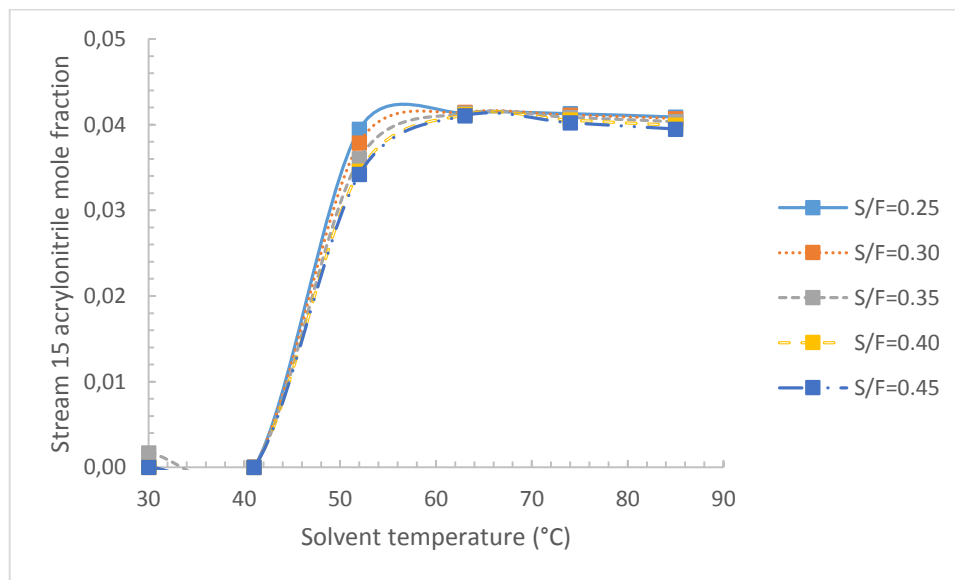


Figure 15. ST effect on stream 15 acrylonitrile molar composition

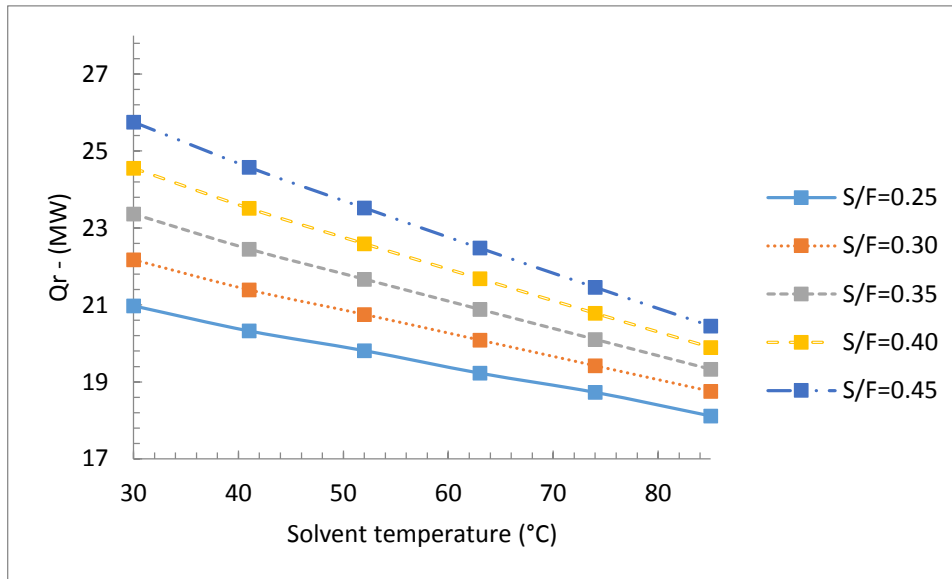


Figure 16. Solvent temperature effect on the reboiler duty

The sensitivity analysis has proved to be a powerful tool in the identification of the parameters that mostly affect the trajectory of the reboiler duty and products specifications. Moreover, it was able to establish the operational range of the variables and their role in the operating flexibility. Through this technique it was possible to realize that the reboiler duty is a strong function of the solvent feed ratio, feed and solvent temperature. However, it is not able to determine the combined effects of these three variables neither the shape of this multifunctional relationship. Therefore, the use of Response Surface Methodology is indicated.

5 Optimization through RSM

The aim of the optimization is to search for the optimal operating point involving relevant variables that will result in a minimum energy consumption. The searching space must be constrained by process specifications: acetonitrile in distillate and acrylonitrile in stream 15 shall not be higher than 100 ppm and 0.1% molar, respectively.

The optimization was carried out by using the response surface methodology (RSM) to generate the adequate functional relationship among the three variables (RSF, ST and FT) and their limits identified by the sensitivity analysis. It was performed a composite design with central point for these three variables. The heat duty for each point was determined by simulation. Table 6 illustrates the levels of the variables and Table 7 the full factorial planning.

Table 6. Variables and levels.

| Variable | Level | | | | |
|----------|---------|-------|-------|-------|---------|
| | (-1.68) | (-1) | 0 | (+1) | (+1.68) |
| RSF | 0.316 | 0.35 | 0.40 | 0.45 | 0.484 |
| ST (°C) | 38.64 | 40.00 | 42.00 | 44.00 | 45.36 |
| FT (°C) | 52.18 | 60.00 | 71.50 | 83.00 | 90.82 |

Table 7. Factorial planning matrix

| Simulations | RSF | ST | FT | Heat duty (MW) |
|-------------|-------|-------|-------|----------------|
| 1 | -1 | -1 | -1 | 26.09 |
| 2 | -1 | -1 | 1 | 20.88 |
| 3 | -1 | 1 | -1 | 25.71 |
| 4 | -1 | 1 | 1 | 20.49 |
| 5 | 1 | -1 | -1 | 29.24 |
| 6 | 1 | -1 | 1 | 24.03 |
| 7 | 1 | 1 | -1 | 28.67 |
| 8 | 1 | 1 | 1 | 23.45 |
| 9 | -1.68 | 0 | 0 | 22.29 |
| 10 | 1.68 | 0 | 0 | 27.38 |
| 11 | 0 | -1.68 | 0 | 25.24 |
| 12 | 0 | 1.68 | 0 | 24.45 |
| 13 | 0 | 0 | -1.68 | 29.16 |
| 14 | 0 | 0 | 1.68 | 20.40 |
| 15 | 0 | 0 | 0 | 24.84 |

The quadratic model shown in Equation 1 represents the resulting functional relationship among the three relevant variables (RSF, ST and FT) and the reboiler duty. ANOVA (Analysis of Variance) results for this model are presented in Table 8. It can be seen that the optimization in the quadratic form fits quite well the data generated by the simulation since the correlation coefficient (R^2) is equal to 0.9999. Highlighted terms refer to the variables that present significant contribution. The designation (L) and (Q) represents the linear and quadratic contributions respectively. The P-values reveal the statistical significance of each model term. If it is higher than 0.05 the model term can be considered as non-significant. Test F is a ratio of systematic variances. The more this ratio deviates from 1, the stronger the evidence that the model is statistically significant. These conclusions can also be reached by analyzing the Pareto diagram shown in Figure 17, which enables to visually identify the important effects and compare the relative magnitudes between them. By analyzing these statistical information, one can conclude that the quadratic terms in RSF and ST parameters, and their interactions with FT can be eliminated without loss of significance. Therefore, the regression can be simplified as shown in Equation 2.

$$Qr = 0.3231 * 10^2 + 0.3179 * 10^2x - 1.302 * 10^{-3}y - 21.67 * 10^2z - 58.48 * 10^{-2}x^2 + 21.03 * 10^{-5}y^2 - 21.83 * 10^{-5}z^2 - 24.88 * 10^{-2}yx + 12.32 * 10^{-4}xz - 7.096 * 10^{-5}yz \quad (1)$$

Where, x is RSF, y represents ST and z is FT.

Table 8. ANOVA

$R^2 = 0.9999$ (Optimization); 3 Factors.

| Factors | SS | MS | F | p |
|---------------------------|----------------------|-----------------------|------------------------|------------------------|
| <u>1 - RSC (L)</u> | <u>31.652</u> | <u>31.6521</u> | <u>249582</u> | <u>0.000000</u> |
| RSC (Q) | 0.0001 | 0.0001 | 0.8 | 0.408700 |
| <u>2 - TS (L)</u> | <u>0.7724</u> | <u>0.77230</u> | <u>6090.3</u> | <u>0.000000</u> |
| TS (Q) | 0.0000 | 0.00001 | 0.1 | 0.759400 |
| <u>3- TC (L)</u> | <u>92.770</u> | <u>92.7700</u> | <u>731506.3</u> | <u>0.000000</u> |
| <u>TC (Q)</u> | <u>0.0047</u> | <u>0.00474</u> | <u>37.3</u> | <u>0.000876</u> |
| <u>(1) by (2)</u> | <u>0.0174</u> | <u>001740</u> | <u>137.4</u> | <u>0.000230</u> |
| (1) by (3) | 0.0000 | 0.00001 | 0.1 | 0.815500 |
| (2) by (3) | 0.0000 | 0.00003 | 0.2 | 0.658260 |
| Erro | 0.0083 | 0.00013 | | |
| Total SS | 125.21 | | | |

Where: SS = sum of squares , MS= mean square; F= test F, p=p-values

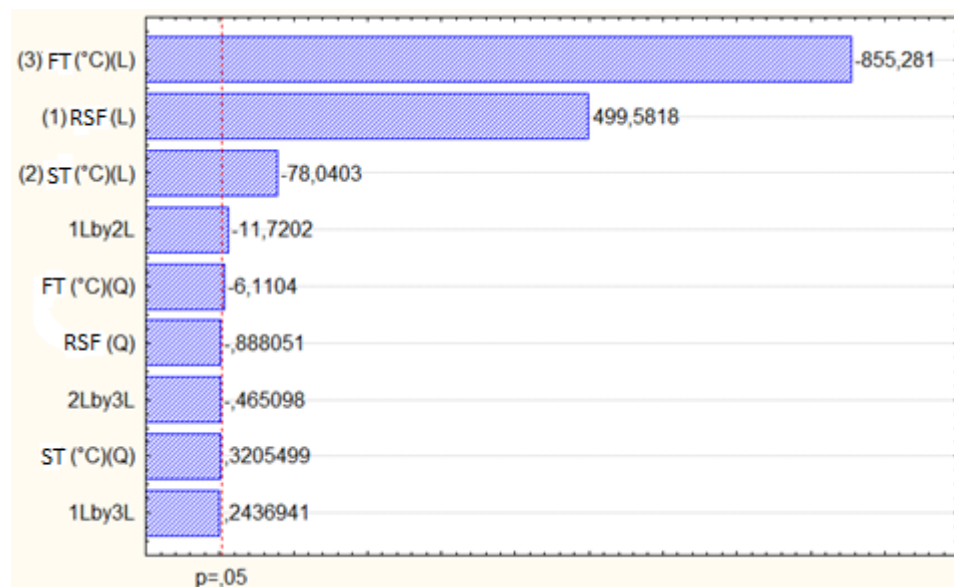


Figure 17. Pareto diagram

$$Qr = 0.3231 * 10^2 + 0.3179 * 10^2 x - 1.302 * 10^{-3} y - 21.67 * 10^2 z - 21.83 * 10^{-5} z^2 - 24.88 * 10^{-2} yx \quad (2)$$

The reboiler duty response surfaces are illustrated in Figures 18 to 20, which confirm the expected behavior: high feed and solvent temperatures and small RSF lead to a minimum energy consumption.

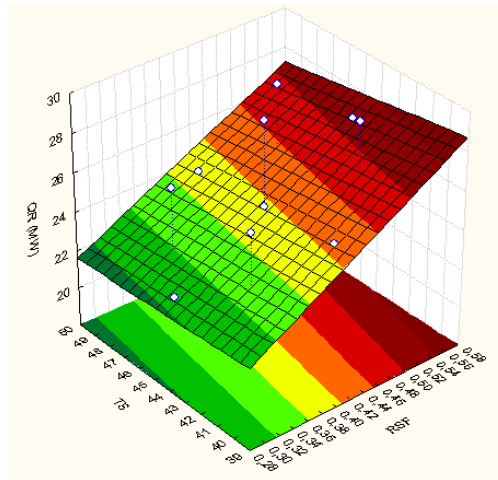


Figure 18. Reboiler duty dependence on solvent temperature and RSF ratio with feed temperature as the central point

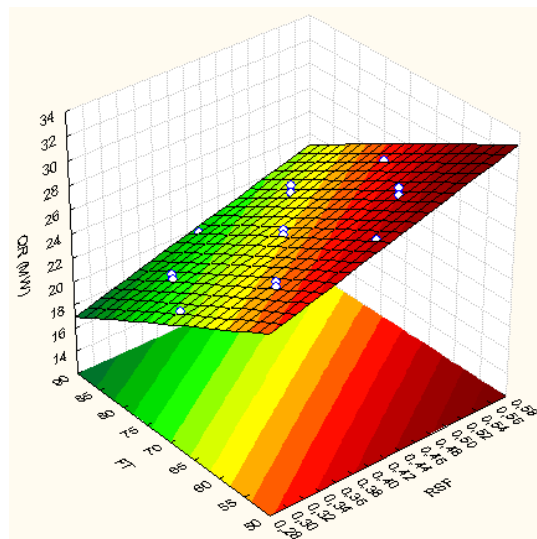


Figure 19. Reboiler duty dependence on feed temperature and RSF ratio with solvent temperature as the central point

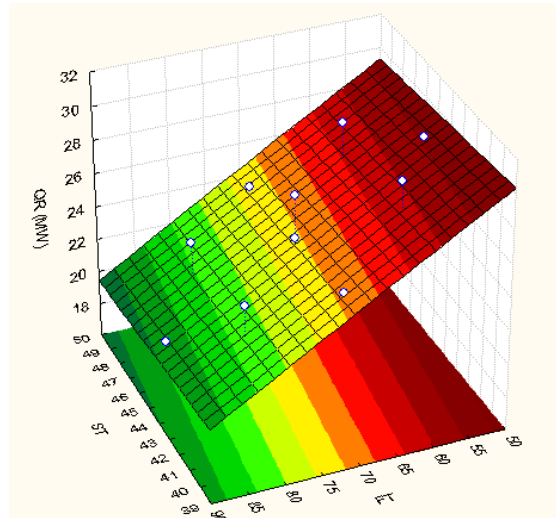


Figure 20. Reboiler duty dependence on feed temperature and solvent temperature with RSF ratio as the centralpoint

By applying the nonlinear minimization method GRG (generalized reduced gradient) using Equation 2 as the objective function, it is possible to find the values of the RSF, ST and FT that provide the minimum heat duty, as shown in Table 9. It can be seen that a reduction of 9.65% in the reboiler duty is possible. However, this optimal point would imply in operating with higher feed and solvent temperatures. Although there are heat exchangers and heat sources available in the unit, a plant layout analysis and a study of technical and economical viability are still necessary in order to establish if the changes in the operating point are advantageous or not.

Table 9. Optimal operating conditions.

| | <u>Optimal operating point</u> | <u>Operating point</u> | <u>Relative deviation (%)</u> |
|---------|--------------------------------|------------------------|-------------------------------|
| RSF | 0.350 | 0.388 | 9.80 |
| ST (°C) | 43.67 | 43.00 | 1.56 |
| FT (°C) | 82.56 | 75.00 | 10.08 |
| Qr (MW) | 20.69 | 22.90 | 9.65 |

6 Concluding remarks

This work presents a systematic methodology for the selection of the optimal operating conditions for an industrial acrylonitrile recovery unit based on the minimum energy consumption and products specifications as process restrictions. The optimization is based on the application of the Response Surface Methodology (RSM) and statistical analyses methods.

Unit models and simulation has been validated against plant data and information. As the complex quaternary system composed of acrylonitrile, acetonitrile, water and

hydrocyanic acid presents azeotropes and form two liquid phases in some trays of the extractive distillation column, adequate thermodynamic models had to be chosen. Binary parameters for the Redlich-Kwong equation of state and NRTL model were adjusted with mean errors of about . Pressure drop along the distillation columns and stage efficiency have been considered and calculated temperatures profile were in good agreement with planta data as depicted by the mean error of 2.0%. The developed model has proven to be able to capture the plant behavior in terms of temperature, flow rates and compositions trajectories.

A sensitivity analyses is used to identify the set of parameters which highly affects the energy consumption while keeping products specifications. It was found that solvent-feed ratio, and solvent and feed temperatures are these variables. Their operating ranges and role in the operational flexibility were also established. It was also concluded that the process behavior is very flexible in terms of feed and solvent stages position.

The optimal operating point and the multifunctional relationship among the three parameters and the reboiler duty are determined by applying the response surface methodology (RSM) and statistical analyses techniques as ANOVA. Results suggest that the optimum operating point is: solvent temperature of 43.67 °C, feed temperature of 82.56 °C and solvent/feed mass ratio of 0.35. Besides, feed stage may vary from 22 to 30 and solvent stage from 1 to 4. In this case, energy savings can reach up to 10%. Although, further studies need to be conducted in order to reach definite conclusions.

In general, the main contribution of this study is to show that even for old industrial facilities an efficient energy management with the use of optimization strategies can ensure greater environmental sustainability and economy.

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