Acrylonitrile Recovery System by Extractive Distillation: Simulation and Optimization

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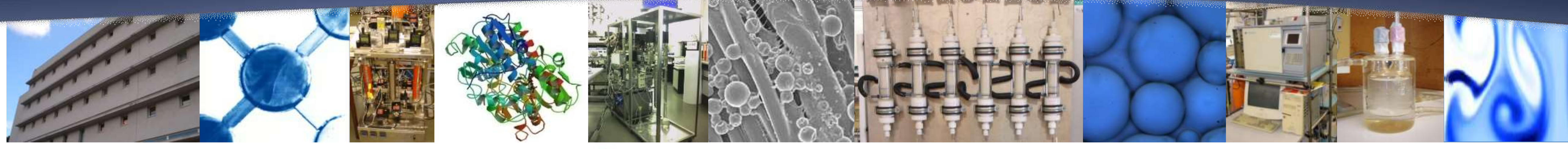

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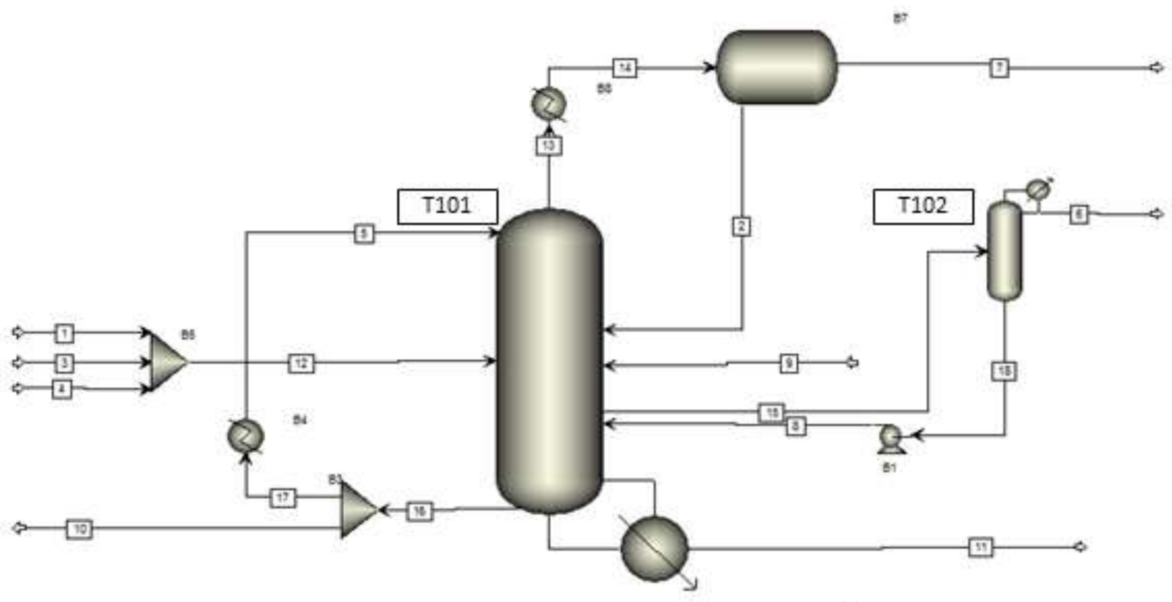
1. Introduction

- Acrylonitrile 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 acrylonitrile production process generates a wide variety of nitrogen compounds with similar physical and chemical characteristics, requiring a large amount of energy to separate.
- In this work, we simulate an acrylonitrile recovery unit, identifying the main operating variables that affect the energy consumption of the process.
- The simulations were performed at the Aspen Plus process simulator, as well as thermodynamic modeling of the system, which was based on experimental data collected in literature.
- The variables that affect the energy consumption of the system were identified by a parametric sensitivity analysis. The optimization of the optimal conditions were made using a statistical method in response surface.
- The results are presented only for variables that were significant for the energy consumption of the system.

2. Acrylonitrile Recovery System



1. Mix of nitrogen compounds.
2. T101 Reflux.
3. Mix of nitrogen compounds.
4. Mix of nitrogen compounds.
5. Solvent (water) recovered.
6. Acetonitrile aqueous mixture.
7. Acrylonitrile aqueous mixture.
8. Solvent (water) recovered.
9. Mixture of nitrogen compounds.
10. Aqueous effluent.
11. Aqueous effluent.
12. Mixture of nitrogen compounds.
13. Distillate vapor phase.
14. Distillate liquid phase.
15. Removing side.
16. Mixture of nitrogen compounds.
17. Mixture of nitrogen compounds.
18. Solvent (water) recovered.

3. Thermodynamic Modelling

The vapor phase deviations to ideality were considered by the Redlich-Kwong equation of state, while for the liquid phase the NRTL excess Gibbs energy model was selected. Several models have been tested within the Aspen platform, but that combination performed better. Information about the collected data to estimate and validate the thermodynamic model is given in table. The procedure used to make estimates of the parameters of the thermodynamic model, when necessary, is shown below.

System	Data type	Data Points	Source
Acrylonitrile + Acetonitrile	VLE	7	Blackford and York, 1965
Acrylonitrile + Hydrocyanic Acid	VLE	17	Sokolov et al., 1966
Acrylonitrile + Water	VLE	10	Gmehling et al., 1991
Acetonitrile + Hydrocyanic Acid	VLE	34	Gmehling et al., 1984
Acetonitrile + Water	VLE	11	Blackford and York, 1965
Hydrocyanic Acid + Water	VLE	18	Gmehling et al., 1991
Acrylonitrile + Acetonitrile + Water	VLE and LLE	40	Volpicelli, 1968; Sazonov et al., 2007

Temperature and composition calculation of the binary ← Thermodynamic model

Comparison between the model and experimental data ← Experimental data

Calculate the relative error to the experimental data

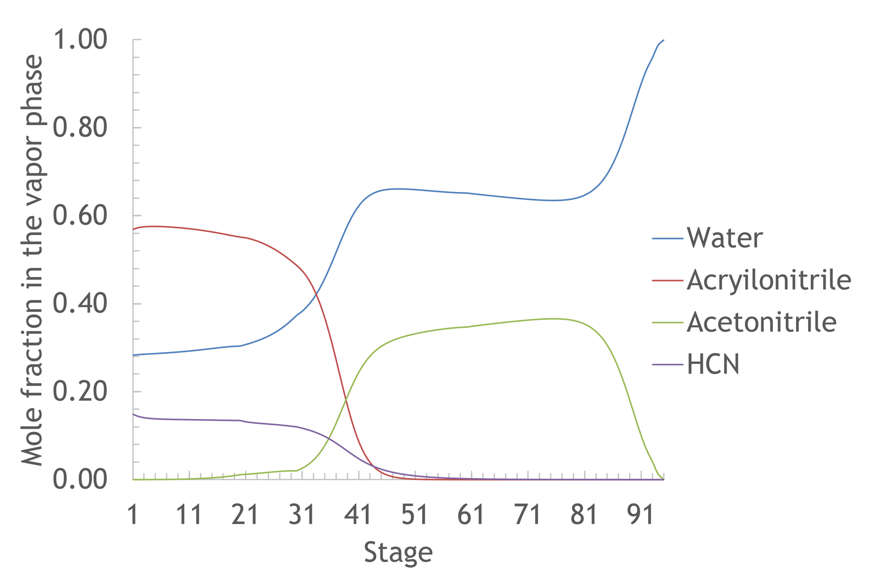
Erro ≤ 0,0001

Yes → Thermodynamic model is set

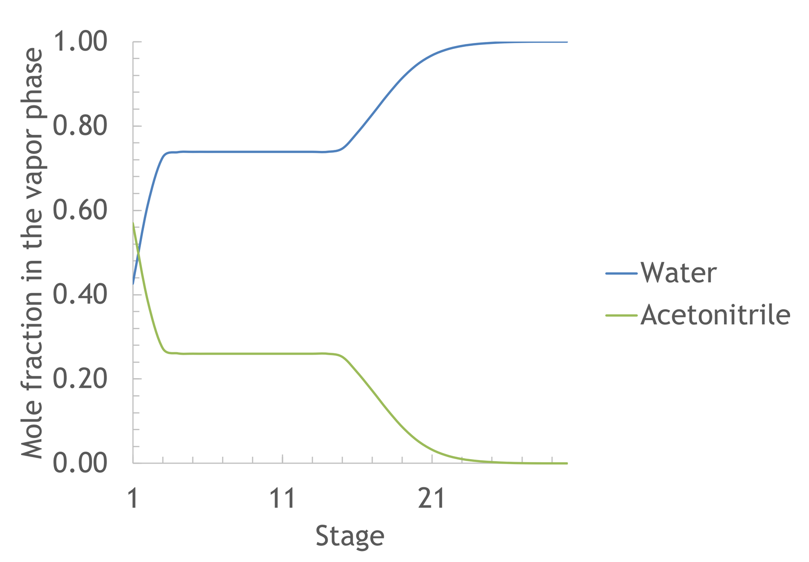
No → Parameter estimation of thermodynamic model → Thermodynamic model

4. Results

Simulation

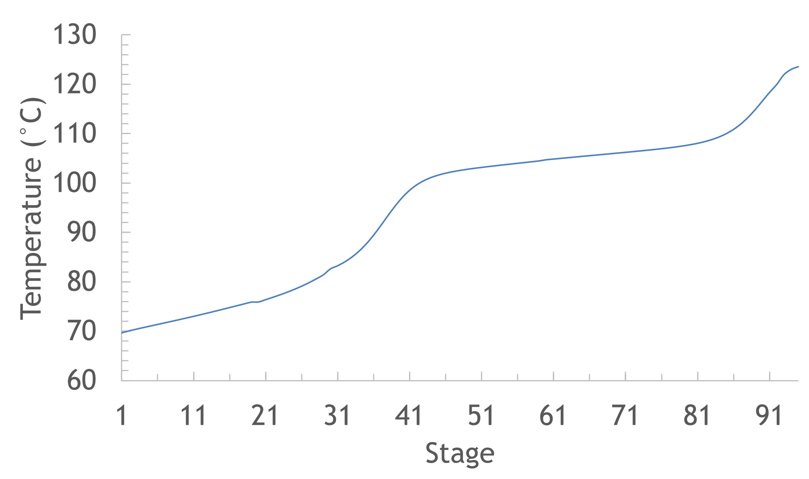


Composition Profile Acrylonitrile Extractive Distillation



Composition profile of the absorption column

Validation

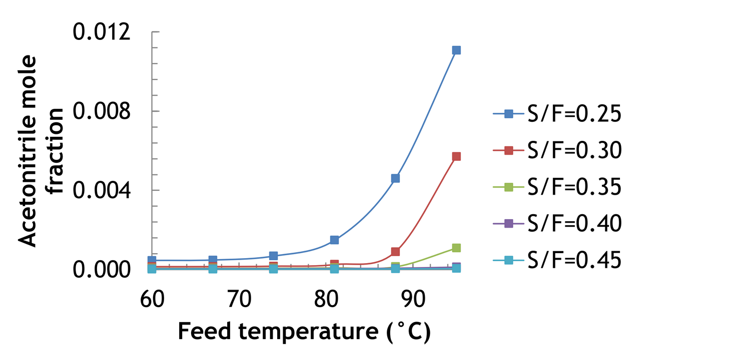


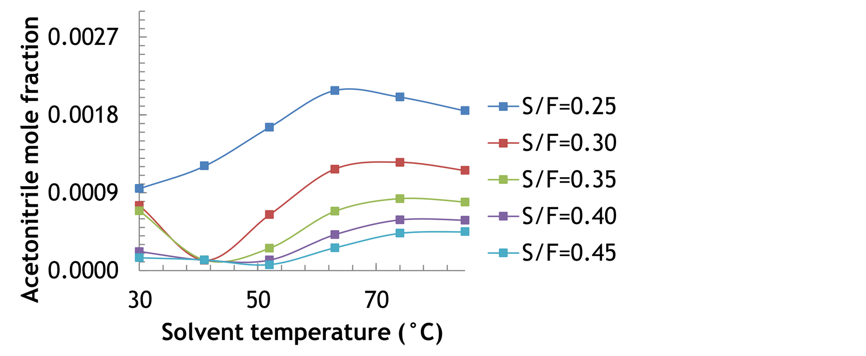
Temperature Profile Acrylonitrile Extractive Distillation

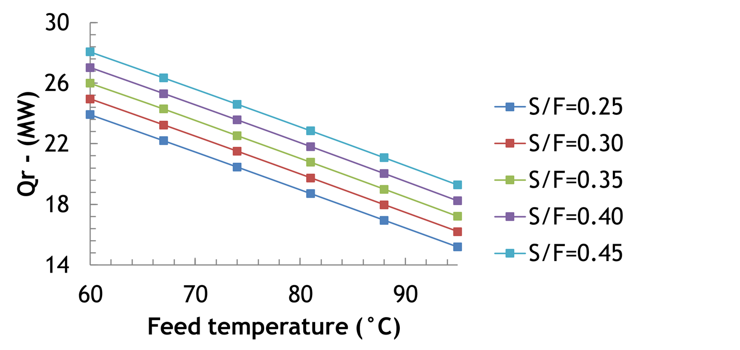
Relative deviations between the calculated and measured temperatures in different stages of the extractive distillation column.

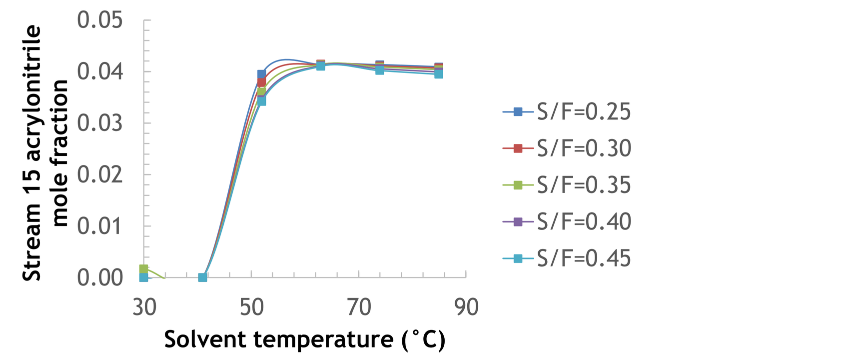
Stage	Deviation (%)
1	10.26
30	1.46
33	1.05
34	1.36
35	1.48
37	1.76
50	0.92
90	1.49
93	0.48
94	0.70
95	1.03

Sensitivity Analysis





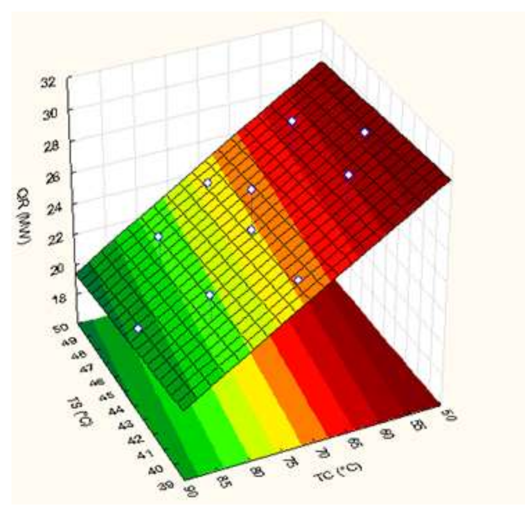




Optimization

Objective function to be minimized

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



Optimal operating conditions

RSF	0.350
ST (°C)	44.50
FT (°C)	80.56
Qr (MW)	20.69

5. Conclusions

- In order to do so, a thermodynamic approach based on the NRTL excess Gibbs energy model and Redlich-Kwong equation of state has been developed, pressure drop along the distillation columns considered and stage efficiency evaluated.
- Calculated temperature profile in the extractive distillation column has been compared with data from an industrial plant, showing very satisfactory agreement.
- From the sensibility analysis, solvent to feed mass ratio, and solvent and feed temperatures are the main variables interfering in the value of the reboiler duty.
- From the optimization, variables should follow or be changed to: Feed stage range: 22 to 30, Solvent stage range: 1 to 4, Solvent temperature: 44.50 ºC, Feed temperature: 80.56 ºC, Solvent to feed mass ratio: 0.350.
- Performing these modifications the reboiler duty will be approximately 20.69 MW, about 10% inferior to the value calculated using the actual operating conditions in the recovery system.

References

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