Separation of Acetonitrile and N-Propanol via Distillation

Mr. Ivica MARJANOVIC
UPMC – Université Pierre et Marie Curie, Paris – CAPGEMINI, Paris

Background & Description:

Acetonitrile and n-propanol are commonly used in chemical industries, particularly in chromatography and electrochemical applications. Their azeotropic behavior under atmospheric pressure makes conventional distillation ineffective for separation. This project focuses on the simulation of their separation using a two-column distillation process.

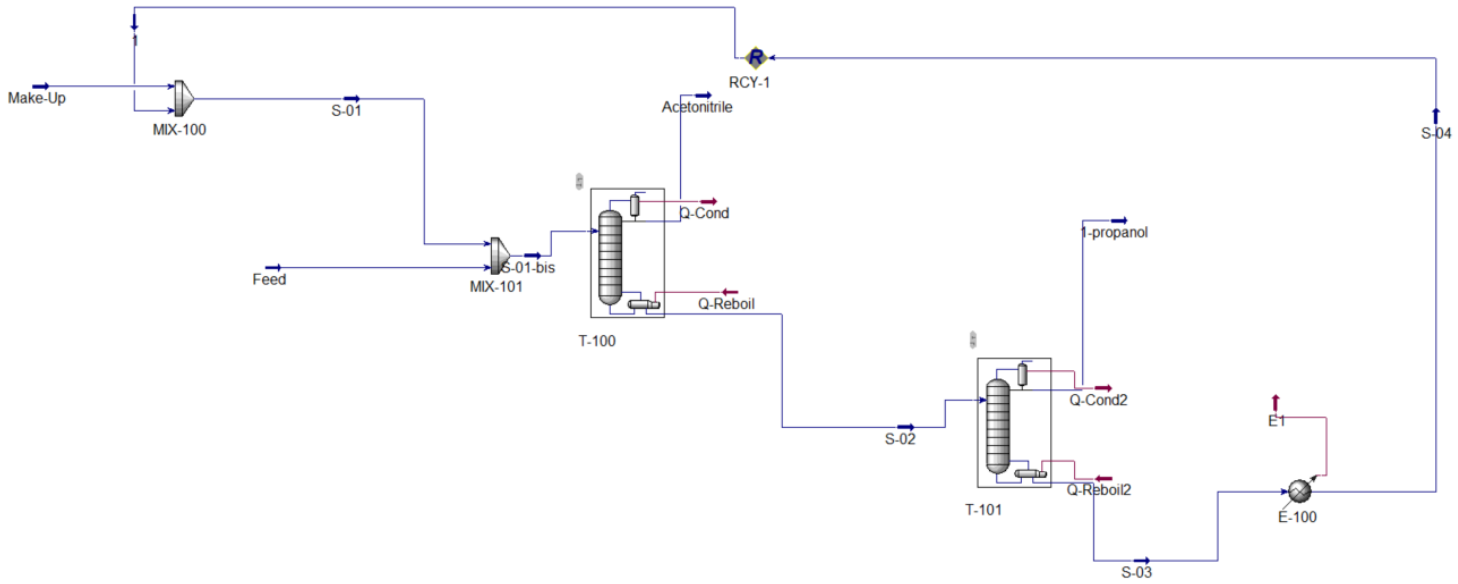
The process includes:

1. **First Column (Column 1)**: Designed to recover acetonitrile as the top product with a target purity of 97.25 mol%. The 1-propanol is retained in the bottoms at 99 mol%. This separation was simulated using Aspen HYSYS, starting with a ShortCut Column to estimate design parameters (number of stages, reflux ratio) and finalized with a Rigorous Distillation Column for detailed simulation and validation.
2. **Second Column (Column 2)**: Used to further separate 1-propanol from the heavier component (DMSO – dimethyl sulfoxide). A high-purity 1-propanol distillate was achieved (~99.1 mol%), with the bottom stream still containing ~98.9 mol% of 1-propanol, indicating a minimal loss to the bottom. Due to the low separation gradient, this column was simulated directly using a Rigorous Distillation model.

The simulation successfully achieved the separation objectives through conventional distillation without the use of extractive entrainers. The first column effectively removed acetonitrile, while the second provided fine purification of 1-propanol. Due to the very small composition difference between top and bottom products in Column 2, the use of Rigorous Distillation was necessary. The NRTL model proved suitable for accurately modeling the VLE behavior of the mixture. This process design may serve as a simplified alternative to extractive distillation, depending on purity requirements and energy constraints.

Thermodynamic package: The NRTL (Non-Random Two-Liquid) model was selected for its ability to accurately handle non-ideal mixtures involving polar components like acetonitrile and alcohols.

Flowsheet



Results:

Master Property Tableau								
Object	**Feed**	**Make-up**	**S-01-bis**	**S-02**	**Acetonitrile (P)**	**1-propanol (P)**	**S-04**	**1 (R)**
T (°C)	**25.00**	**95.00**	**36.06**	**98.50**	**82.04**	**97.03**	**100.8**	**95**
P (bar)	**1.013**	**1.013**	**1.013**	**1.013**	**1.013**	**1.013**	**1.013**	**1.013**
Molar Flow Kgmol/h	**22.43**	**1.152e-2**	**25.09**	**6.33**	**18.76**	**3.72**	**2.61**	**2.61**
Molar Flow (1-Propaol)	**4.16**	**0**	**6.48**	**5.96**	**0.53**	**3.69**	**2.26**	**2.26**
Molar Flow (AcetNit)	**18.27**	**0**	**18.27**	**0.03**	**18.23**	**0.03**	**0**	**0**
Molar Flow (DMS)	**0**	**1.152e-2**	**0.34**	**0.34**	**0**	**0**	**0.34**	**0.34**

Nb : Insignificant quantities (<0) of components in the product streams can be considered negligible, effectively approximating them to zero without impacting the overall process results or conclusions (see flowsheet).

References: Wang, H., Xue, L., Su, W., Li, X., Li, Y., & Li, C. (2018). Design and control of acetonitrile/N-propanol separation system via extractive distillation using N-methyl pyrrolidone as entrainer. Separation Science and Technology, 53(15), 2444-24