Modeling an Extractive Distillation Process in Aspen HYSYS: A Two-Column Phenol-Solvent System

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Background & Description:

This project focuses on simulating the extractive distillation of n-heptane and toluene using phenol as a high-boiling solvent in Aspen HYSYS, a commercial chemical process simulation platform. Since n-heptane and toluene have very similar boiling points, conventional distillation becomes inefficient. To overcome this, a selective solvent (phenol) is introduced to enhance the relative volatility between the components, allowing for effective separation.

Aspen HYSYS does not include a dedicated extractive distillation module. Therefore, a modular workaround was implemented using:

- Two Shortcut Columns (DSTWU) for preliminary analysis
- A phenol recycle loop for solvent recovery
- And ultimately, a transition to rigorous distillation columns for accurate simulation of the separation steps

The simulation workflow is divided into two key separation stages:

1. Primary Extractive Distillation

In the first column, a binary feed of n-heptane and toluene is combined with a phenol solvent stream. The presence of phenol enhances the volatility difference, favoring n-heptane to be recovered as the top product.

- Feed stream: 50 mol% n-heptane / 50 mol% toluene at 100.7 °C and 1 bar
- Solvent stream: 100% phenol at 180.4 °C and 1 bar (60 kmol/h)
- Top product: Predominantly n-heptane (mole fraction ≈ 0.9878)
- Bottom product: Mixture of toluene and phenol

2. Solvent Recovery and Toluene Purification

The second column receives the bottom stream from the first unit and separates toluene and phenol:

- Top product: High-purity toluene (≈ 99.05%)
- Bottom product: Phenol (≈ 99.999%), suitable for recycling

A mixer blends the recovered phenol with a make-up stream to compensate for losses. A recycle loop ensures solvent consistency in the process.

Thermodynamic package: Due to the unavailability of the UNIFAC model in Aspen HYSYS, the NRTL (Non-Random Two-Liquid) model was selected to accurately represent vapor–liquid equilibrium (VLE) in this non-ideal system.

- Accurately models non-ideal liquid mixtures
- Effective for polar solvents (like phenol) and non-polar hydrocarbons
- Proven convergence stability in distillation operations

Conclusion:

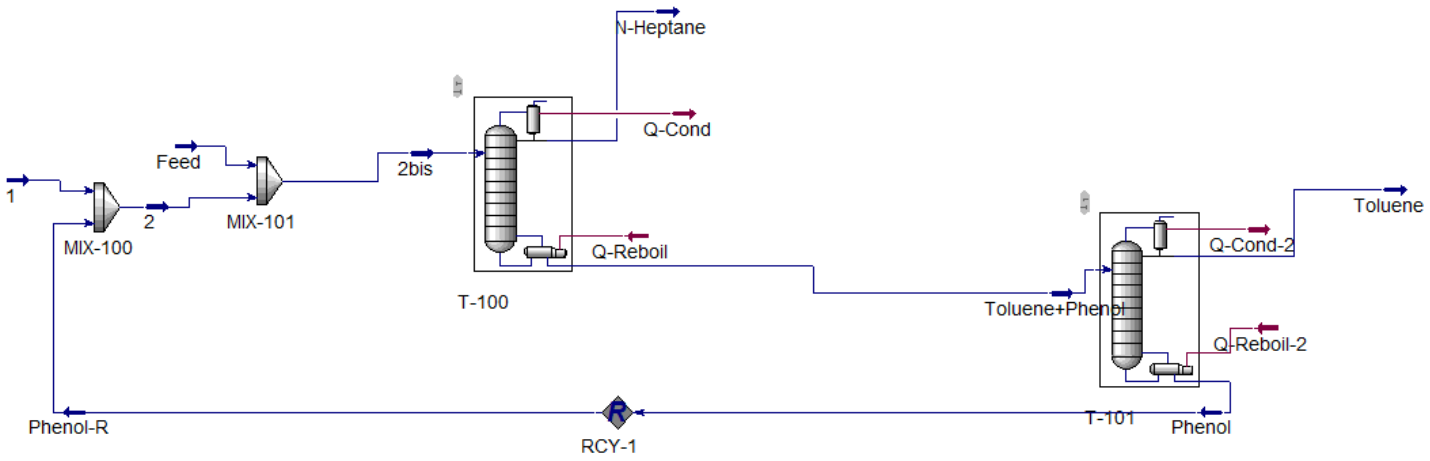
This simulation demonstrates that Aspen HYSYS, despite lacking a dedicated extractive distillation module, can successfully model complex solvent-based separations through a modular, stepwise approach.

- The use of phenol as an extractive solvent effectively improves the separation of n-heptane and toluene, which have very close boiling points.
- Shortcut Columns provided an initial design framework and operating targets.
- Subsequent Rigorous Distillation Columns enabled detailed analysis of stage requirements, thermal duties, and component purities.
- The NRTL property package captured much of the non-ideal behavior between polar (phenol) and non-polar (hydrocarbon) components.

However, simulation results indicate that n-heptane was not completely removed from the toluene–phenol mixture in the first extractive column. As a result, a small amount of n-heptane remains in the distillate of the second column, which was intended to yield high-purity toluene. This residual presence slightly reduces the purity of the recovered toluene.

This deviation may be attributed to the thermodynamic model limitations. While NRTL is suitable for many non-ideal systems, it may not perfectly capture all interactions in highly non-ideal ternary systems involving strong solvents like phenol. Future work could explore the use of alternative models, such as UNIFAC, if available, or implement parameter regression for more accurate VLE representation.

Overall, the approach demonstrates the feasibility of simulating extractive distillation systems in Aspen HYSYS using standard unit operations and opens possibilities for further refinement in process design and thermodynamic modeling.



Results:

Master Property Tableau					
Object	**Feed**	**N-Heptane**	**T+P**	**Toluene**	**Phenol**
T (°C)	**100.7**	**98.36**	**115.4**	**105.6**	**181.1**
P (bar)	**1**	**1**	**1**	**1**	**1**
Molar Flow	**100.0**	**41.74**	**118.7**	**58.26**	**60.39**
Mole Fract (n-Heptane)	**0.5**	**0.9498**	**0.0873**	**0.1778**	**0**
Mole Fract (Phenol)	**0**	**0**	**0.5090**	**0**	**1**
Mole Fract (Toluene)	**0.5**	**0.0502**	**0.4037**	**0.8222**	**0**

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: https://lms.nchu.edu.tw/sysdata/doc/c/ca9cbcaa03cb9d9f/pdf.pdf