Modeling a Reactive Distillation Process in Aspen HYSYS: A Sequential Reactor–Column Approach

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Background & Description:

This project focuses on simulating the metathesis of cis-2-pentene into cis-2-butene and cis-2-hexene using Aspen HYSYS, a commercial chemical process simulator. Due to the absence of a dedicated reactive distillation module in Aspen HYSYS, a sequential approach was developed involving a chemical reactor followed by a distillation column. The objective was to reproduce the process described in the literature, particularly by Housam Binous and Ahmed Bellagi.

The studied reaction is as follows:

2 cis-2-pentene→ cis-2-butene + cis-2-hexene

The process is carried out in two main steps:

1. **Reaction**: A Conversion Reactor (RCSTR) is used to convert cis-2-pentene with 100% conversion efficiency at 73.2 °C and 304 kPa. The reaction is modeled as a conversion reaction, assuming complete transformation of the reactant.
2. **Separation**: The vapor and liquid products of the reactor are combined using a Mixer, and the resulting stream is fed into a Distillation Column. This column separates::
    - **cis-2-butene** as the **top product** (more volatile).
    - **cis-2-hexene** as the **bottom product**.

The system was modeled using the Peng-Robinson thermodynamic model, selected for its compatibility with light hydrocarbons and non-polar olefin systems. While the simulation does not employ a true reactive distillation column, the two-step strategy effectively mimics the behavior of such a system within the limitations of HYSYS.

Thermodynamic package: The Peng-Robinson equation of state was selected as the thermodynamic model due to:

- Its reliability with non-polar hydrocarbons
- Its compatibility with vapor-liquid equilibrium (VLE) behavior in olefins
- Its availability and stability in Aspen HYSYS simulations

Challenges & Convergence: While the shortcut column (DSTWU) converged easily and provided useful estimates (reflux ratio, number of stages), the rigorous distillation column required proper specification of:

- Feed stage
- Reflux ratio
- Distillate or bottoms flow rate

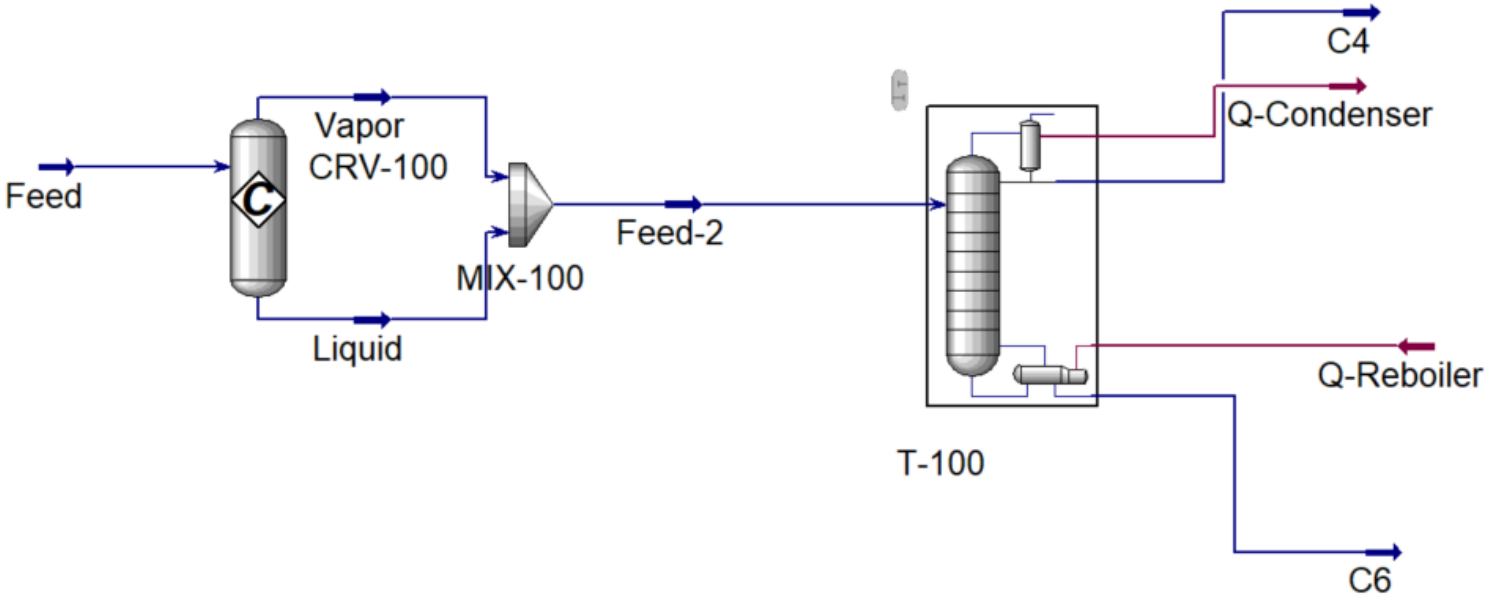
A reflux ratio of 10 and distillate rate of ~50 kmol/h allowed the column to converge and meet the purity targets from literature.

Conclusion:

This simulation successfully reproduces the reactive distillation behavior using a reactor–column sequence in Aspen HYSYS. The results confirm that:

- Complete conversion of cis-2-pentene can be modeled via a Conversion Reactor
- The distillation column can effectively separate the metathesis products under standard conditions
- Aspen HYSYS, although lacking a direct reactive distillation block, can simulate the full process via modular assembly

This approach can be applied to other reactive separation systems, offering flexibility and insight into reaction–separation interactions using widely available simulation tools.



Results:

Master Property Tableau				
Object	**Feed**	**Feed-2**	**Top Product (C4)**	**Bottom Prod (C6)**
T (°C)	**73.2**	**73.2**	**36.7**	**108.9**
P (kPa)	**304**	**304**	**304**	**304**
Molar Flow	**100.00**	**100.00**	**49.92**	**50.08**
Molar Flow (Pent)	**100.00**	**0**	**0**	**0**
Molar Flow (C4)	**0**	**50.00**	**49.81**	**0.19**
Molar Flow (C6)	**0**	**50.00**	**0.11**	**49.89**

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: Binous, H., & Bellagi, A. (2013). Simulation of The Separation of Industrially Important Hydrocarbon Mixtures by Different Distillation Techniques Using Mathematica©. Advances in Systems Engineering Research, 47-78. ISBN: 978-1-62948-310-8