Modeling the Production of Toluene by Dehydrogenation of Normal Heptane : A Reactor–Flash Separator Approach

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Background & Description:

This project focuses on simulating the catalytic dehydrogenation of normal heptane (n-heptane) to produce toluene and hydrogen using Aspen HYSYS, a commercial chemical process simulator. The simulation models a typical process consisting of a heater, a conversion reactor, and a flash separator. The objective is to replicate a feasible industrial configuration for toluene production by partial dehydrogenation of n-heptane using a Cr_2O_3 catalyst.

The studied reaction is:

$$\mathbf{CH_3(CH_2)_5CH_3 \rightarrow C_6H_5CH_3 + 4H_2}$$

The process is carried out in two main steps:

1. **Reaction**: The feed (n-heptane) is heated from 18 °C to 427 °C using a Heater. It is then sent to a Conversion Reactor, which operates isothermally and converts 15 mol% of the n-heptane into toluene. This conversion level reflects typical industrial operation, where complete conversion is not always desired for economic and catalyst life reasons.
2. **Separation**: The reactor outlet is cooled to 18 °C and introduced into a Flash Separator operating at 1 atm (101.3 kPa). In the flash, the hydrogen gas is separated from the liquid phase containing unreacted n-heptane and the produced toluene.

Thermodynamic package: The simulation uses the Peng-Robinson equation of state, selected for its strong performance with:

- Non-polar hydrocarbons and light gases
- Accurate vapor-liquid equilibrium (VLE) behavior for systems containing hydrogen and aromatics
- Broad availability and robustness in Aspen HYSYS simulations

Challenges & Convergence: The simulation required careful setup, particularly regarding:

- Defining the correct stoichiometry and fractional conversion in the Conversion Reactor
- Ensuring proper vapor–liquid separation conditions in the flash unit
- Selecting appropriate pressure and temperature specifications across units to maintain convergence

Despite these challenges, the model converged successfully by starting with realistic estimates for feed flow rates and product separation.

Results:

- Toluene was successfully produced with a 15% conversion of n-heptane
- Hydrogen was effectively separated as the top vapor stream in the flash unit
- Compositional and flow data were obtained for all process streams

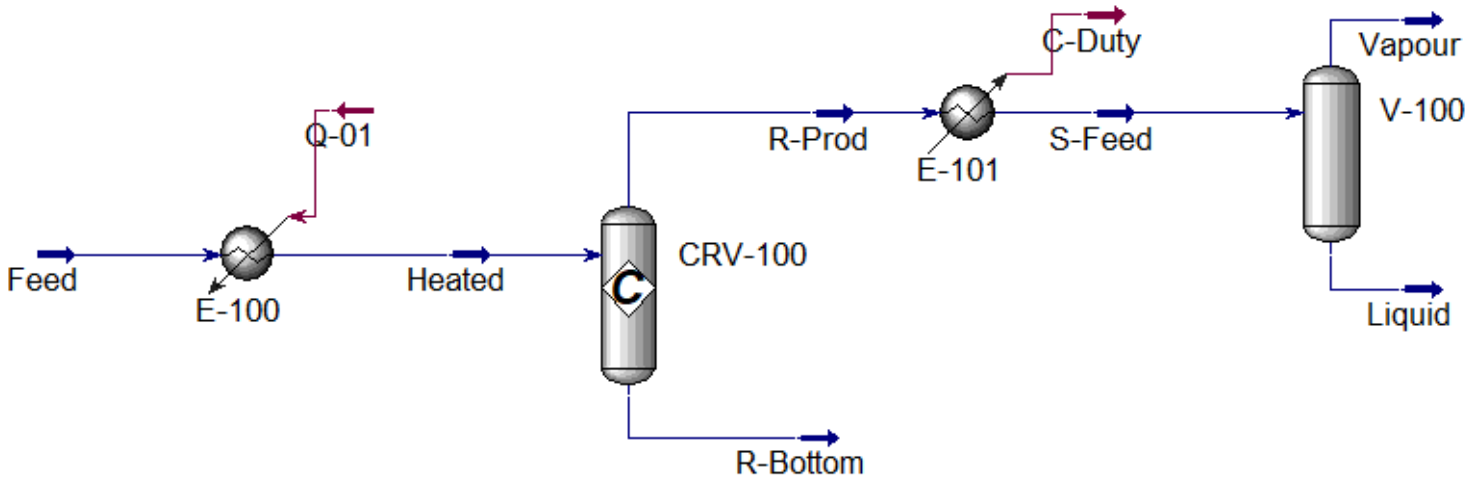
Conclusion:

This Aspen HYSYS simulation confirms that:

- The Conversion Reactor can effectively model the partial dehydrogenation of n-heptane
- A Flash Separator is sufficient to isolate the hydrogen from heavier hydrocarbon products
- Aspen HYSYS, though lacking a specific reactive distillation block, allows full modeling of this process using basic unit operations

This modular approach can be extended to simulate similar reaction–separation processes, offering flexibility and insight into integrated chemical systems using readily available tools in HYSYS.

Flowsheet



Results:

Master Property Tableau							
Object	**Feed**	**Heated**	**R-Bottom**	**R-Prod**	**S-Feed**	**Vapour**	**Liquid**
T (°C)	**18.33**	**426.7**	**300.6**	**300.6**	**18.33**	**18.33**	**18.33**
P (bar)	**1.013**	**1.013**	**1.013**	**1.013**	**1.013**	**1.013**	**1.013**
Molar Flow (kmole/h)	**34.52**	**34.52**	**0**	**55.23**	**55.23**	**21.64**	**33.59**
Mole Fract (Hydrogen)	**0**	**0**	**0.3771**	**0.3750**	**0.3750**	**0.9558**	**0.0009**
Mole Fract (n-Heptane)	**1**	**1**	**0.5294**	**0.5313**	**0.5313**	**0.0384**	**0.8488**
Mole Fract (Toluene)	**0**	**0**	**0.0935**	**0.0938**	**0.0938**	**0.0058**	**0.1504**

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: "HYSYS:An Introduction to Chemical Engineering Simulation " by Mohd Kamaruddin Abd Hamid Chapter-13 Page no-146.