PRODUCTION OF N-OCTANE FROM ETYLENE AND I-BUTANE Contributor

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Background:

N-octane is a colorless liquid having density less than of water and with a gasoline-like odor. The octane rating of a fuel determines the extent of compression of air-fuel mixture before ignition. Gasoline with an optimal octane rating performs best in an engine designed to run on that octane level. The widespread use of octane involves as fuels and fuel additives, intermediates and as solvents for product formation.

Description of flowsheet:

The thermodynamic model used in this flowsheet is the Raoults law equation of state as it accounts for feed materials operating at high pressure. The reactor used is a conversion reactor that performs the energy and mass balances based on the stoichiometry and the specified conversion.

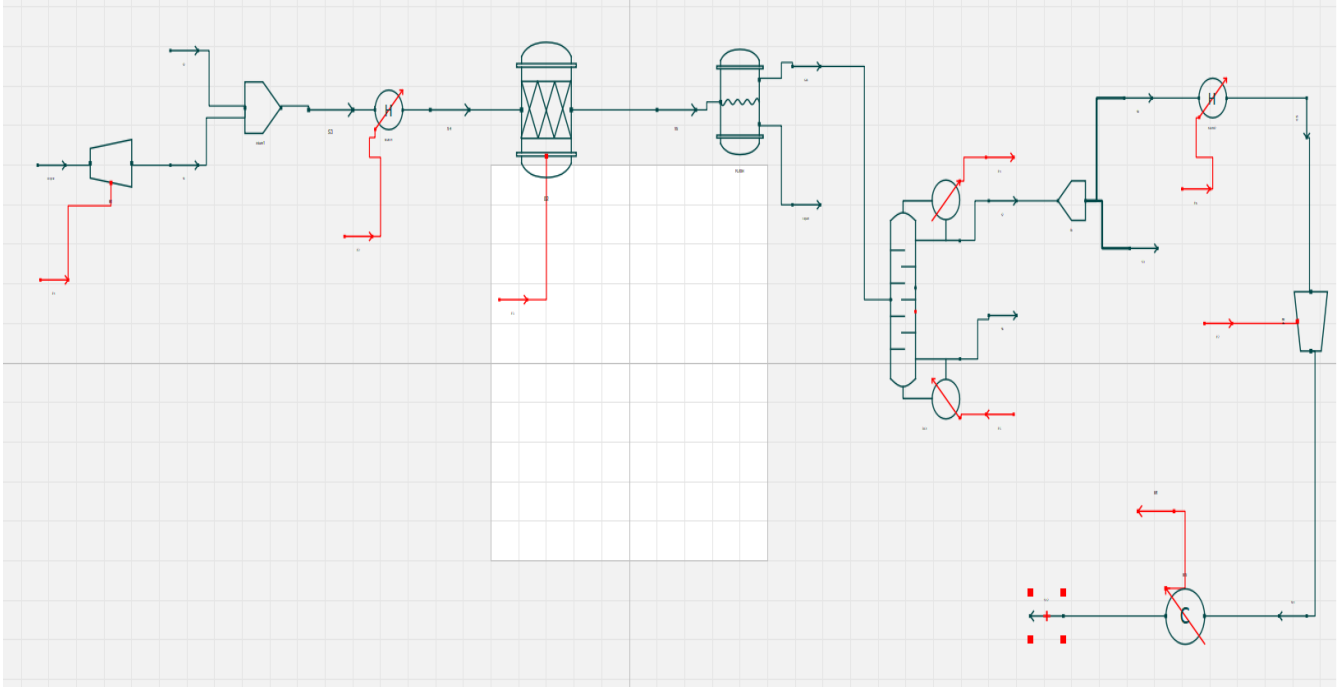
Reactions Involved: $2C_2H_4(ethylene) + C_4H_{10}(i\text{-}butane) \rightarrow C_8H_{18}(n\text{-}octane)$

The feed stream consisting of ethylene and i-butane in stoichiometric proportions (along with nitrogen and n-butane as inerts) is fed to the conversion reactor at 366.15 K and 137895 Pa. The other stream coming out of the reactor is passed through a flash column . A flash column is used to separate the gas and liquid phase products. After that the gas phase product is sent to Distillation Column where it further get purified and from top product it sent to splitter wher it split into two product. One product is again sent to compressor to increase its pressure.

The distillate stream contains some unconverted raw material that is recycled back. The recycle system consists of a purge stream, a compressor and a heater with a 10% purging performed to avoid trapping of unconverted feed. The compressor is used to match the pressure of the distillate stream to that of the feed stream. A cooler unit is used to cool down the temperature of the stream that has increased due to compression to match the reactor operating temperature. The outlet of the cooler is passed through a recycle unit and finally mixed with the feed stream. The stream coming out of recycle unit (R-1 in flowsheet) has a higher pressure (+4 psia) and a lower temperature (-5℃ after passing through expander) than that of needed for the feed stream. Hence, it is passed through an adiabatic expander and a recycle preheater before being mixed with the feed stream.

The flowsheet is integrated in such a way that the condenser duty is recycled and fed to meet the reboiler duty needs; much in a similar way the energy stream coming out of the cooler is recycled to the preheater.

Flowsheet:



Results:

Stream	Temperature (K)	Pressure (Pa)	Molar Flow (mol/s)	Mole Fraction N-Octane
S4	366.15	137895	0.8481	0.0316
Liquid	366.15	137895	3.4846	0.9649
S6	313.85	101325	0.00237	0.7713

Conclusion:

N-octane is produced with 96% purity from the condensate stream of the distillation column.

Reference:

- Foo, Dominic Chwan Yee, Murugan Selvan, and Michael Lynn McGuire. "Integrate process simulation and process synthesis." *Chemical engineering progress* 101, no. 10 (2005): 25-29.