PRODUCTION OF N-OCTANE FROM ETYLENE AND I-BUTANE

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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 Peng-Robinson 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:

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

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 93℃ and 20 psia. The other stream coming out of the reactor which is ethylene rich is passed through a shortcut distillation column. A shortcut distillation column is used which performs the calculations based on the Fenske-Underwood-Gilliland model. The condenser chosen is a partial condenser with the light key component chosen as ethylene (0.0015 mole fraction) and heavy key component as n-octane (0.28 mole fraction).

The distillate stream contains some unconverted raw material that is recycled back. The recycle system consists of a purge stream, a compressor and a cooler 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.

Results:

STREAM	TEMPERATURE (K)	PRESSURE (Pa)	MOLAR FLOW (mol/s)	Mole fraction N-octane
Reactor Feed	365.256	137895	9.61996	0.0326
3	365.256	89631.8	2.53409	0.9699
Condensate	349.699	101325	0.29358	0.9427

Conclusion:

N-octane is produced with 94.27% 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.