Pentane isomerization for Naphtha stream

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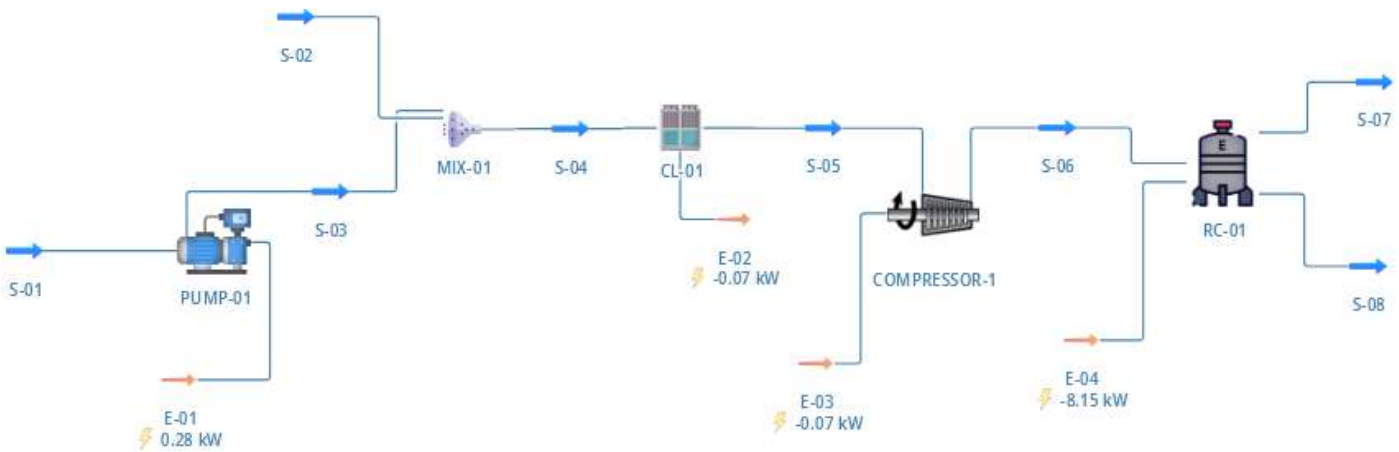
Background & Description:

Naphtha stream taken from the fractionated distillation column, in oil refining contains a major portion of n-pentane (48.9 %), which has a research octane number (RON) of 61.7. This n-pentane can be isomerized to give i-pentane, which has a research octane number (RON) of 92.3. The process requires a naphtha stream at atmospheric conditions, which is pressurized to 1311.6 kPa by the pump. This stream is mixed with hydrogen, having a molar flow 1.5 times that of n-pentane, in a mixer. This well-mixed stream is then sent to a cooler which reduces the temperature of the mixture to -100 C and hence is pressurized to 2 MPa by an adiabatic compressor working at 50% efficiency.

This treated feed stream enters an equilibrium reactor, working on the Redlich-Kwong state model, where n-pentane is isomerized to i-pentane with the standard Gibb's free energy of reaction equal to -5237 kJ/kmol of n-pentane at a temperature of -125 C. During this process, the maximum concentration of i-pentane at the reactor it is contained by the thermodynamic equilibrium between the three species, namely pentane, neopentane, and isopentane. Various pressure and temperature combinations were tested and the optimum result was obtained at the specified conditions with the achieved conversion of 96.5082% and isomerization extent of 2.47006 kmol/hr.

Units used: Temperature in C, Pressure in kPa, Molar flux in kmole/h, Mass flux in kg/h, Volumetric flow in m3/h and Density in kg/m3.

Flowsheet:



Naphtha treatment for pentane polymerization flowsheet

Results:

Naphtha Stream		
Object	**S-01**	**Unit**
Temperature	25	C
Pressure	101.325	kPa
Mass Flow	386.767	kg/h
Molar Flow	5.234	kmol/h
Volumetric Flow	0.621981	m3/h
Density (Mixture)	621.831	kg/m3
Molar Enthalpy (Mixture)	-27095.5	kJ/kmol
Mole Fractions		
Ethane	0.0032	
Propane	0.001	
N-butane	0.0008	
Isobutane	0.0048	
N-pentane	0.489	
Isopentane	0.3686	
N-hexane	0.1278	
N-heptane	0.0028	
N-nonane	0.0019	
N-dodecane	0.0001	

Reactor Outlet		
Object	**S-08**	**Unit**
Temperature	-125	C
Pressure	2000	kPa
Mass Flow	386.838	kg/h
Molar Flow	5.27026	kmol/h
Volumetric Flow	0.509815	m3/h
Density (Mixture)	758.781	kg/m3
Molar Enthalpy (Mixture)	-47007.9	kJ/kmol
Mole Fractions		
Ethane	0.003167254	
Propane	0.000993	
N-butane	0.000794492	
Isobutane	0.004766916	
N-pentane	0.016957341	
Isopentane	0.83474074	
N-hexane	0.12692053	
N-heptane	0.002780732	
N-nonane	0.001886925	
N-dodecane	9.93E-05	
Hydrogen	0.006892769	

Table 1: Streamwise Results for the Pentane isomerization for Naphtha stream