Production of Cyclohexane

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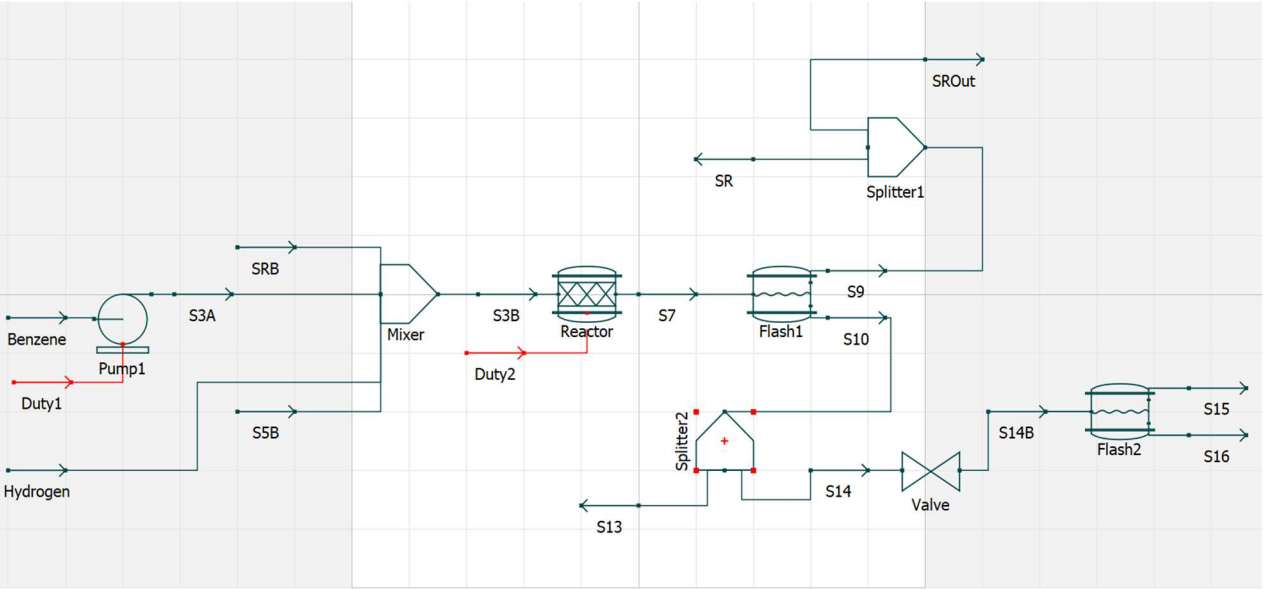
In this project, a liquid benzene stream at 311K is first pumped from 103.4 kPa to 23.1MPa, which is mixed with a hydrogen stream (at 322K and 23.1MPa, also contains trace amounts of nitrogen). There are two recycle streams also present from the upper and lower sections. The mixed stream goes into a **conversion reactor** where the main reaction takes place (with 99.85% conversion).

As opposed to the DWSIM sheet, this is an *isothermal* reactor, so a cooler is not necessary. The vapor-liquid mixture is sent to Flash-1 where is separates into vapor and liquid streams respectively. The vapor stream is split by the splitter into a ratio of (0.9918:0.0082) giving a hydrogen enriched stream in `SROut' while the latter is recycled back from the top.

The liquid stream from Flash-1 is also split into a ratio of (0.62:0.38) into S14 and S13. The S13 stream is brought back to 23.1MPa with a pump and recycled back. The S14 stream is exhausted through a valve to 103.4kPa, after which it is flashed again in Flash-2. The final liquid stream S16 is the product of the process, enriched in cyclohexane.



Flowsheet in OMEdit

All the results obtained are tabulated in the following table: (OpenModelica, Raoult's Law)

Streams	Temperature (K)	Pressure (Pa)	Total flowrate (mol/s)	Mole Fractions (hydrogen, nitrogen, cyclohexane, benzene)
Benzene	310.928	103421	11.61	(0, 0, 0, 1)
Hydrogen	322.039	2.31×10^6	35.76	(0.99704, 0.00296, 0, 0)
SROut	314.559	2.2×10^6	1.07	(0.875, 0.112798, 0.0118, 1.08×10^{-5})
S15	314.556	103421	~0	(6.5×10^{-12}, 0.747, 0.25192, 0.00023)
S16	314.556	103421	11.5943	(1.09×10^{-5}, 1.61×10^{-5}, 0.999053, 0.000931)

The results from DWSIM are as follows: (Raoult's Law)

Streams	Temperature (K)	Pressure (Pa)	Total flowrate (mol/s)	Mole Fractions (hydrogen, nitrogen, cyclohexane, benzene)
Benzene	310.928	103421	11.6094	(0, 0, 0, 1)
Hydrogen	322.039	2.3097×10^6	35.7582	(0.99704, 0.00296, 0, 0)
SROut	322.043	2.0684×10^6	0.9758	(0.8749, 0.1082, 0.0168, 1.55×10^{-5})
S15	323.335	103421	~0	(0.893, 0.10946, 0.0175, 1.6148×10^{-5})
S16	323.335	103421	11.5955	(0.0002236, 1.739×10^{-5}, 0.998828, 0.000931)

It is visible that the values are in good agreement. However, due to convergence issues, a lot of start values needed to be provided in the OM Chemical Simulator.