Production of Heptenes from Propylene and Butenes

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Background:

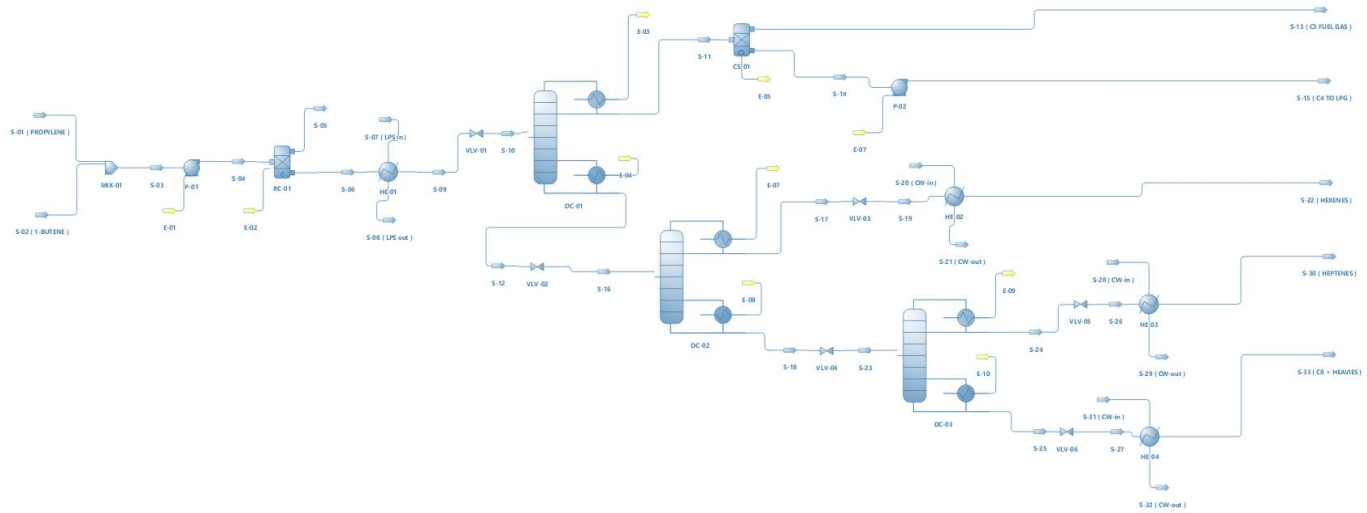
1-heptene finds its application mainly as a high-octane blending agent for gasoline or in plasticizer production. It is also used in the organic synthesis of perfumes, dyes and resins.
The simulated process converts a mixture of C_3 and C_4 unsaturated hydrocarbons to 1-heptene and other heavier unsaturated products.
Four primary reactions occur in the reactor:

- $C_3H_6 + C_3H_6 \rightarrow C_6H_{12}$ (1-hexene)
- $C_3H_6 + C_4H_8 \rightarrow C_7H_{14}$ (1-heptene)
- $C_4H_8 + C_4H_8 \rightarrow C_8H_{16}$ (1-octene)
- $C_3H_6 + 2C_4H_8 \rightarrow C_6H_{12}$ (1-undecene)

Description:

In the simulation, two fluid packages are used. The Soave-Redlich-Kwong (SRK) fluid package is used to model all the streams containing hydrocarbons while the Steam Tables (IAPWS-IF97) fluid package is used to model cooling water (cw) and low-pressure steam (lps) flowing through the heat exchangers. The C5 System of units is used in which temperature has unit °C, pressure has unit bar and molar flowrate is in kmol/hr.
The two feed streams, one containing propane and propylene (C3 feed) and the other containing isobutane, N-butane, isobutene and 1-butene (C4 feed) are first mixed together by mixer MIX-01 and fed to the conversion reactor RC-01 at a pressure 8 bar. The four primary reactions mentioned above occur in the reactor. The reactor effluent is vaporized partially before feeding it to the first distillation column DC-01. The feed enters the distillation column at a pressure 5.8 bar and the unreacted C3 and C4 components are removed as the top product after which it is sent to the component splitter to separate C3 and C4 component mixture. From the component splitter, the vapor phase C3 component stream is sent as a fuel gas at a temperature 45°C and pressure 5 bar. The liquid phase C4 stream is sent to LPG storage at a temperature 45°C and pressure 6.5 bar. The bottom product from the first distillation column DC-01 is again partially vaporized and sent to the second distillation column DC-02 to separate 1-hexene as top product. The feed to the second distillation column DC-02 is at a pressure of 2.5 bar. The liquid stream containing 1-hexene is cooled to a temperature 45°C and has pressure 1.7 bar. The bottom product from the second distillation column DC-02 is further partially vaporized and sent to the third distillation column DC-03 to separate 1-heptene from 1-octene and 1-undecene. The feed to the third distillation column is at a pressure of 2 bar. The liquid stream containing 1-heptene obtained as the product is at a temperature 45°C and pressure 1.2 bar.

Flowsheet:



Process Flowsheet for Production of Heptenes from Propylene and Butene

Results:

Object	S-33 (C8 + HEAVIES)	S-30 (HEPTENES)	S-27	S-26	S-25	S-24	S-23	S-22 (HEXENES)	S-19	S-16
Temperature	45	45	147.04	95.1985	153.129	107.036	125.886	45	72.2279	117.537
Pressure	1.7	1.2	1.7	1.2	2	1.5	2	1.7	1.7	2.5
Molar Flow	10.5051	25.8007	10.5051	25.8007	10.5051	25.8007	36.3058	22.3891	22.3891	58.6949
Molar Fraction (Vapor)	0	0	0.0596128	0	0	0	0.0782101	0	0.0372012	0.303745
Molar Flow (Mixture) / Propane	1.70834E-54	9.48991E-24	1.70834E-54	9.48991E-24	1.70834E-54	9.48991E-24	9.49042E-24	0.000195268	0.000195268	0.000195266
Molar Flow (Mixture) / Propylene	2.44124E-59	1.35575E-27	2.44124E-59	1.35575E-27	2.44124E-59	1.35575E-27	1.35582E-27	1.76675E-07	1.76675E-07	1.76673E-07
Molar Flow (Mixture) / Isobutane	3.84243E-41	3.04305E-16	3.84243E-41	3.04305E-16	3.84243E-41	3.04305E-16	3.04322E-16	0.13729	0.13729	0.137288
Molar Flow (Mixture) / N-butane	1.74754E-36	8.93802E-14	1.74754E-36	8.93802E-14	1.74754E-36	8.93802E-14	8.9385E-14	0.736306	0.736306	0.736297
Molar Flow (Mixture) / Isobutene	6.50559E-40	7.34795E-16	6.50559E-40	7.34795E-16	6.50559E-40	7.34795E-16	7.34834E-16	0.0710619	0.0710619	0.071061
Molar Flow (Mixture) / 1-butene	8.05335E-39	6.09355E-15	8.05335E-39	6.09355E-15	8.05335E-39	6.09355E-15	6.09387E-15	0.430828	0.430828	0.430822
Molar Flow (Mixture) / 1-hexene	4.91136E-10	0.250387	4.91136E-10	0.250387	4.91136E-10	0.250387	0.250401	20.7499	20.7499	21
Molar Flow (Mixture) / 1-heptene	0.798272	25.4611	0.798272	25.4611	0.798272	25.4611	26.2606	0.26356	0.26356	26.5244
Molar Flow (Mixture) / 1-octene	7.31908	0.0891963	7.31908	0.0891963	7.31908	0.0891963	7.40732	2.49644E-08	2.49644E-08	7.40737
Molar Flow (Mixture) / 1-undecene	2.38775	4.17221E-19	2.38775	4.17221E-19	2.38775	4.17221E-19	2.38743	9.67473E-28	9.67473E-28	2.38745

S-15 (C4 TO LPG)	S-14	S-13 (C3 FUEL GAS)	S-12	S-11	S-10	S-06	S-04	S-03	S-02 (1-BUTENE)	S-01 (PROPYLENE)	
45.2041	45.1126	45.1126	149.694	45.1126	94.228	45	25.7432	25.6824	25.505	24.8626	C
6.5	5.5	5.5	5.8	5.5	5.8	7.7	8	7.3	3	11.6	bar
116.356	116.356	2.99995	58.6949	119.356	178.051	178.051	237.83	237.83	163.21	74.62	kmol/h
0	0	1	0	0	0.676963	0	0	0	0	0	
0.559976	0.559976	2.99995	0.000195266	3.55992	3.56	3.56	3.56	3.56	0	3.56	kmol/h
0.00710606	0.00710606	0	1.76673E-07	0.00710606	0.007106	0.007106	71.06	71.06	0	71.06	kmol/h
29.3037	29.3037	0	0.137288	29.3037	29.44	29.44	29.44	29.44	29.44	0	kmol/h
33.6748	33.6748	0	0.736297	33.6748	34.41	34.41	34.41	34.41	34.41	0	kmol/h
8.19921	8.19921	0	0.071061	8.19921	8.27	8.27	8.27	8.27	8.27	0	kmol/h
44.403	44.403	0	0.430822	44.403	44.8323	44.8323	90.95	90.95	90.95	0	kmol/h
0.207863	0.207863	0	21	0.207863	21.2093	21.2093	0.14	0.14	0.14	0	kmol/h
0.000482118	0.000482118	0	26.5244	0.000482118	26.5267	26.5267	0	0	0	0	kmol/h
2.38175E-07	2.38175E-07	0	7.40737	2.38175E-07	7.40788	7.40788	0	0	0	0	kmol/h
6.56462E-16	6.56462E-16	0	2.38745	6.56462E-16	2.38762	2.38762	0	0	0	0	kmol/h

References:

Analysis, Synthesis and Design of Chemical Processes. (Fourth Edition), Turton, Bailie, Whiting, Shaeitwitz and Bhattacharya – Appendix B (Information for the Preliminary Design of Fifteen Chemical Processes)