Production of Heptenes from Propylene and Butenes

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Background:

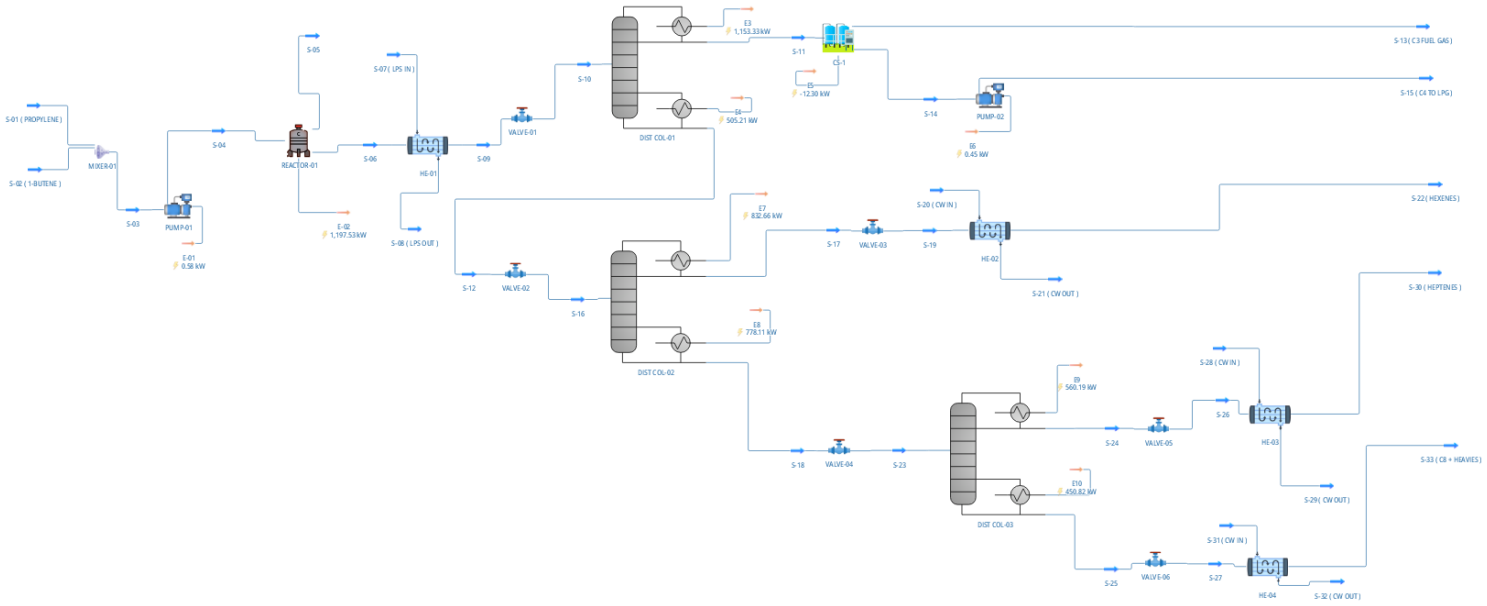
1-heptene finds its application mainly as a high-octane blending agent for gasoline or in plasticizer production. It is also used in the organic synthesis of perfumes, dyes and resins.
The simulated process converts a mixture of C_3 and C_4 unsaturated hydrocarbons to 1-heptene and other heavier unsaturated 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	147.055	99.2426	153.145	107.086	136.171	45	73.538	139.577
Pressure	1.7	1.2	1.7	1.2	2	1.5	2.5	1.7	1.7	4.5
Molar Flow	10.51	25.754	10.51	25.754	10.51	25.754	36.264	22.436	22.436	58.7
Molar Flow (Mixture) / Propane	1.41467E-38	1.38558E-16	1.41467E-38	1.38558E-16	1.41467E-38	1.38558E-16	1.38557E-16	0.00041222	0.00041222	0.000412227
Molar Flow (Mixture) / Propylene	9.5076E-43	4.6512E-20	9.5076E-43	4.6512E-20	9.5076E-43	4.6512E-20	4.65117E-20	4.15757E-07	4.15757E-07	4.15763E-07
Molar Flow (Mixture) / Isobutane	4.1846E-29	3.32742E-11	4.1846E-29	3.32742E-11	4.1846E-29	3.32742E-11	3.32739E-11	0.158331	0.158331	0.158333
Molar Flow (Mixture) / N-butane	6.67522E-26	1.56375E-09	6.67522E-26	1.56375E-09	6.67522E-26	1.56375E-09	1.56374E-09	0.701773	0.701773	0.701784
Molar Flow (Mixture) / Isobutene	1.80559E-28	3.70752E-11	1.80559E-28	3.70752E-11	1.80559E-28	3.70752E-11	3.70749E-11	0.0754462	0.0754462	0.0754473
Molar Flow (Mixture) / 1-butene	1.75799E-27	2.71917E-10	1.75799E-27	2.71917E-10	1.75799E-27	2.71917E-10	2.71915E-10	0.451382	0.451382	0.451389
Molar Flow (Mixture) / 1-hexene	5.91012E-08	0.216322	5.91012E-08	0.216322	5.91012E-08	0.216322	0.21632	20.7743	20.7743	20.9909
Molar Flow (Mixture) / 1-heptene	0.793873	25.4584	0.793873	25.4584	0.793873	25.4584	26.2521	0.274403	0.274403	26.5262
Molar Flow (Mixture) / 1-octene	7.32853	0.0792918	7.32853	0.0792918	7.32853	0.0792918	7.40796	2.01125E-06	2.01125E-06	7.40789
Molar Flow (Mixture) / 1-undecene	2.3876	3.82212E-19	2.3876	3.82212E-19	2.3876	3.82212E-19	2.38764	6.4839E-20	6.4839E-20	2.38762
Molar Flow (Mixture) / Water	0	0	0	0	0	0	0	0	0	0

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)	
45.2075	45.1159	45.1159	149.632	45.1159	94.2157	45	25.3767	25.3161	25	24.8622	C
6.5	5.5	5.5	5.8	5.5	5.8	7.7	8	7.3	3	11.6	bar
116.351	116.351	2.99966	58.7	119.351	178.051	178.051	237.83	237.83	163.21	74.62	kmol/h
0.559923	0.559923	2.99966	0.000412227	3.55958	3.56	3.56	3.56	3.56	0	3.56	kmol/h
0.00710558	0.00710558	0	4.15763E-07	0.00710558	0.007106	0.007106	71.06	71.06	0	71.06	kmol/h
29.2816	29.2816	0	0.158333	29.2816	29.44	29.44	29.44	29.44	29.44	0	kmol/h
33.7082	33.7082	0	0.701784	33.7082	34.41	34.41	34.41	34.41	34.41	0	kmol/h
8.19455	8.19455	0	0.0754473	8.19455	8.27	8.27	8.27	8.27	8.27	0	kmol/h
44.3809	44.3809	0	0.451389	44.3809	44.8323	44.8323	90.95	90.95	90.95	0	kmol/h
0.218437	0.218437	0	20.9909	0.218437	21.2093	21.2093	0.14	0.14	0.14	0	kmol/h
0.0005052	0.0005052	0	26.5262	0.0005052	26.5267	26.5267	0	0	0	0	kmol/h
2.51518E-07	2.51518E-07	0	7.40789	2.51518E-07	7.40788	7.40788	0	0	0	0	kmol/h
7.1626E-16	7.1626E-16	0	2.38762	7.1626E-16	2.38762	2.38762	0	0	0	0	kmol/h
0	0	0	0	0	0	0	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)