Methyl propionate synthesis in the Lucite Alpha process

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Process Description-

The simulation of the Lucite Alpha process was based on the process information available from the patents. The process flow sheet for the simulation is shown in Fig. 1. Ethylene and carbon monoxide gas feeds are compressed to a pressure of 40 bar. During compression, the gas feeds need to be cooled to prevent the temperature from exceeding 200 °C. Methanol is also pressurized to 40 bar, using a liquid pump. The reactor is a continuously stirred tank reactor (CSTR) operated at 100 °C and 40 bar, in which gas–liquid contact is maximized through agitation of the reaction mixture and gas re-circulation. The reaction is exothermic, with the stoichiometry shown in reaction. The heat production by the exothermic reaction will require cooling of the reactor.

The output of the reactor is a solution of methyl propionate and methanol in which the catalyst is dissolved. Subsequently, the solution is decompressed to atmospheric pressure and partially evaporated by a flash unit at 64 °C. The solution that remains is returned to the reactor to allow the catalyst to be recycled. The part of the solution that was evaporated, a mixture of methyl propionate and methanol, is then fed to a distillation column. The distillation column was simulated in Aspen Plus using a RadFrac unit, with 80 equilibrium stages, a reflux ratio of 1.5 and operating at atmospheric pressure. The feed enters at stage 10. A 95% (m/m) solution of methyl propionate is obtained as bottom product, at 79 °C. As methyl propionate and methanol form an azeotrope at approximately 45% methanol and 55% methyl propionate, a mixture of both components is recovered as top product at 52 °C and recycled.

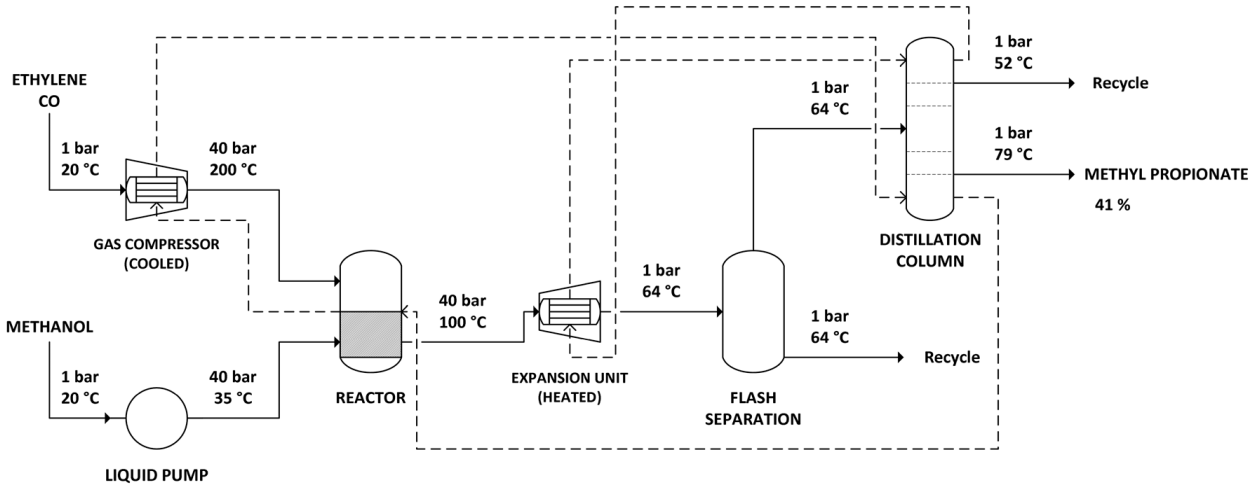
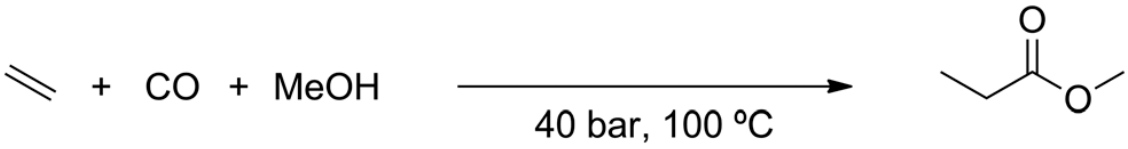


Fig.1 Process flow sheet of methyl propionate synthesis in the Lucite Alpha process.



Reaction- Methyl propionate synthesis in the Lucite Alpha process.

Result-

	PROPERTIES TABLE		
Feed	Temperature	25	C
Feed	Pressure	1	bar
Feed	Molar Flow	35.674	mol/s
Feed	Molar Fraction (Mixture) / Carbon monoxide	0.5	
Feed	Molar Fraction (Mixture) / Ethylene	0.5	
Methyl Propinate	Temperature	70.6719	C
Methyl Propinate	Pressure	1.01325	bar
Methyl Propinate	Molar Fraction (Mixture) / Ethylene	2.04E-23	
Methyl Propinate	Molar Flow (Mixture) / Carbon monoxide	0	mol/s
Methyl Propinate	Molar Flow (Mixture) / Methanol	14.1839	mol/s
Methyl Propinate	Molar Fraction (Mixture) / Methyl propionate	0.5	
Methanol	Temperature	20	C
Methanol	Pressure	1	bar
Methanol	Molar Flow	31.2092	mol/s
Methanol	Molar Flow (Mixture) / Methanol	31.2092	mol/s

References-

- https://pubs.rsc.org/en/Content/ArticleLanding/2017/RE/C7RE00094D#!divAbstract