production of butadiene from ethanol

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a two-step reaction process, which takes a 92% ethanol stream (by mole fraction)and produces a 95% 1,3-butadiene stream, was designed for this project.The process first passes ethanol through a catalyticdehydrogenation reactor to convert ethanol to acetaldehyde and hydrogen. A conversion reactor(acetaldehyde reactor) was used to determine the reaction rates and operating conditions of the reactor. The acetaldehyde intermediate is further reacted with ethanol in a butadiene reactor to form butadiene.

reactions involved :

$CH_3CH_2OH \rightarrow CH_3CHO + H_2$

$2CH_3CHO \rightarrow CH_3(CH)_3O + H_2O$

$CH_3(CH)_3O + C_2H_5OH \rightarrow CH_2CHCHCH_2 + H_2O + CH_3CHO$

$CH_3CH_2OH + CH_3CHO \rightarrow CH_2CHCHCH_2 + 2H_2O$

$2CH_3CH_2OH \rightarrow CH_2CHCHCH_2 + H_2 + 2H_2O$

uses of butadiene produced:

Butadiene is a very versatile raw material and is used to make synthetic rubbers, polymer resins, and a wide variety of other chemical intermediates. More than 75% of the butadiene produced goes into synthetic rubber products. The major uses include production of styrene- butadiene rubber (30% to 35%), polybutadiene rubber (20% to 22%), adiponitrile (12% to 15%), styrene-butadiene latex (10%), neoprene rubber (5% to 6%), acrylonitrile-butadiene-styrene resins (5% to 6%), and nitrile rubber (3%). Other uses include production of specialty polymers

Flow sheet description:

DWSIM flow sheet involves two conversion reactors: acetaldehyde reactor and butadiene reactor and stream mixer is used to mix both obtained acetaldehyde and ethanol feed and sent into the butadiene reactor to convert it into butadiene and distillation column(shortcut distillation) where both butadiene and other heavy products such as heavy water ;ethyl acetate; diethyl ether ;hydrogen are separated in distillate stream and heavy products stream respectively.

Hence 1,3-butadiene is formed from ethanol .

Results obtained:

final distillate results			
Object	heavy bottoms	distillate	
Temperature	364.681	255.237	K
Pressure	101325	101325	Pa
Mass Flow	0.000434437	1.96597	kg/s
Molar Flow	0.0185247	36.3416	mol/s
Volumetric Flow	1.0772E-06	0.0052099	m3/s
Mixture Molar Weight	23.4517	54.0971	kg/kmol
Molar Flow (Mixture) / Acetaldehyde	1.07028E-05	0.364275	mol/s
Mass Flow (Mixture) / Acetaldehyde	4.71488E-07	0.0160473	kg/s
Molar Fraction (Liquid Phase 1) / Acetaldehyde	0.000648719	0.0100237	
Molar Fraction (Aqueous Phase) / Acetaldehyde	0	0	
Mass Flow (Solid Phase) / Acetaldehyde	0	0	kg/s
Molar Fraction (Mixture) / 1,3-butadiene	0.01	0.946585	
Mass Fraction (Mixture) / 1,3-butadiene	0.0230653	0.946495	
Molar Fraction (Vapor Phase) / 1,3-butadiene	0.163766	0.543638	Molar
Fraction (Liquid Phase 1) / 1,3-butadiene	0.0111486	0.946585	
Molar Fraction (Mixture) / HeavyWater	0.737364	0.01	
Mass Fraction (Mixture) / HeavyWater	0.629701	0.00370214	
Molar Flow (Mixture) / HeavyWater	0.0136595	0.363416	mol/s
Mass Flow (Mixture) / HeavyWater	0.000273565	0.00727831	kg/s
Molar Fraction (Liquid Phase 2) / HeavyWater	0	0	
Molar Fraction (Aqueous Phase) / HeavyWater	0	0	
Mass Fraction (Vapor Phase) / HeavyWater	0.323424	6.32044E-06	

Conclusion:

Hence from the results table it is observed .9465(appr 95%)of1,3-butadiene is obtained from ethanol and other byproducts are obtained in other proportions.

Thank you

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