Production of Pure Liquid Hydrogen using Water-Gas Shift Reaction

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Background & Description:

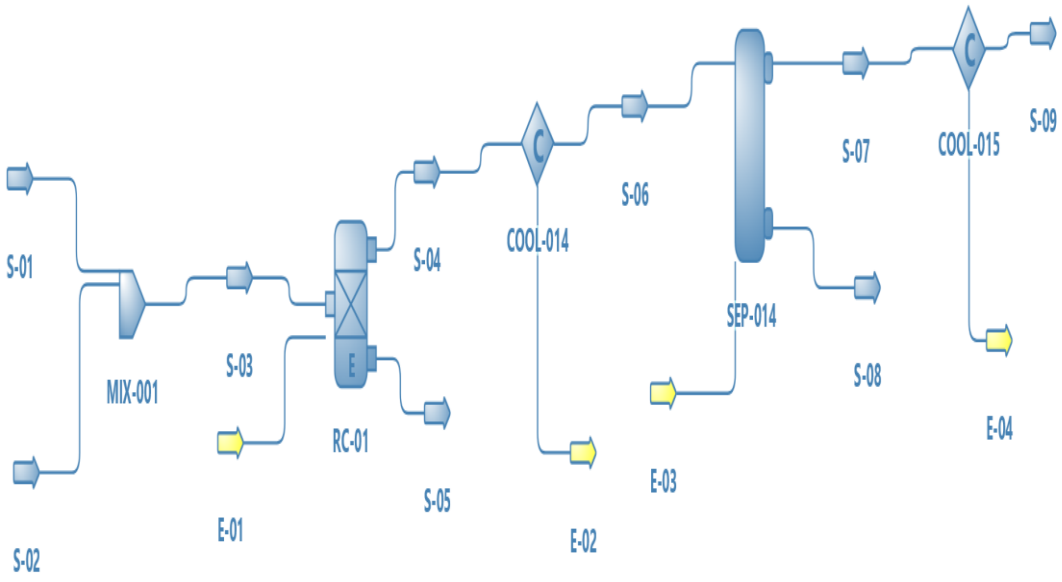
Water Gas Shift reaction is one of the most important ways of producing pure hydrogen in chemical industry as it provides a cheap and effective way for industrial uses like ammonia synthesis. The future is focused on the idea of Hydrogen Economy; hence producing pure hydrogen from WGSR is beneficial. WSGR also helps in increasing the battery of fuel cells with hydrogen production and reducing the concentrations of carbon monoxide.

The water gas shift reaction is as follows:

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \qquad \Delta H^0_{298} = -41.1 \text{ kJ /mol}$$

It involves the reaction of Carbon Monoxide with steam to form carbon dioxide and hydrogen. It is an equilibrium reaction with equilibrium constant equal to 6.80 and a conversion rate of approximately 80%. The initial amount of carbon monoxide and steam are 25 mol/h and 100 mol/h. Both CO and H_2O are mixed and sent to an equilibrium reactor where they are reacted in vapour phase. After reaction, the vapour phase products are passed through a condenser/cooler where the vapour phase mol fraction dropped to 0.29 (ideally 0.2). The outlet stream is passed to a separator where the vapour stream contains 0.99 mole fraction of hydrogen and liquid stream is let out. The hydrogen stream is again passed through a cooler which is liquefies the pure hydrogen. Approximately 36 mol/h of liquid hydrogen are formed.

Flowsheet:



Results:

MATER PROPERTY TABLE										
Object	S-09	S-08	S-07	S-06	S-05	S-04	S-03	S-02	S-01	
Temperature	-252.664	-240.35	-240.35	-240.35	469.65	469.65	81.1208	100	25	C
Pressure	101.32	101.32	101.32	101.32	101.32	101.32	101.32	101.325	101.32	kPa
Mass Flow	74.3498	2727.28	74.3498	2801.63	0	2801.63	2801.63	1261.07	1540.56	kg/h
Molar Flow	36.882	88.118	36.882	125	0	125	125	70	55	kmol/h
Volumetric Flow	1.05381	8.02011	96.2369	104.257	0	7619.09	3586.96	2124.71	1344.8	m3/h
Vapor Phase Molar Fraction	0	5.40168E-18	1	0.295056	0	1	0.991347	1	1	
Energy Flow	-6.78312E+06	-7.18983E+07	-5.81265E+06	-7.7711E+07	0	4.81147E+07	4.13168E+06	4.14328E+06	-11596.8	kJ/d

Conclusion:

Pure Hydrogen was produced successfully from carbon monoxide and steam via water-shift reaction. The conversion is approximately 80% which indicates a good yield.
Furthermore, if the cooler/condenser 1 can change the vapour fraction to less than 0.29 so as to yield better results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