Water-Gas shift reaction

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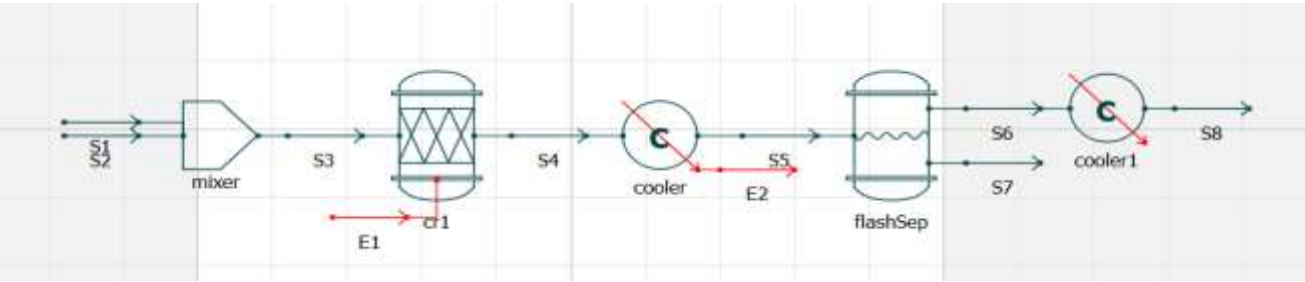
Problem Statement: Production of Pure Liquid Hydrogen using Water-Gas Shift Reaction

System of unit: The system of units taken in this flowsheet are SI.

Thermodynamic package: Raoult's law

Background and 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 + H2O ⇔ CO2 + H2. (ΔH 0 298= -41.1 kJ /mol) It involves the reaction of Carbon Monoxide with steam to form carbon dioxide and hydrogen. It is an equilibrium reaction with conversion rate of approximately 80%. The initial amount of carbon monoxide and steam are 15.278 mol/s and 19.444 mol/s. Both CO and H2O are mixed and sent to an conversion 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 0.36. The outlet stream is passed to a separator where the vapour stream contains 0.9745 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 12.1818 mol/s of liquid hydrogen are formed.

Flowsheet:



Results:

OpenModelica results:

Object	S1	S2	S3	S4	S5	S6	S7	S8
Pressure (Pa)	101320	101325	101322	101322	101322	101322	101322	101322
Mass Flow (kg/s)	427.937	350.284	778.221	778.221	778.221	33.479	744.746	33.479
Molar Flow (mol/s)	15.278	19.444	34.722	34.722	34.722	12.5004	22.2216	12.5004
Mole fraction(Hydrogen)	0	0	0	0.352254	0.352254	0.9745	0.00221	0.9745

DWSIM results:

Object	S1	S2	S3	S4	S5	S6	S7	S8
Pressure (Pa)	101320	101325	101322	101322	101322	101322	101322	101322
Mass Flow (kg/s)	427.937	350.297	778.221	778.234	778.234	20.6334	757.6006	20.6334
Molar Flow (mol/s)	15.2778	19.444	34.7222	34.7222	34.7222	10.2355	24.4867	10.2355
Mole fraction(Hydrogen)	0	0	0	0.35227192	0.35227192	1	0.081519	1

Conclusion: Hydrogen was produced successfully from carbon monoxide and steam via water-shift reaction. The conversion is approximately 82% which indicates a good yield. Furthermore, if the cooler can change the vapour fraction to less than 0.36 so as to yield better results.