Autothermal Reforming of Methane for Hydrogen Production

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Background:

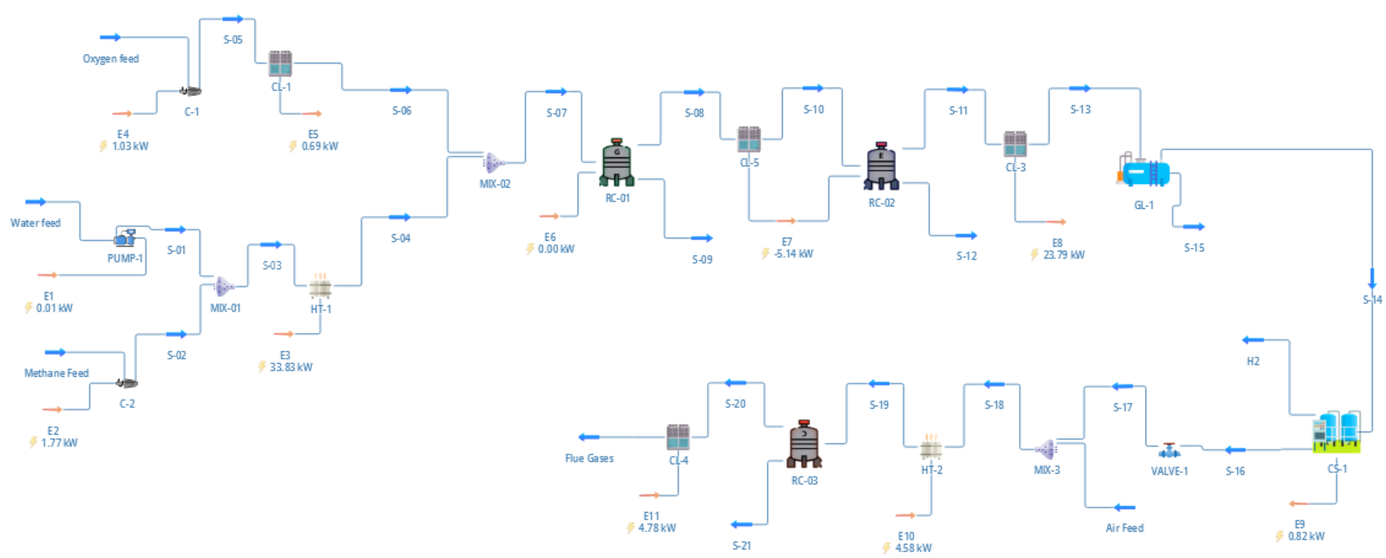
Beside the conventional steam methane reforming, autothermal reforming (ATR) is one of the advanced processes of hydrogen production which combines steam reforming and partial oxidation of methane to produce syngas (mixture of H_2 and CO). Unlike conventional steam reforming which is strongly endothermic and needs external heat, ATR balances endothermic reforming with exothermic oxidation. This makes it a thermoneutral or slightly exothermic process. This makes the process generally more compact, simpler and more system efficient than partial oxidation of hydrocarbons.

Description

The autothermal reforming process involves steam methane reforming, partial oxidation, the water–gas shift reaction, pressure swing adsorption (PSA), and tail-gas combustion. In the DWSIM simulation, 1 kmol/hr of methane and 2 kmol/hr of water are supplied at 5 bar and mixed in MIX-02, while 0.55 kmol/hr of oxygen is maintained at 5 bar and 100°C before entering the mixer. The combined stream enters a Gibbs reactor where the reactions occur adiabatically, producing syngas at around 769.05°C and 4.85 bar. The syngas is then cooled to 270°C and fed to an isothermal water–gas shift reactor operating at the same temperature, where the pressure drops to 4.67 bar and hydrogen rises to about 55%. The stream is cooled to 50°C and sent to a gas–liquid separator to remove excess water. The vapor stream, containing around 71.24% hydrogen, is sent to the PSA unit, which operates at high efficiency to deliver pure hydrogen and a tail gas. This tail gas is mixed with air, preheated to 250°C, and combusted, reaching nearly 443.34°C. The released heat is recovered, and the final flue gas is discharged at about 200°C to avoid condensation.

Thermodynamic Package: Peng-Robinson 1978 (PR78)

The flowsheet:



Results:

Object	S-06	S-05	S-04	S-03	S-02	S-01	O_2 feed	H_2O feed	CH_4 Feed	
Temperature	100	247.178	350	41.1423	186.882	8.96399	25	25	25	°C
Pressure	5	5	5	5	5	5	1	1	1	bar
Molar Flow	0.55	0.55	3	3	1	2	0.55	2	1	kmol/hr
Molar Fraction (Mixture)/ CH_4	0	0	0.33	0.33	1	0	0	0	1	
Molar Fraction (Mixture)/ O_2	1	1	0	0	0	0	1	0	0	
Molar Fraction (Mixture)/ CO_2	0	0	0	0	0	0	0	0	0	
Molar Fraction (Mixture)/ CO	0	0	0	0	0	0	0	0	0	
Molar Fraction (Mixture) / H_2O	0	0	0.67	0.67	0	1	0	1	0	
Molar Fraction (Mixture)/ H_2	0	0	0	0	0	0	0	0	0	
Molar Fraction (Mixture)/ N_2	0	0	0	0	0	0	0	0	0	

Object	S-15	S-14	S-13	S-12	S-11	S-10	S-09	S-08	S-07	
Temperature	50	50	50	270	270	270	769.051	769.051	320.117	°C
Pressure	4.67	4.67	4.67	4.67	4.67	4.85	4.85	4.85	5	bar
Molar Flow	1.12115	3.79614	4.91729	0	4.91729	4.91729	0	4.91729	3.55	kmol/hr
Molar Fraction (Mixture)/ CH_4	8.83E-10	0.0106	0.00818304	0	0.008183	0.008183	0	0.0081830	0.28169	
Molar Fraction (Mixture)/ O_2	4.03E-14	1.91E-09	1.47E-09	0	1.47E-09	1.47E-09	0	1.47E-09	0.15493	
Molar Fraction (Mixture)/ CO_2	0.000523	0.24417	0.188619	0	0.188619	0.093127	0	0.093127	0	
Molar Fraction (Mixture)/ CO	1.19E-08	0.008501	0.00656246	0	0.006562	0.102054	0	0.102054	0	
Molar Fraction (Mixture) / H_2O	0.999474	0.0242569	0.24663	0	0.24663	0.342121	0	0.342121	0.56338	
Molar Fraction (Mixture)/ H_2	2.54E-06	0.712443	0.550006	0	0.550006	0.454514	0	0.454514	0	
Molar Fraction (Mixture)/ N_2	0	0	0	0	0	0	0	0	0	

Object	Flue Gases	S-21	S-20	S-19	S-18	S-17	S-16	H_2	
Temperature	200	443.343	443.343	250	25.5264	43.1876	50	50	°C
Pressure	1.01325	1.01325	1.01325	1.01325	1.01325	2.67	4.67	4.67	bar
Molar Flow	1.76127	0	1.76127	1.77507	1.77507	1.1457	1.1457	2.65044	kmol/hr
Molar Fraction (Mixture)/ CH_4	0.018277	0	0.018277	0.022669	0.022669	0.035121	0.035121	0	
Molar Fraction (Mixture)/ O_2	0.0580679	0	0.058068	0.074458	0.074458	6.32E-09	6.32E-09	0	
Molar Fraction (Mixture)/ CO_2	0.540368	0	0.540368	0.52218	0.52218	0.809031	0.809031	0	
Molar Fraction (Mixture)/ CO	0.00879443	0	0.008794	0.018179	0.018179	0.028166	0.028166	0	
Molar Fraction (Mixture) / H_2O	0.0676264	0	0.067626	0.051939	0.051939	0.08047	0.08047	0	
Molar Fraction (Mixture)/ H_2	0.024569	0	0.024569	0.030473	0.030473	0.047212	0.047212	1	
Molar Fraction (Mixture)/ N_2	0.282298	0	0.282298	0.280103	0.280103	0	0	0	

References:

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