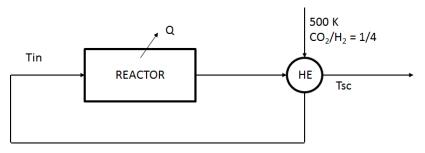
## INDUSTRIAL ORGANIC CHEMISTRY- July 11th, 2017

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A possible way to exploit hydrogen produced by water hydrolysis is the production of methane according to the Sabatier reaction ( $CO_2 + 4 H_2 \rightarrow CH_4 + 2 H_2O$ ). A simplified process layout consists of a heat exchanger (HE), where the fresh feed at 500 K is heated up using the reactor effluents, and of a reactor where a conversion of 95% of  $CO_2$  is achieved when operated at 8 atm. The formation of CO is also experienced in the reactor.



## By assuming that:

- The reacting mixture is an ideal mixture of ideal gases
- The thermodynamic equilibrium is reached at the outlet of the reactor (species present at equilibrium: CO<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>O, CO)
- The heat exchanger is ideal and the heat losses are negligible
- The reactor is designed to remove 7000 cal/mol of charge
- The fresh feed is at 500 K and the molar ratio between CO2 and H2 is 1:4
- The pressure drop is negligible
- 1. Evaluate the composition and the temperature of the stream leaving the reactor

H <sub>2</sub> O	$H_2$	
CH <sub>4</sub>	СО	
CO <sub>2</sub>	Temperature	

2.	Evaluate the	e temperature	of the stream	entering th	e reactor (	$T_{in}$	1

Temperature			

3. Evaluate the temperature of the stream leaving the heat exchanger (T<sub>sc</sub>)

## Thermodynamic data:

Sabatier reaction:

$$K_{eq}(T) = \exp\left(\frac{1}{1.987} \left(\frac{56000}{T^2} + \frac{34633}{T} - 16.4 \ln T + 0.00557 T\right) + 33.165\right)$$
 where T in [K]

Water gas shift reaction:  $\Delta G_{WGS}^{0}(T) = -8514 + 7.71 \cdot T$  [cal/mol] where T in [K]

Reference state: ideal gas at 1 atm

	∆H <sup>0</sup> ғ(298K)	Ср
	[cal/mol]	[cal/mol]
H <sub>2</sub>	0	2207
CO	-26420	2253
CO <sub>2</sub>	-94050	3284
CH <sub>4</sub>	-17890	3438
H <sub>2</sub> O	-57800	2662

Heat capacity can be assumed constant in the range of temperature of interest.