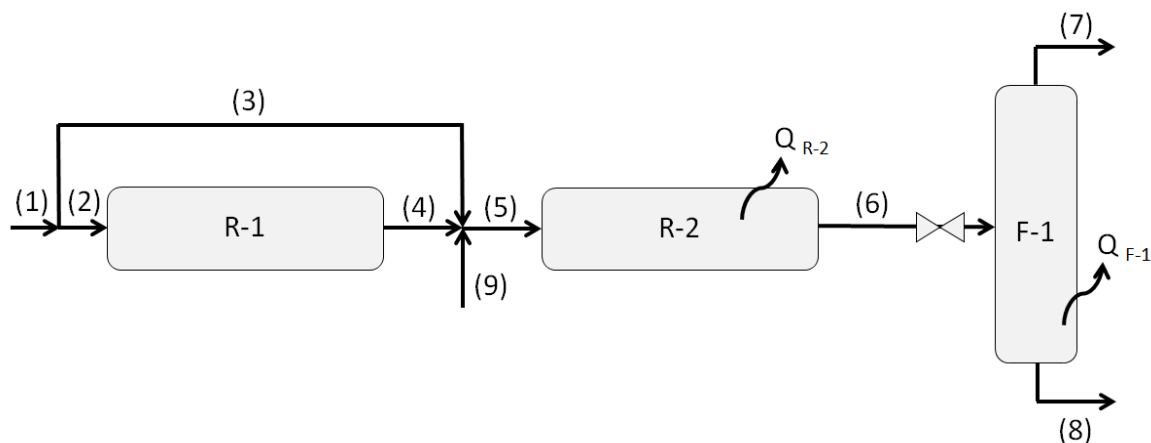# Methanol synthesis: simplified ICI layout

A simplified layout of an ICI process for the methanol production consists of two reactors in series with intermediate quench. The fresh feed (1) with known composition and at T = 453 K is split in two streams: the first (2) is sent to the first adiabatic reactor (R-1) where CO and H_2 are converted to methanol. The stream (4) leaving the reactor is mixed with the remaining feed (3) and with a make-up stream (9) consisting of pure CO_2 (at 453 K) to obtain a temperature of stream (5) equal to 520 K and sent to the second reactor (R-2). The stream (6) leaving the reactor is isoenthalpically laminated and sent to an isothermal methanol condenser (F-1).

By assuming:

- At 70 bar the gas mixture is ideal and consists of real gas. As a first approximation, a $K_\phi^{MeOH} = \frac{\phi_{MeOH}}{\phi_{H_2}^2 \phi_{CO}} = 0.7$ and $K_\phi^{WGS} = \frac{\phi_{CO_2}\phi_{H_2}}{\phi_{H_2O}\phi_{CO}} = 1.2$ can be assumed for the evaluation of the K_p of the methanol synthesis and of the WGS, respectively. At 10 bar the vapor phase is an ideal mixture of ideal gas; the liquid mixture is ideal with negligible Poynting correction.

- The pressure in each reactor is equal to 70 bar and pressure drops are negligible, while the separator works at 10 bar.

- The reactor R-1 is designed to work with a conversion of CO equal to the 90% of the equilibrium one at the adiabatic temperature. CO_2 and H_2O are not present at the outlet of R-1.

- The molar fraction of CO_2 in stream (5) is equal to 0.15

- The reactor R-2 is designed to achieve thermodynamic equilibrium at the temperature of 570 K.

- The methanol condenser (F-1) is designed to obtain a recovery efficiency of methanol equal to 70 % in stream (8)

- As a first approximation, supercritical components can be assumed as not dissolved in the liquid.

It is required to evaluate:

1. The temperature and the composition (molar fractions) of the stream leaving reactor R-1
2. The ratio between stream (3) and stream (2) and the ratio between stream (9) and stream (2)
3. The composition (molar fractions) of the stream (6) leaving reactor R-2, the heat exchanged in the reactor per mol of stream (2) and the overall conversion of CO in the reacting section
4. The extent of vaporization, the flash temperature and the molar composition of the liquid and vapor streams leaving the flash
5. The state of stream (6) before the lamination valve (for this calculation consider the ideal gases hypothesis) and the heat removed per mole of stream (6) in condenser (F-1)

<u>Data</u>:

<u>Molar fractions and temperature:</u>

	CH_4	H_2	CO	CO_2	T [K]
Stream (1)	0.05	0.75	0.20	0	453
Stream (9)	0	0	0	1	453

<u>Thermodynamic data</u> (reference state: ideal gas at 1 atm)

Methanol synthesis:	$\Delta G_R^0(T) = -22828 + 56.02 \cdot T$	[cal/mol] where T in [K]
Water gas shift reaction:	$\Delta G_{R,WGS}^0(T) = -8514 + 7.71 \cdot T$	[cal/mol] where T in [K]

Species	$\Delta H^0_F(298K)$ [cal/mol]	C_p^L [cal/mol/K]	$\Delta h_i^{vap}@T_{boil,n}$ [cal/mol]	C_p^V coefficients				Antoine coefficients		
				a	b x 10³	c x 10⁶	d x 10⁹	A	B	C
H_2	0			6.483	2.215	-3.298	1.826			
CO	-26420			7.373	-3.070	6.662	-3.037			
CO_2	-94050			4.728	17.54	-13.38	4.097			
CH_4	-17890			4.598	12.450	2.860	-2.709			
H_2O	-57800	19.09	8395	7.701	0.4595	2.521	-0.859	6.2096	2354.731	7.559
CH_3OH	-48080	18.05	9436	5.062	16.94	6.179	-6.811	5.2041	1581.34	-33.50

$C_{p,i}^V(T) = a_i + b_i \cdot T + c_i \cdot T^2 + d_i \cdot T^3$ [cal/mol/K] – gas phase

ANTOINE EQ: $\log_{10} p^0(T) = A - \frac{B}{C+T}$, where: T [K] - $p^0(T)$ [bar]