Equilibrio de gas de síntesis Base 1 kmol de entrada al convertidor CO + 2H2 = CH3OH

Composición

$y_{0CH3OH} = 0,02$

$y_{0H2} = [1 - y_{0CH3OH} - y_{0I}] \cdot 2 / 3$

$y_{0CO} = [1 - y_{0CH3OH} - y_{0I}] \cdot 1 / 3$

$y_{0I} = 0,1$

Condiciones de entrada

$P = 100 \text{ [atm]} \cdot \left| 1,01325 \cdot \frac{\text{bar}}{\text{atm}} \right|$

Constante de equilibrio para la reacción 3H2 +CO = CH3OH

Call **NASA**['CH3OH' ; T : CP_{CH3OH} ; H_{CH3OH} ; S_{CH3OH}]

$R = 8,314 \text{ [kJ/kmol-K]}$

$$-R \cdot T \cdot \ln[K_{CH3OH}] = H_{CH3OH} - T \cdot S_{CH3OH} - 2 \cdot \left[\mathbf{h}('H2' ; T = T) - T \cdot \mathbf{s}\left('H2' ; T = T ; P = 1 \text{ [atm]} \cdot \left| 1,01325 \cdot \frac{\text{bar}}{\text{atm}} \right| \right) \right] - \left[\mathbf{h}('CO' ; T = T) - T \cdot \mathbf{s}\left('CO' ; T = T ; P = 1 \text{ [atm]} \cdot \left| 1,01325 \cdot \frac{\text{bar}}{\text{atm}} \right| \right) \right]$$

$$y_{CH3OH} = \frac{y_{0CH3OH} + \alpha}{1 - 2 \cdot \alpha}$$

$$y_{H2} = \frac{y_{0H2} - 2 \cdot \alpha}{1 - 2 \cdot \alpha}$$

$$y_{CO} = \frac{y_{0CO} - \alpha}{1 - 2 \cdot \alpha}$$

$$K_{CH3OH} = \frac{P}{1 \text{ [bar]}} \cdot \frac{y_{CH3OH}}{\left[\frac{P}{1 \text{ [bar]}} \cdot y_{H2} \right]^2 \Big/ \frac{P}{1 \text{ [bar]}} \cdot y_{CO}}$$

$$\text{Conversion} = 1 - \frac{y_{CO}}{y_{0CO}}$$

$t_C = T - 273,15 \text{ [K]}$

SOLUTION
Unit Settings: [kJ]/[K]/[bar]/[kmol]/[degrees]

$\alpha = 0,1072$
$CP_{CH3OH} = 65,25$ [kJ/kmol-K]
$K_{CH3OH} = 0,0002963$
$R = 8,314$ [kJ/kmol-K]
Conversion = 0,1922
$H_{CH3OH} = -185933$ [kJ/kmol]
$P = 101,3$ [bar]
$S_{CH3OH} = 274,7$ [kJ/kmol-K]

$T = 573{,}1$ [K]
$y_{0CH3OH} = 0{,}02$
$y_{0H2} = 0{,}5867$
$y_{CH3OH} = 0{,}1619$
$y_{H2} = 0{,}4739$

$t_C = 300$ [C]
$y_{0CO} = 0{,}2933$
$y_{0I} = 0{,}1$
$y_{CO} = 0{,}2369$

No unit problems were detected.

Parametric Table: Table 1

	t_C [C]	y_{CH3OH}	Conversion
Run 1	*180*	*0,6069*	*0,7951*
Run 2	*193,3*	*0,5692*	*0,7441*
Run 3	*206,7*	*0,5262*	*0,6858*
Run 4	*220*	*0,4783*	*0,6209*
Run 5	*233,3*	*0,4262*	*0,5504*
Run 6	*246,7*	*0,3713*	*0,476*
Run 7	*260*	*0,3153*	*0,4001*
Run 8	*273,3*	*0,2603*	*0,3255*
Run 9	*286,7*	*0,2084*	*0,2553*
Run 10	*300*	*0,1619*	*0,1922*