Cálculo del equilibrio líquido-vapor (dewpoint) de una mezcla de gas de síntesis y agua a alta presión (P = 30 atm).
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Se utiliza la ecuación de Redlich-Kwong modificada por De Santis & al. Ind. Eng. Chem. Proc. Des. Dev. 13, 1974
según el artículo Enthalpy and Dew Point Calculations for Aqueous Gas Mixtures Produced in Coal Gasification and Similar Processes
B. Rittmann, H. Knapp, J.M. Prausnitz, Ind, Eng. Chem. Proc. Des. Dev. 21, 1982.

$P = R*T/(v-b) - a(T)/T^{1}/2/v/(v+b)$

	b_i	a_{ii}	P_c (atm)	T_c (K)
H2O	0,0146	35	218,3	647,4
CH4	45,8	190,7		
H2	20,2/(1+44,2/2,016/T)	43,6/(1+21,8/2,016/T)	quantum effects	
CO	34,5	133		
CO2	0,0297	46,0	72,9	304,2
N2	0,02678	15,462	33,5	126,2
A	48,0	151,2		

Para vapor de agua $a(T) = (93{,}415 - 1{,}99798E4/T+1{,}473169E7/T^{2} + 7{,}47112E9/T^{3)}$ *y* $a_0 = 35$
Su derivada es : $da/dT = (1{,}99798E4/T^{2}-2*1{,}473169E7/T^{3}-3*7{,}47112E9/T^{4)}$
Para CO2 gas $a(T) = (-7{,}97203 + 5{,}04354E4/T - 9{,}77329E6/T^{2}+ 5{,}19402E8/T^{3)}$ *y* $a_0 = 46$
Su derivada es : $da/dT = (-5{,}0435E4/T^{2}+2*9{,}77329E6/T^{3}-3*5{,}19402E8/T^{4)}$
El pseudoequilibrio en la fase gas de CO2+H2O : $lnK = -11{,}071 + 5953/T - 2746E3/T^{2} + 464{,}6E6/T^{3}$
Los gases son 1= H2O, 2 = CH4, 3 = H2, 4 = CO, 5 = CO2, 6 = N2, 7 = A

Composición gaseosa inicial

$y_{0;1} = 0{,}3204$ *H2O*

$y_{0;2} = 0{,}001785$ *CH4*

$y_{0;3} = 0{,}3967$ *H2*

$y_{0;4} = 0{,}0034$ *CO*

$y_{0;5} = 0{,}1477$ *CO2*

$y_{0;6} = 0{,}1298$ *N2*

$y_{0;7} = 0$ *A*

$b_1 = 0{,}0146$

$$b_2 = 0{,}08664 \cdot 0{,}0820597 \cdot \frac{190{,}7}{45{,}8}$$

$$b_3 = 0{,}08664 \cdot 0{,}0820597 \cdot \left[\frac{\dfrac{43{,}6}{1 + \dfrac{21{,}8}{2{,}016 \cdot T}}}{\dfrac{20{,}2}{1 + \dfrac{44{,}2}{2{,}016 \cdot T}}} \right]$$

$$b_4 = 0{,}08664 \cdot 0{,}0820597 \cdot \frac{133}{34{,}5}$$

$b_5 = 0{,}0297$

$b_6 = 0{,}02678$

$$b_7 = 0{,}08664 \cdot 0{,}0820597 \cdot \frac{151{,}2}{48}$$

$$b_M = y_1 \cdot b_1 + y_2 \cdot b_2 + y_3 \cdot b_3 + y_4 \cdot b_4 + y_5 \cdot b_5 + y_6 \cdot b_6 + y_7 \cdot b_7$$

$$a_1 = 58{,}415 - \frac{19979{,}8}{T} + \frac{1{,}47316 \times 10^7}{T^2} + \frac{7{,}47112 \times 10^9}{T^3}$$

$$a_2 = 0{,}4275 \cdot 0{,}0820597^2 \cdot \frac{190{,}7^{2,5}}{45{,}8}$$

$$a_3 = 0{,}4275 \cdot 0{,}0820597^2 \cdot \left[\frac{\left(\dfrac{43{,}6}{1 + \dfrac{21{,}8}{2{,}016 \cdot T}} \right)^{2,5}}{\dfrac{20{,}2}{1 + \dfrac{44{,}2}{2{,}016 \cdot T}}} \right]$$

$$a_4 = 0{,}4275 \cdot 0{,}0820597^2 \cdot \frac{133^{2,5}}{34{,}5}$$

$$a_5 = -53{,}97203 + \frac{50435{,}4}{T} - \frac{9{,}77329 \times 10^6}{T^2} + \frac{5{,}19402 \times 10^8}{T^3}$$

$$a_6 = 15{,}462$$

$$a_7 = 0{,}4275 \cdot 0{,}0820597^2 \cdot \frac{151{,}2^{2,5}}{48}$$

$$K = \mathbf{exp}\left[\frac{\dfrac{\dfrac{4{,}646 \times 10^8}{T} - 2{,}746 \times 10^6}{T} + 5953}{T} - 11{,}071 \right]$$

$$dK = \frac{-5953}{T^2} + 2 \cdot \frac{2{,}746 \times 10^6}{T^3} - 3 \cdot \frac{4{,}646 \times 10^8}{T^4}$$

$$R = 0{,}0820597$$

$$a_M = \left[y_1 \cdot 35^{0,5} + y_2 \cdot a_2^{0,5} + y_3 \cdot a_3^{0,5} + y_4 \cdot a_4^{0,5} + y_5 \cdot 46^{0,5} + y_6 \cdot a_6^{0,5} + y_7 \cdot a_7^{0,5} \right]^2 + y_1^2 \cdot a_1 + y_5^2 \cdot a_5 + y_1 \cdot y_5 \cdot R^2 \cdot T^{2,5} \cdot K$$

$$DT = \left[\frac{19979{,}8}{T^2} - 2 \cdot \frac{1{,}47316 \times 10^7}{T^3} - 3 \cdot \frac{7{,}47112 \times 10^9}{T^4} \right] \cdot y_1^2 + \left[\frac{-50435}{T^2} + 2 \cdot \frac{9{,}77329 \times 10^6}{T^3} - 3 \cdot \frac{5{,}19402 \times 10^8}{T^4} \right] \cdot y_5^2 + R^2 \cdot T^{1,5} \cdot K \cdot \left[2{,}5 + T \cdot dK \right] \cdot y_1 \cdot y_5$$

$$P = R \cdot \left[\frac{T}{v - b_M} \right] - \left[\frac{\dfrac{\dfrac{a_M}{v}}{v + b_M}}{T^{0,5}} \right]$$

$$\Delta h = \left[P \cdot v - R \cdot T - \left(\left[\frac{1,5 \cdot \frac{a_M}{\sqrt{T}} - DT \cdot \sqrt{T}}{b_M} \right] \cdot \mathbf{ln}\left[\frac{v + b_M}{v} \right] \right) \right] \cdot \left| 101,325 \cdot \frac{\text{J/kmol}}{\text{atm*l/kmol}} \right|$$

$$\mathbf{ln}[\nu_1] = \mathbf{ln}\left[\frac{v}{v - b_M} \right] + \frac{b_1}{v - b_M} - \Bigg[\frac{\frac{2}{R}}{T^{1,5} \cdot b_M} \cdot \Big(y_1 \cdot [35 + a_1] + y_2 \cdot [35 \cdot a_2]^{0,5} + y_3 \cdot [35$$

$$\cdot\, a_3]^{0,5} + y_4 \cdot [35 \cdot a_4]^{0,5} + y_5 \cdot [35 \cdot 46]^{0,5} + \frac{y_5}{2} \cdot R^2 \cdot T^{2,5} \cdot K + y_6 \cdot [35 \cdot a_6]^{0,5} + y_7 \cdot [35$$

$$\cdot\, a_7]^{0,5} \Big) \cdot \mathbf{ln}\left(\frac{v + b_M}{v} \right) \Bigg] + a_M \cdot \frac{\frac{\frac{b_1}{R}}{T^{1,5}}}{b_M^{\ 2}} \cdot \left[\mathbf{ln}\left(\frac{v + b_M}{v} \right) - \left(\frac{b_M}{v + b_M} \right) \right] - \mathbf{ln}\left[P \cdot \frac{v}{R \cdot T} \right]$$

$$\mathbf{ln}[\nu_2] = \mathbf{ln}\left[\frac{v}{v - b_M} \right] + \frac{b_2}{v - b_M} - \Bigg[\frac{\frac{2}{R}}{T^{1,5} \cdot b_M} \cdot \Big(y_1 \cdot [a_2 \cdot 35]^{0,5} + y_2 \cdot a_2 + y_3 \cdot [a_2 \cdot a_3]^{0,5} + y_4$$

$$\cdot\, [a_2 \cdot a_4]^{0,5} + y_5 \cdot [a_2 \cdot 46]^{0,5} + y_6 \cdot [a_2 \cdot a_6]^{0,5} + y_7 \cdot [a_2 \cdot a_7]^{0,5} \Big) \cdot \mathbf{ln}\left(\frac{v + b_M}{v} \right) \Bigg] + a_M$$

$$\cdot\, \frac{\frac{\frac{b_2}{R}}{T^{1,5}}}{b_M^{\ 2}} \cdot \left[\mathbf{ln}\left(\frac{v + b_M}{v} \right) - \left(\frac{b_M}{v + b_M} \right) \right] - \mathbf{ln}\left[P \cdot \frac{v}{R \cdot T} \right]$$

$$\mathbf{ln}[\nu_3] = \mathbf{ln}\left[\frac{v}{v - b_M} \right] + \frac{b_3}{v - b_M} - \Bigg[\frac{\frac{2}{R}}{T^{1,5} \cdot b_M} \cdot \Big(y_1 \cdot [a_3 \cdot 35]^{0,5} + y_2 \cdot [a_3 \cdot a_2]^{0,5} + y_3 \cdot a_3 + y_4$$

$$\cdot\, [a_3 \cdot a_4]^{0,5} + y_5 \cdot [a_3 \cdot 46]^{0,5} + y_6 \cdot [a_3 \cdot a_6]^{0,5} + y_7 \cdot [a_3 \cdot a_7]^{0,5} \Big) \cdot \mathbf{ln}\left(\frac{v + b_M}{v} \right) \Bigg] + a_M$$

$$\cdot\, \frac{\frac{\frac{b_3}{R}}{T^{1,5}}}{b_M^{\ 2}} \cdot \left[\mathbf{ln}\left(\frac{v + b_M}{v} \right) - \left(\frac{b_M}{v + b_M} \right) \right] - \mathbf{ln}\left[P \cdot \frac{v}{R \cdot T} \right]$$

$$\mathbf{ln}[\nu_4] = \mathbf{ln}\left[\frac{v}{v - b_M} \right] + \frac{b_4}{v - b_M} - \Bigg[\frac{\frac{2}{R}}{T^{1,5} \cdot b_M} \cdot \Big(y_1 \cdot [a_4 \cdot 35]^{0,5} + y_2 \cdot [a_4 \cdot a_2]^{0,5} + y_3 \cdot [a_4$$

$$\cdot\, a_3]^{0,5} + y_4 \cdot a_4 + y_5 \cdot [a_4 \cdot 46]^{0,5} + y_6 \cdot [a_4 \cdot a_6]^{0,5} + y_7 \cdot [a_4 \cdot a_7]^{0,5} \Big) \cdot \mathbf{ln}\left(\frac{v + b_M}{v} \right) \Bigg] + a_M$$

$$\cdot \frac{\frac{\frac{b_4}{R}}{T^{1,5}}}{b_M^{\ 2}} \cdot \left[\ln\left(\frac{v + b_M}{v}\right) - \left(\frac{b_M}{v + b_M}\right)\right] - \ln\left[P \cdot \frac{v}{R \cdot T}\right]$$

$$\ln[\nu_5] = \ln\left[\frac{v}{v - b_M}\right] + \frac{b_5}{v - b_M} - \left[\frac{\frac{2}{R}}{T^{1,5} \cdot b_M} \cdot \left(y_1 \cdot [46 \cdot 35]^{0,5} + \frac{y_1}{2} \cdot R^2 \cdot T^{2,5} \cdot K + y_2 \cdot [46\right.\right.$$

$$\cdot a_2]^{0,5} + y_3 \cdot [46 \cdot a_3]^{0,5} + y_4 \cdot [46 \cdot a_4]^{0,5} + y_5 \cdot [46 + a_5] + y_6 \cdot [46 \cdot a_6]^{0,5} + y_7 \cdot [46$$

$$\left.\left. \cdot a_7]^{0,5} \right) \cdot \ln\left(\frac{v + b_M}{v}\right)\right] + a_M \cdot \frac{\frac{\frac{b_5}{R}}{T^{1,5}}}{b_M^{\ 2}} \cdot \left[\ln\left(\frac{v + b_M}{v}\right) - \left(\frac{b_M}{v + b_M}\right)\right] - \ln\left[P \cdot \frac{v}{R \cdot T}\right]$$

$$\ln[\nu_6] = \ln\left[\frac{v}{v - b_M}\right] + \frac{b_6}{v - b_M} - \left[\frac{\frac{2}{R}}{T^{1,5} \cdot b_M} \cdot \left(y_1 \cdot [a_6 \cdot 35]^{0,5} + y_2 \cdot [a_6 \cdot a_2]^{0,5} + y_3 \cdot [a_6\right.\right.$$

$$\left.\left. \cdot a_3]^{0,5} + y_4 \cdot [a_6 \cdot a_4]^{0,5} + y_5 \cdot [a_6 \cdot 46]^{0,5} + y_6 \cdot a_6 + y_7 \cdot [a_6 \cdot a_7]^{0,5} \right) \cdot \ln\left(\frac{v + b_M}{v}\right)\right] + a_M$$

$$\cdot \frac{\frac{\frac{b_6}{R}}{T^{1,5}}}{b_M^{\ 2}} \cdot \left[\ln\left(\frac{v + b_M}{v}\right) - \left(\frac{b_M}{v + b_M}\right)\right] - \ln\left[P \cdot \frac{v}{R \cdot T}\right]$$

$$\ln[\nu_7] = \ln\left[\frac{v}{v - b_M}\right] + \frac{b_7}{v - b_M} - \left[\frac{\frac{2}{R}}{T^{1,5} \cdot b_M} \cdot \left(y_1 \cdot [a_7 \cdot 35]^{0,5} + y_2 \cdot [a_7 \cdot a_2]^{0,5} + y_3 \cdot [a_7\right.\right.$$

$$\left.\left. \cdot a_3]^{0,5} + y_4 \cdot [a_7 \cdot a_4]^{0,5} + y_5 \cdot [a_7 \cdot 46]^{0,5} + y_6 \cdot [a_7 \cdot a_6]^{0,5} + y_7 \cdot a_7 \right) \cdot \ln\left(\frac{v + b_M}{v}\right)\right] + a_M$$

$$\cdot \frac{\frac{\frac{b_7}{R}}{T^{1,5}}}{b_M^{\ 2}} \cdot \left[\ln\left(\frac{v + b_M}{v}\right) - \left(\frac{b_M}{v + b_M}\right)\right] - \ln\left[P \cdot \frac{v}{R \cdot T}\right]$$

$P = 30$ [atm]

$$\log[f_s] = 3,8926 - \frac{494,34}{T} - \frac{461730}{T^2} + \frac{3,8535 \times 10^7}{T^3}$$

$$\log[P_w] = 6,0034 - \frac{2869,6}{T} + \frac{442350}{T^2} - \frac{7,6887 \times 10^7}{T^3}$$

$$v_W = \left[4,3257 - 0,033622 \cdot T + 0,00012464 \cdot T^2 - 2,0255 \times 10^{-7} \cdot T^3 + 1,2549 \times 10^{-10} \cdot T^4\right] \cdot \frac{18,016}{1000}$$

$$f_w = f_s \cdot \mathbf{exp}\left[\frac{v_W}{8314{,}3 \cdot T} \cdot (P - P_w) \cdot 10^5\right]$$

$$f_1 = \nu_1 \cdot y_1 \cdot P$$

$$f_w = f_1$$

$F = 0{,}1$ *Relación molar de agua líquida de entrada a gas y a una T = 273,15 + 60 para el agua líquida de quench*

$$\text{Entrada} = y_{0;1} \cdot \mathbf{h}[\text{'H2O'}; T=500] + y_{0;2} \cdot \mathbf{h}[\text{'CH4'}; T=500] + y_{0;3} \cdot \mathbf{h}[\text{'H2'}; T=500] + y_{0;4} \cdot \mathbf{h}[\text{'CO'}; T=500] + y_{0;5} \cdot \mathbf{h}[\text{'CO2'}; T=500] + y_{0;6} \cdot \mathbf{h}[\text{'N2'}; T=500] + y_{0;7} \cdot \mathbf{h}[\text{'Argon'}; T=500; P=1] + F \cdot [\mathbf{h}(\text{'H2O'}; T=273{,}15 + 60) + \mathbf{h}(\text{'Water'}; T=273{,}15 + 60; x=0) - \mathbf{h}(\text{'Water'}; T=273{,}15 + 60; x=1)]$$

Composición gaseosa

$y_1 = \frac{y_{0;1} + x}{1 + x}$ *H2O*

$y_2 = \frac{y_{0;2}}{1 + x}$ *CH4*

$y_3 = \frac{y_{0;3}}{1 + x}$ *H2*

$y_4 = \frac{y_{0;4}}{1 + x}$ *CO*

$y_5 = \frac{y_{0;5}}{1 + x}$ *CO2*

$y_6 = \frac{y_{0;6}}{1 + x}$ *N2*

$y_7 = \frac{y_{0;7}}{1 + x}$ *A*

$$\text{Salida} = [y_1 \cdot \mathbf{h}(\text{'H2O'}; T=T) + y_2 \cdot \mathbf{h}(\text{'CH4'}; T=T) + y_3 \cdot \mathbf{h}(\text{'H2'}; T=T) + y_4 \cdot \mathbf{h}(\text{'CO'}; T=T) + y_5 \cdot \mathbf{h}(\text{'CO2'}; T=T) + y_6 \cdot \mathbf{h}(\text{'N2'}; T=T) + y_7 \cdot \mathbf{h}(\text{'Argon'}; T=T; P=1) + \Delta h] \cdot [1 + x] + [F - x] \cdot [\mathbf{h}(\text{'H2O'}; T=T) + \mathbf{h}(\text{'Water'}; T=T; x=0) - \mathbf{h}(\text{'Water'}; T=T; x=1)]$$

Entrada = Salida *El proceso de mezcla y obtención del equilibrio líquido-vapor es adiabático*

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

a_M = 38,43	b_M = 0,0188
Δh = -464,4 [kJ/kmol]	dK = -0,003078
DT = -0,0833	Entrada = -157848 [kJ/kmol]
F = 0,1	f_1 = 9,008
f_s = 8,909	f_w = 9,008
K = 0,001821	P = 30 [atm]
P_w = 9,565 [bar]	R = 0,08206
Salida = -157848 [kJ/kmol]	T = 451,3 [K]
v = 1,205	v_W = 0,02028
x = 0,02981	

22 potential unit problems were detected.

Arrays Table

	a_i	b_i	y_i	ν_i	$y_{0;i}$
1	167,7	0,0146	0,3401	0,883	0,3204
2	31,57	0,0296	0,001733	1,018	0,001785
3	1,768	0,01571	0,3852	1,043	0,3967
4	17,02	0,02741	0,003302	1,029	0,0034
5	15,45	0,0297	0,1434	0,9852	0,1477
6	15,46	0,02678	0,126	1,031	0,1298
7	16,86	0,0224	0	1,025	0

Parametric Table: Table 2

	T [K]	f_1	f_w
Run 1	*450*	*8,843*	*8,743*
Run 2	*450,1*	*8,845*	*8,765*
Run 3	*450,2*	*8,847*	*8,787*
Run 4	*450,3*	*8,849*	*8,808*
Run 5	*450,4*	*8,852*	*8,83*
Run 6	*450,6*	*8,854*	*8,852*
Run 7	*450,7*	*8,856*	*8,874*
Run 8	*450,8*	*8,859*	*8,896*
Run 9	*450,9*	*8,861*	*8,918*
Run 10	*451*	*8,863*	*8,94*