

Cálculo del equilibrio líquido-vapor de una mezcla de gas de síntesis y amoníaco líquido a alta presión.

Se calcula el dew point y la composición del líquido, dada la composición en fase gas .

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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 Calculation of Vapor-Liquid Equilibria for the system NH3-N2-H2-A-CH4

C.G..Alesandrini, S. Lynn, J.M. Prausnitz, Ind, Eng. Chem. Proc. Des. Dev. 11, 1972.

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

	b_i	a_{ij}	P_c (atm)	T_c (K)
NH3	24,33		111,3	405,5
CH4		45,8		190,7
H2	$20,2 / (1 + 44,2 / 2,016 / T)$	$43,6 / (1 + 21,8 / 2,016 / T)$		quantum effects
N2	0,02678	15,462	33,5	126,2
A		48,0	151,2	

Para amoníaco $a(T) = 24,33 + 0,5017E6 \cdot T^{-3/2}$ y $a_0 = 24,33$

Su derivada es : $da/dT = (-3/2 \cdot 0,5017E6 / T^{-5/2})$

Los gases son 1= NH3, 2 = CH4, 3 = H2, 4 = N2, 5 = A

Composición gaseosa

$$y_1 = 0,08 \quad \text{NH3}$$

$$y_2 = 0,088 \quad \text{CH4}$$

$$y_3 = 0,598 \quad \text{H2}$$

$$y_4 = 0,199 \quad \text{N2}$$

$$y_5 = 0,035 \quad \text{A}$$

$$b_1 = 0,08664 \cdot 0,0820597 \cdot \frac{405,5}{111,3}$$

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

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

$$b_4 = 0,02678$$

$$b_5 = 0,08664 \cdot 0,0820597 \cdot \frac{151,2}{48}$$

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

$$a_1 = \frac{501700}{T^{1,5}}$$

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

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

$$a_4 = 15,462$$

$$a_5 = 0,4275 \cdot 0,0820597^2 \cdot \frac{151,2^{2,5}}{48}$$

$$R = 0,0820597 \text{ [atm}\cdot\text{m}^3/\text{kmol}\cdot\text{K]}$$

$$a_M = \left[y_1 \cdot 24,33^{0,5} + y_2 \cdot a_2^{0,5} + y_3 \cdot a_3^{0,5} + y_4 \cdot a_4^{0,5} + y_5 \cdot a_5^{0,5} \right]^2 + y_1^2 \cdot a_1$$

$$DT = \frac{-3}{2} \cdot \frac{501700}{T^{\left[\frac{-5}{2} \right]}} \cdot y_1^2$$

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

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

$$\ln [v_1] = \ln \left[\frac{v}{v - b_M} \right] + \frac{b_1}{v - b_M} - \left[\frac{\frac{2}{R}}{T^{1,5} \cdot b_M} \cdot (y_1 \cdot [24,33 + a_1] + y_2 \cdot [24,33 \cdot a_2]^{0,5} + y_3$$

$$\cdot [24,33 \cdot a_3]^{0,5} + y_4 \cdot [24,33 \cdot a_4]^{0,5} + y_5 \cdot [24,33 \cdot a_5]^{0,5}) \cdot \ln \left(\frac{v + b_M}{v} \right) \right] + a_M \cdot \frac{\frac{b_1}{R}}{b_M^2 T^{1,5}}$$

$$\cdot \left[\ln \left(\frac{v + b_M}{v} \right) - \left(\frac{b_M}{v + b_M} \right) \right] - \ln \left[P \cdot \frac{v}{R \cdot T} \right]$$

$$\ln [v_2] = \ln \left[\frac{v}{v - b_M} \right] + \frac{b_2}{v - b_M} - \left[\frac{\frac{2}{R}}{T^{1,5} \cdot b_M} \cdot (y_1 \cdot [a_2 \cdot 24,33]^{0,5} + y_2 \cdot a_2 + y_3 \cdot [a_2 \cdot a_3]^{0,5}$$

$$+ y_4 \cdot [a_2 \cdot a_4]^{0,5} + y_5 \cdot [a_2 \cdot a_5]^{0,5}) \cdot \ln \left(\frac{v + b_M}{v} \right) \right] + a_M \cdot \frac{\frac{b_2}{R}}{b_M^2 T^{1,5}} \cdot \left[\ln \left(\frac{v + b_M}{v} \right) - \left(\frac{b_M}{v + b_M} \right) \right]$$

$$- \ln \left[P \cdot \frac{v}{R \cdot T} \right]$$

$$\ln [v_3] = \ln \left[\frac{v}{v - b_M} \right] + \frac{b_3}{v - b_M} - \left[\frac{\frac{2}{R}}{T^{1.5} \cdot b_M} \cdot (y_1 \cdot [a_3 \cdot 24,33]^{0.5} + y_2 \cdot [a_3 \cdot a_2]^{0.5} + y_3 \cdot a_3 + y_4 \cdot [a_3 \cdot a_4]^{0.5} + y_5 \cdot [a_3 \cdot a_5]^{0.5}) \cdot \ln \left(\frac{v + b_M}{v} \right) \right] + a_M \cdot \frac{\frac{b_3}{R}}{b_M^2} \cdot \left[\ln \left(\frac{v + b_M}{v} \right) - \left(\frac{b_M}{v + b_M} \right) \right] - \ln \left[P \cdot \frac{v}{R \cdot T} \right]$$

$$\ln [v_4] = \ln \left[\frac{v}{v - b_M} \right] + \frac{b_4}{v - b_M} - \left[\frac{\frac{2}{R}}{T^{1.5} \cdot b_M} \cdot (y_1 \cdot [a_4 \cdot 24,33]^{0.5} + y_2 \cdot [a_4 \cdot a_2]^{0.5} + y_3 \cdot [a_4 \cdot a_3]^{0.5} + y_4 \cdot a_4 + y_5 \cdot [a_4 \cdot a_5]^{0.5}) \cdot \ln \left(\frac{v + b_M}{v} \right) \right] + a_M \cdot \frac{\frac{b_4}{R}}{b_M^2} \cdot \left[\ln \left(\frac{v + b_M}{v} \right) - \left(\frac{b_M}{v + b_M} \right) \right] - \ln \left[P \cdot \frac{v}{R \cdot T} \right]$$

$$\ln [v_5] = \ln \left[\frac{v}{v - b_M} \right] + \frac{b_5}{v - b_M} - \left[\frac{\frac{2}{R}}{T^{1.5} \cdot b_M} \cdot (y_1 \cdot [a_5 \cdot 24,33]^{0.5} + y_2 \cdot [a_5 \cdot a_2]^{0.5} + y_3 \cdot [a_5 \cdot a_3]^{0.5} + y_4 \cdot [a_5 \cdot a_4]^{0.5} + y_5 \cdot a_5) \cdot \ln \left(\frac{v + b_M}{v} \right) \right] + a_M \cdot \frac{\frac{b_5}{R}}{b_M^2} \cdot \left[\ln \left(\frac{v + b_M}{v} \right) - \left(\frac{b_M}{v + b_M} \right) \right] - \ln \left[P \cdot \frac{v}{R \cdot T} \right]$$

$P = 200$ [atm]

$$\beta_1 = \frac{v_{\text{Crit}} ['\text{Ammonia}']}{R} \cdot \left[1 - 0,89 \cdot \mathbf{AcentricFactor}^{0.5} ('\text{Ammonia}') \right] \cdot \exp \left[6,9547 - 76,2853 \cdot \frac{T}{T_{\text{Crit}} ('\text{Ammonia}')} + 191,306 \cdot \left(\frac{T}{T_{\text{Crit}} ('\text{Ammonia}')} \right)^2 - 203,5472 \cdot \left(\frac{T}{T_{\text{Crit}} ('\text{Ammonia}')} \right)^3 + 82,7631 \cdot \left(\frac{T}{T_{\text{Crit}} ('\text{Ammonia}')} \right)^4 \right]$$

$$F = x_1 \cdot v_{\text{Crit}} ['\text{Ammonia}'] + x_2 \cdot v_{\text{Crit}} ['\text{CH4}'] + x_3 \cdot v_{\text{Crit}} ['\text{H2}'] + x_4 \cdot v_{\text{Crit}} ['\text{N2}'] + x_5 \cdot v_{\text{Crit}} ['\text{Argon}']$$

$$G = R \cdot [x_1 \cdot T_{\text{Crit}} ('Ammonia') + x_2 \cdot T_{\text{Crit}} ('CH4') + x_3 \cdot T_{\text{Crit}} ('H2') + x_4 \cdot T_{\text{Crit}} ('N2') + x_5 \cdot T_{\text{Crit}} ('Argon')]$$

$$H = 1 - 0,89 \cdot [x_1 \cdot \text{AcentricFactor} ('Ammonia') + x_2 \cdot \text{AcentricFactor} ('CH4') + x_3 \cdot \text{AcentricFactor} ('H2') + x_4 \cdot \text{AcentricFactor} ('N2') + x_5 \cdot \text{AcentricFactor} ('Argon')]^{0,5}$$

$$J = \exp \left[6,9547 - 72,2853 \cdot T \cdot \frac{R}{G} + 191,306 \cdot \left(T \cdot \frac{R}{G} \right)^2 - 203,5472 \cdot \left(T \cdot \frac{R}{G} \right)^3 + 82,7631 \cdot \left(T \cdot \frac{R}{G} \right)^4 \right]$$

$$J2 = \exp \left[6,9547 - 72,2853 \cdot T \right]$$

$$\cdot \left(\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4'] + 191,306 \cdot \left[T \cdot \left(\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right) \right]^2 - 203,5472 \cdot \left[T \cdot \left(\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right) \right]^3 + 82,7631 \cdot \left[T \cdot \left(\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right) \right]^4} \right)^2$$

$$H2 = 1 - 0,89 \cdot [x_1 \cdot \text{AcentricFactor} ('Ammonia') + x_3 \cdot \text{AcentricFactor} ('H2') + x_4 \cdot \text{AcentricFactor} ('N2') + x_5 \cdot \text{AcentricFactor} ('Argon')]^{0,5}$$

$$\begin{aligned} DJ2 = J2 \cdot & \left[-72,2853 \cdot T \cdot \left(\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} - T_{\text{Crit}} ['CH4'] \cdot \left[\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right]^2 \right) \right. \\ & + 191,306 \cdot T^2 \cdot \left(2 \cdot \left[\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right]^2 - 2 \cdot T_{\text{Crit}} ['CH4'] \right. \\ & \cdot \left. \left[\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right]^3 \right) - 203,5472 \cdot T^3 \cdot \left(3 \cdot \left[\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right]^3 - 3 \right. \\ & \cdot T_{\text{Crit}} ['CH4'] \cdot \left[\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right]^4 \right) + 82,7631 \cdot T^4 \cdot \left(4 \cdot \left[\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right]^4 \right. \\ & \left. \left. - 4 \cdot T_{\text{Crit}} ['CH4'] \cdot \left[\frac{R}{G - R \cdot x_2 \cdot T_{\text{Crit}} ['CH4']} \right]^5 \right) \right] \end{aligned}$$

$$\beta_2 = \beta_1$$

$$+ \left[\frac{v ('Ammonia'; T=T; x=0)}{413,88343 - 5,3949156 \cdot T + 0,029121251 \cdot T^2 - 0,000069651858 \cdot T^3 + 6,3228243 \times 10^{-8} \cdot T^4} \right]$$

$$\cdot 1000 \cdot \left[\left([H - x_2 \cdot v_{\text{Crit}} ('CH4')] \cdot \left[\frac{J2}{G - R \cdot x_2 \cdot T_{\text{Crit}} ('CH4')} \right] \right) \cdot v_{\text{Crit}} ('CH4') - \left([F - x_2 \right.$$

$$\cdot v_{\text{Crit}} ('CH4')] \cdot H2 \cdot J2 \cdot R \cdot \frac{T_{\text{Crit}} ['CH4']}{[G - R \cdot x_2 \cdot T_{\text{Crit}} ('CH4')]^2} \right] + [F - x_2 \cdot v_{\text{Crit}} ('CH4')]$$

$$\cdot \left[G - R \cdot x_2 \cdot T_{\text{Crit}} ('CH4') \cdot \frac{-0,89}{2} \cdot \text{AcentricFactor} ('CH4') \cdot \left(\frac{0,89}{1 - H2} \right) + \left([F - x_2 \cdot v_{\text{Crit}} ('CH4')] \cdot \left[\frac{J2}{G - R \cdot x_2 \cdot T_{\text{Crit}} ('CH4')} \right] \right) \right]$$

$$J3 = \exp \left[6,9547 - 72,2853 \cdot T \right]$$

$$\cdot \left(\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} + 191,306 \cdot \left[T \cdot \left(\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} \right) \right]^2 - 203,5472 \cdot \left[T \cdot \left(\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} \right) \right]^3 \right)$$

$$H3 = 1 - 0,89 \cdot [x_1 \cdot \mathbf{AcentricFactor} ('Ammonia') + x_2 \cdot \mathbf{AcentricFactor} ('CH4') + x_4 \cdot \mathbf{AcentricFactor} ('N2') + x_5 \cdot \mathbf{AcentricFactor} ('Argon')]^{0,5}$$

$$\begin{aligned} DJ3 = J3 \cdot & \left[-72,2853 \cdot T \cdot \left(\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} - T_{\text{Crit}} ['H2'] \cdot \left[\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} \right]^2 \right) \right. \\ & + 191,306 \cdot T^2 \cdot \left(2 \cdot \left[\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} \right]^2 - 2 \cdot T_{\text{Crit}} ['H2'] \cdot \left[\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} \right]^3 \right) \\ & - 203,5472 \cdot T^3 \cdot \left(3 \cdot \left[\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} \right]^3 - 3 \cdot T_{\text{Crit}} ['H2'] \cdot \left[\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} \right]^4 \right) \\ & \left. + 82,7631 \cdot T^4 \cdot \left(4 \cdot \left[\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} \right]^4 - 4 \cdot T_{\text{Crit}} ['H2'] \cdot \left[\frac{R}{G - R \cdot x_3 \cdot T_{\text{Crit}} ['H2']} \right]^5 \right) \right] \end{aligned}$$

$$\beta_3 = \beta_1 + \left[\frac{v ('Ammonia'; T=T; x=0)}{-203,3942 + 2,4117042 \cdot T - 0,0084697111 \cdot T^2 + 0,000010233186 \cdot T^3 + 0 \cdot T^4} \right] \cdot 1000$$

$$\cdot \left[\left([H - x_3 \cdot v_{\text{Crit}} ('H2')] \cdot \left[\frac{J3}{G - R \cdot x_3 \cdot T_{\text{Crit}} ('H2')} \right] \right) \cdot v_{\text{Crit}} ('H2') - \left([F - x_3 \cdot v_{\text{Crit}} ('H2')] \cdot H3 \right) \right]$$

$$\cdot J3 \cdot R \cdot \frac{T_{\text{Crit}} ['H2']}{[G - R \cdot x_3 \cdot T_{\text{Crit}} ('H2')]^2} + [F - x_3 \cdot v_{\text{Crit}} ('H2')]$$

$$\cdot \left[G - R \cdot x_3 \cdot T_{\text{Crit}} ('H2') \cdot \frac{-0,89}{2} \cdot \mathbf{AcentricFactor} ('H2') \cdot \left(\frac{0,89}{1 - H3} \right) + \left([F - x_3 \cdot v_{\text{Crit}} ('H2')] \cdot \left[G - R \cdot x_3 \cdot T_{\text{Crit}} ('H2') \right] \right) \right]$$

$$J4 = \exp \left[6,9547 - 72,2853 \cdot T \right]$$

$$\cdot \left(\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} + 191,306 \cdot \left[T \cdot \left(\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} \right) \right]^2 - 203,5472 \cdot \left[T \cdot \left(\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} \right) \right]^3 \right)$$

$$H4 = 1 - 0,89 \cdot [x_1 \cdot \mathbf{AcentricFactor} ('Ammonia') + x_2 \cdot \mathbf{AcentricFactor} ('CH4') + x_3 \cdot \mathbf{AcentricFactor} ('H2') + x_5 \cdot \mathbf{AcentricFactor} ('Argon')]^{0,5}$$

$$\begin{aligned}
 DJ4 = & J4 \cdot \left[-72,2853 \cdot T \cdot \left(\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} - T_{\text{Crit}} ['N2'] \cdot \left[\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} \right]^2 \right) \right. \\
 & + 191,306 \cdot T^2 \cdot \left(2 \cdot \left[\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} \right]^2 - 2 \cdot T_{\text{Crit}} ['N2'] \cdot \left[\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} \right]^3 \right) \\
 & - 203,5472 \cdot T^3 \cdot \left(3 \cdot \left[\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} \right]^3 - 3 \cdot T_{\text{Crit}} ['N2'] \cdot \left[\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} \right]^4 \right) \\
 & \left. + 82,7631 \cdot T^4 \cdot \left(4 \cdot \left[\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} \right]^4 - 4 \cdot T_{\text{Crit}} ['N2'] \cdot \left[\frac{R}{G - R \cdot x_4 \cdot T_{\text{Crit}} ['N2']} \right]^5 \right) \right]
 \end{aligned}$$

$$\begin{aligned}
 \beta_4 = & \beta_1 + \left[\frac{v ('Ammonia'; T=T; x=0)}{460 - 6,0849 \cdot T + 0,032672 \cdot T^2 - 0,000077657 \cdot T^3 + 6,99 \times 10^{-8} \cdot T^4} \right] \cdot 1000 \cdot \left([H - x_4 \right. \\
 & \cdot v_{\text{Crit}} ('N2')] \cdot \left[\frac{J4}{G - R \cdot x_4 \cdot T_{\text{Crit}} ('N2')} \right] \cdot v_{\text{Crit}} ('N2') - ([F - x_4 \cdot v_{\text{Crit}} ('N2')] \cdot H_4 \cdot J4 \cdot R \\
 & \cdot \left. \frac{T_{\text{Crit}} ['N2']}{[G - R \cdot x_4 \cdot T_{\text{Crit}} ('N2')]^2} \right) + [F - x_4 \cdot v_{\text{Crit}} ('N2')] \\
 & \cdot \left[G - R \cdot x_4 \cdot T_{\text{Crit}} ('N2') \cdot \frac{-0,89}{2} \cdot \mathbf{AcentricFactor} ('N2') \cdot \left(\frac{0,89}{1 - H_4} \right) + ([F - x_4 \cdot v_{\text{Crit}} ('N2')] \cdot \left[G - R \cdot x_4 \cdot \right. \right. \\
 & \left. \left. T_{\text{Crit}} ('N2')] \right) \right]
 \end{aligned}$$

$$\begin{aligned}
 J5 = & \exp \left[6,9547 - 72,2853 \cdot T \right. \\
 & \cdot \left(G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon'] + 191,306 \cdot \left[T \cdot \left(\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right) \right]^2 - 203,5472 \cdot \left[T \cdot \left(G - R \cdot x_5 \cdot \right. \right. \\
 & \left. \left. T_{\text{Crit}} ['Argon'] \right) \right]^3 \right) - 203,5472 \cdot T^3 \cdot \left(3 \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^3 - 3 \cdot T_{\text{Crit}} ['Argon'] \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^4 \right) \\
 & \left. + 82,7631 \cdot T^4 \cdot \left(4 \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^4 - 4 \cdot T_{\text{Crit}} ['Argon'] \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^5 \right) \right]
 \end{aligned}$$

$$\begin{aligned}
 H5 = & 1 - 0,89 \cdot [x_1 \cdot \mathbf{AcentricFactor} ('Ammonia') + x_2 \cdot \mathbf{AcentricFactor} ('CH4') + x_3 \cdot \mathbf{AcentricFactor} ('H2') \\
 & + x_4 \cdot \mathbf{AcentricFactor} ('N2')]^{0,5}
 \end{aligned}$$

$$\begin{aligned}
 DJ5 = & J5 \cdot \left[-72,2853 \cdot T \cdot \left(\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} - T_{\text{Crit}} ['Argon'] \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^2 \right) \right. \\
 & + 191,306 \cdot T^2 \cdot \left(2 \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^2 - 2 \cdot T_{\text{Crit}} ['Argon'] \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^3 \right) \\
 & - 203,5472 \cdot T^3 \cdot \left(3 \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^3 - 3 \cdot T_{\text{Crit}} ['Argon'] \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^4 \right) \\
 & \left. + 82,7631 \cdot T^4 \cdot \left(4 \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^4 - 4 \cdot T_{\text{Crit}} ['Argon'] \cdot \left[\frac{R}{G - R \cdot x_5 \cdot T_{\text{Crit}} ['Argon']} \right]^5 \right) \right]
 \end{aligned}$$

$$\beta_5 = \beta_1$$

$$+ \left[\frac{v ('Ammonia' ; T=T ; x=0)}{483,54588 - 6,4121276 \cdot T + 0,034018649 \cdot T^2 - 0,000080038523 \cdot T^3 + 7,1411916 \times 10^{-8} \cdot T^4} \right]$$

$$\cdot 1000 \cdot \left[\left([H - x_5 \cdot v_{\text{Crit}} ('Argon')] \cdot \left[\frac{J_5}{G - R \cdot x_5 \cdot T_{\text{Crit}} ('Argon')} \right] \right) \cdot v_{\text{Crit}} ('Argon') - \left([F - x_5 \cdot v_{\text{Crit}} ('Argon')] \cdot H_5 \cdot J_5 \cdot R \cdot \frac{T_{\text{Crit}} ['Argon']}{[G - R \cdot x_5 \cdot T_{\text{Crit}} ('Argon')]^2} \right) \right] + [F - x_5 \cdot v_{\text{Crit}} ('Argon')]$$

$$\cdot \left[G - R \cdot x_5 \cdot T_{\text{Crit}} ('Argon') \cdot \frac{-0,89}{2} \cdot \mathbf{AcentricFactor} ('Argon') \cdot \left(\frac{0,89}{1 - H_5} \right) + \left([F - x_5 \cdot v_{\text{Crit}} ('Argon')] \cdot \left[G - \right. \right. \right]$$

$$f_{1L} = \gamma_1 \cdot x_1 \cdot \mathbf{Fugacity} ['Ammonia' ; T=T ; x=0] \cdot \left| 0,9869 \cdot \frac{\text{atm}}{\text{bar}} \right| \cdot \exp \left[v ('Ammonia' ; T=T ; x=0) \right]$$

$$\cdot \left(\frac{1 + 7 \cdot \beta_1 \cdot \left[P - P_{\text{sat}} ('Ammonia' ; T=T) \cdot \left| 0,9869 \cdot \frac{\text{atm}}{\text{bar}} \right| \right]^{[6 / 7]} - 1}{R \cdot T \cdot 6 \cdot \beta_1} \right)$$

$$\ln \left[\frac{\alpha_2}{1000} \right] = -38,1649 + \frac{19801,2}{T} - \frac{2,88498 \times 10^6}{T^2}$$

$$\ln \left[\frac{\alpha_3}{1000} \right] = -9,87862 + \frac{2904,17}{T} - \frac{177315}{T^2}$$

$$\ln \left[\frac{\alpha_4}{1000} \right] = 4,32945 - \frac{5751,52}{T} + \frac{1,03658 \times 10^6}{T^2}$$

$$\ln \left[\frac{\alpha_5}{1000} \right] = -6,43535 + \frac{2602,91}{T} - \frac{536723}{T^2}$$

$$\ln [H_2] = -1,6701 + \frac{4405,58}{T} - \frac{482973}{T^2}$$

$$\ln [H_3] = -2,29337 + \frac{5294,74}{T} - \frac{521881}{T^2}$$

$$\ln [H_4] = -3,68607 + \frac{5967,36}{T} - \frac{642828}{T^2}$$

$$\ln [H_5] = -0,7941 + \frac{4472,47}{T} - \frac{509281}{T^2}$$

$$\phi = \frac{X_2 \cdot v_{\text{Crit}} [\text{'CH4'}] \cdot \alpha_2^{0.5} + X_3 \cdot v_{\text{Crit}} [\text{'H2'}] \cdot \alpha_3^{0.5} + X_4 \cdot v_{\text{Crit}} [\text{'N2'}] \cdot \alpha_4^{0.5} + X_5 \cdot v_{\text{Crit}} [\text{'Argon'}] \cdot \alpha_5^{0.5}}{1}$$

F

$$\ln [\gamma_1] = v_{\text{Crit}} [\text{'Ammonia'}] \cdot \phi^2$$

$$\ln [\gamma_2] = v_{\text{Crit}} [\text{'CH4'}] \cdot [\phi^2 - 2 \cdot \alpha_2^{0.5} \cdot \phi]$$

$$\ln [\gamma_3] = v_{\text{Crit}} [\text{'H2'}] \cdot [\phi^2 - 2 \cdot \alpha_3^{0.5} \cdot \phi]$$

$$\ln [\gamma_4] = v_{\text{Crit}} [\text{'N2'}] \cdot [\phi^2 - 2 \cdot \alpha_4^{0.5} \cdot \phi]$$

$$\ln [\gamma_5] = v_{\text{Crit}} [\text{'Argon'}] \cdot [\phi^2 - 2 \cdot \alpha_5^{0.5} \cdot \phi]$$

$$f_{2L} = \gamma_2 \cdot X_2 \cdot H_2 \cdot \exp \left[\frac{1}{1000} \cdot (413,88343 - 5,3949156 \cdot T + 0,029121251 \cdot T^2 - 0,000069651858 \cdot T^3 + 6,3228243 \times 10^{-8} \cdot T^4) \cdot \left(\frac{1 + 7 \cdot \beta_2 \cdot \left[P - P_{\text{sat}} (\text{'Ammonia'}; T=T) \cdot \left| 0,9869 \cdot \frac{\text{atm}}{\text{bar}} \right| \right]^{[6/7]} - 1}{R \cdot T \cdot 6 \cdot \beta_2} \right) \right]$$

$$f_{3L} = \gamma_3 \cdot X_3 \cdot H_3 \cdot \exp \left[\frac{1}{1000} \cdot (-203,3942 + 2,4117042 \cdot T - 0,0084697111 \cdot T^2 + 0,000010233186 \cdot T^3 + 0 \cdot T^4) \cdot \left(\frac{1 + 7 \cdot \beta_3 \cdot \left[P - P_{\text{sat}} (\text{'Ammonia'}; T=T) \cdot \left| 0,9869 \cdot \frac{\text{atm}}{\text{bar}} \right| \right]^{[6/7]} - 1}{R \cdot T \cdot 6 \cdot \beta_3} \right) \right]$$

$$f_{4L} = \gamma_4 \cdot X_4 \cdot H_4 \cdot \exp \left[\frac{1}{1000} \cdot (460 - 6,0849 \cdot T + 0,032672 \cdot T^2 - 0,000077657 \cdot T^3 + 6,99 \times 10^{-8} \cdot T^4) \cdot \left(\frac{1 + 7 \cdot \beta_4 \cdot \left[P - P_{\text{sat}} (\text{'Ammonia'}; T=T) \cdot \left| 0,9869 \cdot \frac{\text{atm}}{\text{bar}} \right| \right]^{[6/7]} - 1}{R \cdot T \cdot 6 \cdot \beta_4} \right) \right]$$

$$f_{5L} = \gamma_5 \cdot X_5 \cdot H_5 \cdot \exp \left[\frac{1}{1000} \cdot (483,54588 - 6,4121276 \cdot T + 0,034018649 \cdot T^2 - 0,000080038523 \cdot T^3 + 7,1411916 \times 10^{-8} \cdot T^4) \cdot \left(\frac{1 + 7 \cdot \beta_5 \cdot \left[P - P_{\text{sat}} (\text{'Ammonia'}; T=T) \cdot \left| 0,9869 \cdot \frac{\text{atm}}{\text{bar}} \right| \right]^{[6/7]} - 1}{R \cdot T \cdot 6 \cdot \beta_5} \right) \right]$$

$$f_{1G} = v_1 \cdot y_1 \cdot P$$

$$f_{2G} = v_2 \cdot y_2 \cdot P$$

$$f_{3G} = v_3 \cdot y_3 \cdot P$$

$$f_{4G} = v_4 \cdot y_4 \cdot P$$

$$f_{5G} = v_5 \cdot y_5 \cdot P$$

$$f_{1G} = f_{1L}$$

$$f_{2G} = f_{2L}$$

$$f_{3G} = f_{3L}$$

$$f_{4G} = f_{4L}$$

$$f_{5G} = f_{5L}$$

$$\sigma = \sum_{i=1}^5 [x_i]$$

$$\sigma = 1$$

SOLUTION

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

$$a_M = 7,406$$

$$\Delta h = -9,607E+13$$

$$DJ3 = 0,000002206$$

$$DJ5 = 0,000001487$$

$$F = 0,07583$$

$$f_{1L} = 11,67$$

$$f_{2L} = 15,97$$

$$f_{3L} = 136,8$$

$$f_{4L} = 40,5$$

$$f_{5L} = 6,742$$

$$H = 0,5555$$

$$H3 = 0,5555$$

$$H5 = 0,5555$$

$$J2 = 2,838E-07$$

$$J4 = 2,790E-07$$

$$P = 200 \text{ [atm]}$$

$$R = 0,08206 \text{ [atm}\cdot\text{m}^3/\text{kmol}\cdot\text{K]}$$

$$T = 304,5 \text{ [K]}$$

$$b_M = 0,02029$$

$$DJ2 = 0,000001288$$

$$DJ4 = 0,000001654$$

$$DT = -7,793E+09$$

$$f_{1G} = 11,67$$

$$f_{2G} = 15,97$$

$$f_{3G} = 136,8$$

$$f_{4G} = 40,5$$

$$f_{5G} = 6,742$$

$$G = 32,62$$

$$H2 = 0,5556$$

$$H4 = 0,5557$$

$$J = 2,321$$

$$J3 = 2,775E-07$$

$$J5 = 2,765E-07$$

$$\phi = 0,1869$$

$$\sigma = 1$$

$$v = 0,1335$$

51 potential unit problems were detected.

Arrays Table

	a_i	α_i	b_i	β_i	γ_i	H_i	v_i	x_i	y_i
1	94,42		0,0259	0,0001221	1,003		0,7293	0,974	0,08
2	31,57	14,25	0,0296	0,0001221	0,8731	1977	0,9074	0,007571	0,088
3	1,757	105	0,01589	0,0001221	0,7756	12916	1,144	0,01183	0,598
4	15,46	34,07	0,02678	0,0001221	0,8253	7927	1,018	0,005137	0,199
5	16,86	25,33	0,0224	0,0001221	0,8714	4452	0,9632	0,001475	0,035