② 6.71

Nitrogen at 15 bar and 100K is to be adiabatically flashed to 1 bar. Determine the exiting temperature of nitrogen and the fractions that are vapor and liquid using the Peng-Robinson equation of state.

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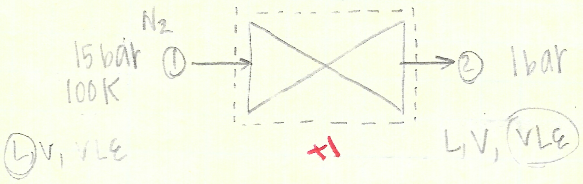

+1 +1

Assumptions: steady state (no info)
no KE/PE change (no info)
no Q/adiabatic (problem)

+3

Mass Balance: $\frac{dN_{sys}}{dt}^{\nearrow ss} = \sum_{k=1}^{K} \dot{n}_k \qquad \dot{N}_1 = -\dot{N}_2 = \dot{N}$

Energy Balance: $\frac{dE_{sys}}{dt}^{\nearrow ss} = \frac{d}{dt}\left[U + M_{sys}\left(\frac{v^2}{2} + gz\right)\right]_{sys} = \dot{Q}^{\nearrow adia} + \dot{W}^{\nearrow \text{Rigid work}} + \sum_{k=1}^{K} \dot{n}_k \left[H_k + \frac{v^2}{2} + gz\right]^{\nearrow \text{no KE/PE change}}$

$0 = \dot{N}(\underline{H}_2 - \underline{H}_1) \qquad \underline{H}_2 = \underline{H}_1 \qquad \boxed{\Delta \underline{H} = 0}$

+5

Entropy Balance: $\frac{dS_{sys}}{dt}^{\nearrow ss} = \frac{\dot{Q}}{T}^{\nearrow adia} + \sum_{k=1}^{K} \dot{N}_k S_k + \dot{S}_{gen}$

$\frac{\dot{S}_{gen}}{\dot{N}} = \underline{S}_2 - \underline{S}_1 = \Delta \underline{S}$

$\Delta \underline{H} = \underline{H}_2^{dep} - \underline{H}_1^{dep} + \Delta \underline{H}^{IG} = 0 \qquad \Delta \underline{H}^{IG} = \int_{T_1}^{T_2} c_p^* \, dT$

$\Delta \underline{S} = \underline{S}_2^{dep} - \underline{S}_1^{dep} + \Delta \underline{S}^{IG} \qquad \Delta \underline{S}^{IG} = \int_{T_1}^{T_2} \frac{c_p^*}{T} dT - R \ln \frac{P_2}{P_1}$

P^{vap} of N_2 @ 100K = $\boxed{7.839 \text{ bar}}$ → stream 1 $\boxed{\text{liquid}}$ +4
$P^{vap} < P = L$

$\underline{H}_1 = \theta_1^L \underline{H}_1^L + \cancel{\theta_1^V \underline{H}_1^V} \qquad \underline{H}_2 = \theta_2^L \underline{H}_2^L + \theta_2^V \underline{H}_2^V$

+1 $\Delta \underline{H} = 0 = \underline{H}_2 - \underline{H}_1 = \theta_2^L \underline{H}_2^L + \theta_2^V \underline{H}_2^V - \underline{H}_1 \qquad (\underline{H}_1 = \underline{H}_1^{dep} + \underline{H}^{IG})$ +1

$\Delta \underline{H} = 0 = \theta_2^L \underline{H}_2^L + \theta_2^V \underline{H}_2^V - \underline{H}_1^{dep} - \underline{H}_1^{IG} \qquad$ where $\underline{H}_2 = \underline{H}_2^{dep} + \underline{H}_2^{IG}$

$P_2 = 1$ bar
$T_c = 126.2$ K
$P_c = 33.9$ bar
$\omega = 0.039$

guess $T_2 = 50$ K

$P = \frac{RT}{\underline{V} - b} - \frac{a(\omega, T_r)}{\underline{V}(\underline{V}+b) + b(\underline{V}-b)}$ +3

$a = \frac{0.45724 (8.314\times10^{-5} \text{ bar m}^3/\text{mol K})^2 (126.2 \text{ K})^2}{(33.9 \text{ bar})} = 1.48\times10^{-6} \frac{\text{bar m}^6}{\text{mol}^2}$

$A = \frac{aP}{(RT)^2} = \frac{\left(1.48\times10^{-6} \frac{\text{bar m}^6}{\text{mol}^2}\right)(1 \text{ bar})}{\left(8.314\times10^{-5} \frac{\text{bar m}^3}{\text{mol K}} \cdot 50 \text{ K}\right)^2}$

$A = 0.085645$

$b = \frac{0.07780 (8.314\times10^{-5} \text{ bar m}^3/\text{mol K})(126.2 \text{ K})}{(33.9 \text{ bar})} = 2.41\times10^{-5} \text{ m}^3/\text{mol}$

$B = \frac{bP}{RT} = \frac{(2.41\times10^{-5} \text{ m}^3/\text{mol})(1 \text{ bar})}{(8.314\times10^{-5} \text{ bar m}^3/\text{mol K})(50 \text{ K})}$ +3

$B = 0.005797$

$\alpha = -(1-B)$ $\quad$ $\beta = (A - 3B^2 - 2B)$ $\quad$ $\gamma = -(AB - B^2 - B^3)$

$\alpha = -(1 - 0.005797)$ $\quad$ $\beta = (0.085645 - 3(0.005797)^2 - 2(0.005797))$ $\quad$ $\gamma = -(0.085 \cdot 0.0057 - 0.0057^2 - 0.0057^3)$

$\alpha = -0.994203$ $\quad$ $\beta = 0.073949$ $\quad$ $\gamma = -0.000463$

$z^3 + \alpha z^2 + \beta z + \gamma = 0$ → cubic equation solver

$x_1 = 0.91367$

* $x_2 = 0.0069$ → use stability criteria to eliminate 1 $\quad$ $C_v > 0,\ \left(\frac{\partial V}{\partial P}\right)_T < 0$

$x_3 = 0.07343$

$$\left(\frac{\partial P}{\partial \underline{V}}\right) = -\frac{RT}{(\underline{V}-b)} + \frac{2a(\underline{V}+b)}{[\underline{V}(\underline{V}+b)+b(\underline{V}-b)]^2} < 0$$

$z_1 = 0.91367$ $\quad$ $z_2 = 0.0069$ $\quad$ $z_3 = 0.07343$

$\underline{V} = \frac{zRT}{P} = \frac{(0.91367)(8.314\times10^{-5})(50)}{(1\ \text{bar})}$ $\quad$ $\underline{V}_2 = 0.000029\ \frac{m^3}{mol}$ $\quad$ $\underline{V}_3 = 0.000305\ m^3/mol$

$\underline{V}_1 = 0.003798\ m^3/mol$

$$\left(\frac{\partial P}{\partial \underline{V}_1}\right) = \frac{(-8.314\times10^{-5}\ m^3\,bar/mol\,K)(50\,K)}{(0.003798\ m^3/mol - 2.41\times10^{-5})} + \frac{2\cdot 1.48\times10^{-6}\ \frac{bar\,m^6}{mol^2}\left(0.003798\ m^3/mol + 2.41\times10^{-5}\ m^3/mol\right)}{[0.003798\ m^3/mol\,(0.003798\ m^3/mol + 2.41\times10^{-5}\ \frac{m^3}{mol}) + 2.41\times10^{-5}(0.003798 - 2.41\times10^{-5})}$$

$\left(\frac{\partial P}{\partial \underline{V}_1}\right) = -1.10 < 0$ $\quad$ (same procedure for $\underline{V}_2$ + $\underline{V}_3$) (estimating) $\quad$ $\left(\frac{\partial P}{\partial \underline{V}_2}\right) = -$ $\quad$ $\left(\frac{\partial P}{\partial \underline{V}_3}\right) = +$ $\quad$ +2

Roots are z_1 + z_2 $\quad$ vapor = 0.91367 (bigger)
liquid = 0.0069 $\quad$ +1

now check fugacity → we want $f^L = f^V$

$$\ln\left(\frac{f(T,P)}{P}\right) = \frac{1}{RT}\int_{\infty}^{\underline{V}}\left[\frac{RT}{\underline{V}} - P\right]d\underline{V} - \ln z + (z-1)$$

$$\ln\left(\frac{f(T,P)}{P}\right) = \frac{1}{RT}\left[RT\ln(\underline{V}) - P\underline{V}\right]_{\infty}^{\underline{V}} - \ln z + (z-1)$$

$$\ln\left(\frac{f(T,P)}{P}\right) = \ln(\underline{V}) - \frac{P\underline{V}}{RT} - \ln z + (z-1)$$

vapor
$z = 0.91367$
$\underline{V} = 0.003798\ m^3/mol$

liquid
$z = 0.0069$
$\underline{V} = 0.000029\ m^3/mol$

$f^V = 0.89019$ $\quad$ $f^L = 0.0006$

software

$f^V > f^L$ equilibrium not satisfied
need to guess higher temp $\quad$ +3

Need to iterations using software + guess higher temp than 50°, but lower than 100° (higher gives img. roots)

$\boxed{f^L = f^V \approx 0.95\ @\ 77°K}$

+3 $\quad$ +1

$$\underline{H}_1^{dep}(100\,K, 15\,bar) = RT(z-1) + \frac{T\left(\frac{da}{dT}\right) - a}{2\sqrt{2}b} \ln\left[\frac{z+(1+\sqrt{2})B}{z+(1-\sqrt{2})B}\right]$$

$$\frac{da}{dT} = -0.45724\frac{R^2 T_c^2}{P_c}\cdot K\cdot\sqrt{\frac{\alpha}{T\cdot T_c}}$$

$$K = 0.37464 + 1.54226(0.039) - 0.26992(0.039)^2 = 0.434$$

$$\frac{da}{dT} = -0.45724\frac{(8.314\times10^{-5}\frac{m^3\,bar}{mol\,K})^2(126.2\,K)^2}{(33.9\,bar)}\cdot 0.434\cdot\sqrt{\frac{1.3478}{(77)(126.2)}}$$

$\frac{da}{dT}(77\,K) = -7.594\times10^{-9}$ $\frac{da}{dT}(100\,K) = -6.016\times10^{-9}$

$B(100\,K) = 0.043481$ $B(77\,K) = 0.003765$ $a = 1.48\times10^{-6}$
$A(100\,K) = 0.3212$ $b = 2.41\times10^{-5}$

$\alpha = -(1-B)$ $\beta = (A-3B^2-2B)$ $\gamma = -(AB-B^2-B^3)$
$\alpha = -0.9565$ $\beta = 0.2256$ $\gamma = -0.011993$

Finding z for state 1

$z^3 + \alpha z^2 + \beta z + \gamma = 0 \rightarrow$ cubic equation solver $z_1 = 0.61807$, $z_2 = 0.0732$, $z_3 = 0.26525$

z for liquid $\rightarrow 0.01-0.2$

$\underline{H}_1^{dep} = -4923.24$ J/mol
$\underline{H}_2^{dep}\,V = -64.10$ J/mol
$\underline{H}_2^{dep}\,L = -5622.96$ J/mol

from software (see work/equation above for manual)

① $\Delta\underline{H}^{IG}(15\,bar, 100) = -5842.13$ J/mol
② $\Delta\underline{H}^{IG}(1\,bar, 77\,K) = -6535.62$ J/mol

from software

$\theta^L + \theta^V = 1$

$$\Delta\underline{H} = 0 = \theta_2^L(\underline{H}_{2L}^{dep} + \underline{H}_{2L}^{IG}) + \theta_2^V(\underline{H}_{2V}^{dep} + \underline{H}_{2V}^{IG}) - \underline{H}_1^{dep} - \underline{H}_1^{IG}$$

$$0 = (x)(-5622.96 + -6535.62) + (1-x)(-64.10 + -6535.62) + 4923.24 + 5842.13$$

$$0 = x(-12158.6) + (1-x)(-6599.72) + 10765.4$$

$\boxed{x = 0.75}$ $\boxed{1-x = .25}$

+2

Answer

$$\boxed{\begin{array}{l} T_2 = 77K \\ \theta_2^L = 0.75 \\ \theta_2^V = 0.25 \end{array}}$$

Description of software
(see manual iteration as well)

① Inputs known P_c, T_c, w
② Guess T
③ calculate α, A, B based on T
④ solve cubic equation
$z^3 - (1-B)z^2 + (A-3B^2-2B)z - (AB-B^2-B^3) = 0$
⑤ calculate fugacity (liquid/vapor)
⑥ calculate departure functions
⑦ check energy balance