Josh Whitehead
Ch En 3853


Midterm 1

1 a) $\boxed{P^{sat} = 0.999\text{ MPa}}$

b) $\boxed{f^{sat} = 0.841\text{ MPa}}$ $\qquad \phi^{sat} = \frac{f^{sat}}{P^{sat}} = \frac{0.841}{0.999} = \boxed{0.842}$

c) $f^{l} \approx \phi^{sat} \cdot P^{sat} \exp\left(\frac{P - P^{sat}}{RT} V^{l}\right)$

$= 0.842 \cdot 0.999 \exp\left(\frac{10 - 0.999}{8.31 \cdot 300} \cdot 80\right) = \boxed{1.12\text{ MPa}}$

d) $Z = 1 + \frac{BP}{RT} = 1 + \frac{-397 \cdot 0.1}{8.31 \cdot 300} = 0.984$

$\ln \phi = \int_0^P (Z-1)\frac{dP}{P} \rightarrow \ln \phi = \int_0^P \frac{B\cancel{P}}{RT}\frac{dP}{\cancel{P}} = \int_0^P \frac{B}{RT} dP$

$\therefore \ln \phi = \frac{B}{RT}\Big]_0^P = \frac{BP}{RT} = -0.0159$

$\phi = \exp(-0.0159) = \boxed{0.984\text{ MPa}}$

Preos_problem1_propane - Excel

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TK | 300

# Peng-Robinson Equation of State (Pure Fluid)

Spreadsheet protected, but no password used.

## Properties

| Gas | $T_c$ (K) | $P_c$ (MPa) | ω |
|---|---|---|---|
| PROPANE | 369.8 | 4.249 | 0.152 |

| Current State | | Roots | | |
|---|---|---|---|---|
| T (K) | 300 | Z | V | fugacity |
| P (MPa) | 0.998886 | | $cm^3$/gmol | MPa |
| answers for three root region | | 0.814974714 | 2035.091 | 0.841426 |
| | | 0.127743853 | 318.992 | |
| | | 0.034737342 | 86.74339 | 0.841426 |
| & for 1 root region | | #NUM! | #NUM! | #NUM! |

Stable Root has a lower fugacity

| Intermediate Calculations | | | |
|---|---|---|---|
| R($cm^3$MPa/molK) | | 8.314472 | |
| $T_r$ | 0.811249 | a (MPa $cm^6$/$gmol^2$) | |
| $P_r$ | 0.235087 | 1142765 | |
| κ | 0.602827 | b ($cm^3$/gmol) | |
| α | 1.123313 | 56.29535 | |
| fugacity ratio | | A | 0.183468 |
| | 1.000001 | B | 0.022544 |

To find vapor pressure, or saturation temperature, see cell A28 for instructions

1

## Solution to Cubic $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$

| $a_2$ | $a_1$ | $a_0$ | p | q |
|---|---|---|---|---|
| -0.97746 | 0.136856 | -0.003616436 | -0.18162 | -0.0282 |

$R = q^2/4 + p^3/27 =$ -2.3E-05

If Negative, three unequal real roots,
If Positive, one real root

## Method 1 - For region with one real root

| P | Q | Root to equation in x |
|---|---|---|
| #NUM! | #NUM! | #NUM! |

Solution methods are summarized in the appendix of the text.

## Method 2 - For region with three real roots

| m | 3q/pm | $3*\theta_1$ | $\theta_1$ | Roots to equation in x | | |
|---|---|---|---|---|---|---|
| 0.492095 | 0.946684 | 0.328013002 | 0.109338 | 0.489156 | -0.19807 | -0.29108 |

Instructions PVT Props Ref State Crit. Props IG Cps rev. info

Yunshan Wang

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2b) $H_2 - H_1 = 40006.91 - 0 \boxed{= 4.00 \times 10^4 \frac{J}{mol}}$

$H_2 - H^{ig} = -180.115 \boxed{= -1.80 \times 10^2 \frac{J}{mol}}$

2c) Closed, Constant P $\therefore$ $\Delta H = Q$

$\Delta H = 40006.91 \frac{J}{mol} \cdot 10\,mol = 400069.1 \frac{J}{mol}$

$\boxed{= 4.00 \times 10^5\ J}$

d) $W_{EC} = -\int_{V_1}^{V_2} P dV = -P\Delta V = -P(V_2 - V_1)$

$V_1 = 112.99208 \frac{cm^3}{gmol}$

$V_2 = 32210.152 \frac{cm^3}{gmol}$

$\therefore W_{EC} = -101325 Pa (32210.152 - 112.99208) \frac{cm^3}{gmol}$

$= -3.25 \times 10^9 \frac{Pa\,cm^3}{gmol} \cdot 10\,\cancel{mol} = -3.25 \times 10^{10}\ Pa\,cm^3$

$W_{EC} = -3.25 \times 10^{10}\ Pa\,cm^3 \cdot \frac{1\,m^3}{1 \times 10^6\,cm^3} \boxed{= 3.25 \times 10^4\ J}$

Preos_problem2_npentane - Excel    Joshua Whitehead

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uhflag | $f_x$ | 0

| | A | B | C | D | E | F | G | H | I | J | K |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Peng-Robinson Equation of State (Pure Fluid) | | | | | Spreadsheet protected, but no password used. | | | | | |
| 2 | Properties | | | | | | | | | | |
| 3 | Gas | $T_c$ (K) | $P_c$ (MPa) | ω | | | Enter Name and Critical | | | | |
| 4 | n-PENTANE | 469.7 | 3.369 | 0.249 | | | Properities on "Props" | | | | |
| 5 | | | | | | | Worksheet. | | | | |
| 6 | Reference State | | For real fluid | | Roots | | | | | | |
| 7 | T (K) | 300 | reference state | | Z | V | fugacity | $H-H^{ig}$ | $U-U^{ig}$ | $S-S^{ig}$ | |
| 8 | P (MPa) | 0.101325 | identifier index | | | $cm^3$/gmol | MPa | J/mol | J/mol | J/molK | |
| 9 | 0 for $H_R$ = 0, 1 for $U_R$ = 0 | | 1 | | 0.957725 | 23576.54 | 0.097203 | -280.498 | -175.049 | -0.58962 | answers for three |
| 10 | 0 | | | | 0.034022 | 837.5217 | | | | | root region |
| 11 | 0 for ig, 1 for real fluid ref | | 2 | | 0.00459 | 112.9921 | 0.071651 | -26444 | -23961.1 | -85.2551 | |
| 12 | 1 | | 3 | | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | & for 1 root region |
| 13 | Identifier Index for reference state row to use from Row 9 - Row 12 (Enter 1, 2, or 3) | | | | | | | | | | |
| 14 | YOU MUST CHOOSE A ROW WITH CALCULABLE NUMBERS, NOT ONE WITH #NUM! | | | | | | | | | | |
| 15 | 2 | | | | | | | | | | |
| 16 | | | | | | | | | | | |
| 17 | | | Z | H(J/mol) | U(J/mol) | S(J/molK) | | | | | |
| 18 | Reference State Values | | 0.00459 | 0 | -11.4489 | 0 | | | | | |
| 19 | Ref State Departures | | | -26444 | -23961.1 | -85.2551 | | | | | |
| 20 | | | | | | | | | | | |
| 21 | Solution to Cubic | | $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$ | | | $R = q^2/4 + p^3/27 =$ | | -6.2E-06 | | | |
| 22 | $a_2$ | $a_1$ | $a_0$ | p | q | If Negative, three unequal real roots, | | | | | |
| 23 | -0.9963367 | 0.03713556 | -0.00015 | -0.29376 | -0.06108 | If Positive, one real root | | | | | |
| 24 | | | | | | | | | | | |
| 25 | | | | | | | Intermediate Calculations | | | | |
| 26 | | | | | | | R($cm^3$MPa/molK) | | 8.314472 | | |
| 27 | Method 1 - For region with one real root | | | | | | $T_r$ | 0.638706 | a (MPa $cm^6$/$gmol^2$) | | |
| 28 | P | Q | Root to equation in x | | | | $P_r$ | 0.030076 | 2732618 | | |

2a

Instructions | PVT | Props | Ref State | Crit. Props | IG Cps | rev. info

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Preos_problem2_npentane - Excel

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P | fx 0.101325

Peng-Robinson Equation of State (Pure Fluid)

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| Properties | | | | Heat Capacity constants from Appendix | | | | ideal gas values | $H^{ig} - H_R^{ig}$ | $U^{ig} - U_R^{ig}$ | $S^{ig} - S_R^{ig}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Gas | $T_c$ (K) | $P_c$ (MPa) | $\omega$ | A | B | C | D | | J/mol | J/mol | J/molK |
| n-PENTANE | 469.7 | 3.369 | 0.249 | -3.626 | 4.87E-01 | -2.58E-04 | 5.31E-08 | | 0 | 0 | 0 |

| Current State | | Roots | | Stable Root has a lower fugacity | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| T (K) | 300 | Z | V | fugacity | H | U | S | $H-H^{ig}$ | $U-U^{ig}$ | $S-S^{ig}$ |
| P (MPa) | 0.101325 | | $cm^3$/gmol | MPa | J/mol | J/mol | J/molK | J/mol | J/mol | J/molK |
| answers for three root region | | 0.957725 | 23576.543 | 0.097202 | 26163.53 | 23774.64 | 84.66546 | -280.498 | -175.049 | -0.58962 |
| | | 0.0340218 | 837.52172 | | 19540.44 | 19455.57 | 51.09943 | -6903.6 | -4494.12 | -34.1557 |
| | | 0.00459 | 112.99208 | 0.07156 | 0 | -11.4489 | 0 | -26444 | -23961.1 | -85.2551 |
| & for 1 root region | | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! |

fugratio
1.358324

If thermodynamic property calculations give a #NUM! error for both root regions in the table above, fix the "reference state index indentifier" on "Ref State" page.

Solution to Cubic $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$

| $a_2$ | $a_1$ | $a_0$ | p | q |
|---|---|---|---|---|
| -0.9963367 | 0.03713556 | -0.00015 | -0.29376 | -0.06108 |

$R = q^2/4 + p^3/27 =$ -6.2E-06
If Negative, three unequal real roots,
If Positive, one real root

Intermediate Calculations

| | | | |
|---|---|---|---|
| R($cm^3$MPa/molK) | 8.314472 | | |
| $T_r$ | 0.638706 | a (MPa $cm^6$/$gmol^2$) | |
| $P_r$ | 0.030076 | 2732618 | |
| $\kappa$ | 0.741927 | b ($cm^3$/gmol) | |
| $\alpha$ | 1.320169 | 90.18035 | |
| | | A | 0.044502 |
| | | B | 0.003663 |

Method 1 - For region with one real root

| P | Q | Root to equation in x |
|---|---|---|
| #NUM! | #NUM! | #NUM! |

Method 2 - For region with three real roots

2b

H1

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Preos_problem2_npentane - Excel

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D8 | cm3/gmol

# Peng-Robinson Equation of State (Pure Fluid)

Spreadsheet protected, but no password used.

| Properties | | | | Heat Capacity constants from Appendix | | | | ideal gas values | $H^{ig} - H_R^{ig}$ | $U^{ig} - U_R^{ig}$ | $S^{ig} - S_R^{ig}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Gas | $T_c$ (K) | $P_c$ (MPa) | ω | A | B | C | D | | J/mol | J/mol | J/molK |
| n-PENTANE | 469.7 | 3.369 | 0.249 | -3.626 | 4.87E-01 | -2.58E-04 | 5.31E-08 | | 13742.99 | 12911.55 | 39.31115 |

| Current State | | Roots | | Stable Root has a lower fugacity | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| T (K) | 400 | Z | V | fugacity | H | U | S | $H-H^{ig}$ | $U-U^{ig}$ | $S-S^{ig}$ |
| P (MPa) | 0.101325 | | $cm^3$/gmol | MPa | J/mol | J/mol | J/molK | J/mol | J/mol | J/molK |
| answers for three root region | | 0.9813292 | 32210.152 | 0.099462 | 40006.91 | 36743.22 | 124.2702 | -180.115 | -118.02 | -0.29599 |
| | | 0.011391 | 373.88497 | | 28467.91 | 28430.03 | 76.7798 | -11719.1 | -8431.21 | -47.7864 |
| | | 0.0045324 | 148.76587 | 0.815373 | 19080.87 | 19065.8 | 54.46258 | -21106.2 | -17795.4 | -70.1037 |
| & for 1 root region | | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! | #NUM! |

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0.121983

If thermodynamic property calculations give a #NUM! error for both root regions in the table above, fix the "reference state index indentifier" on "Ref State" page.

Solution to Cubic $Z^3 + a_2Z^2 + a_1Z + a_0 = 0$

| $a_2$ | $a_1$ | $a_0$ | p | q |
|---|---|---|---|---|
| -0.99725252 | 0.01567765 | -5.07E-05 | -0.3158266 | -0.0683 |

$R = q^2/4 + p^3/27 =$ -3.9E-07

If Negative, three unequal real roots,

If Positive, one real root

| Intermediate Calculations | | | |
|---|---|---|---|
| R($cm^3$MPa/molK) | 8.314472 | | |
| $T_r$ | 0.851607 | a (MPa $cm^6$/$gmol^2$) | |
| $P_r$ | 0.030076 | 2313722 | |
| κ | 0.741927 | b ($cm^3$/gmol) | |
| α | 1.117794 | 90.18035 | |
| | | A | 0.021195 |
| | | B | 0.003747 |

Method 1 - For region with one real root

| P | Q | Root to equation in x |
|---|---|---|
| #NUM! | #NUM! | #NUM! |

Method 2 - For region with three real roots

2b

$H_2$

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Instructions PVT Props Ref State Crit. Props IG Cps rev. info

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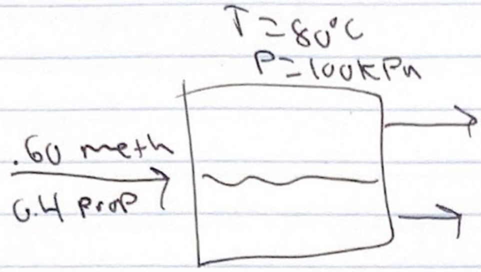
3a)




$$x_1 P_1^{sat} + (1-x_1) P_2^{sat} = P$$

$$x_1 \cdot 181 + (1-x_1) 50.8 = 100$$

$$181 x_1 + 50.8 - 50.8 x_1 = 100$$

$$(181 - 50.8) x_1 = 49.2$$

$$\boxed{x_1 = 0.377}$$

$$y_1 = \frac{x_1 \cdot P_1^{sat}}{P} = \frac{0.377 \cdot 181}{100} = \boxed{0.684}$$

$$\frac{V}{F} = \frac{z_1 - x_1}{y_1 - x_1} = \frac{0.6 - 0.377}{0.684 - 0.377} = 0.725$$

$$\dot{V} = 100 \frac{mol}{sec} \cdot 0.725 = \boxed{72.5 \frac{mol}{sec}}$$

b) $P_{max} = P_{bubble} = 1.2892 \text{ bar} = 128.92 = \boxed{129. \text{ kPa}}$

$P_{min} = P_{dew} = 0.8937 \text{ bar} = \boxed{89.4 \text{ kPa}}$

$$P_{bubble} = x_1 \cdot P_1^{sat} + x_2 \cdot P_2^{sat} = 0.6(1.81 \text{ bar}) + 0.4(0.508 \text{ bar})$$

$$P_{dew} = \frac{1}{\frac{y_1}{P_1^{sat}} + \frac{y_2}{P_2^{sat}}} = \frac{1}{\frac{0.6}{1.81 \text{ bar}} + \frac{0.4}{0.508 \text{ bar}}}$$

Module7_bubble_dew_point - Excel

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I22

# Given xi, T, calculate bubble point Pressure

| | A | B | C | Pi_sat (bar) | xi | Pi_sat*xi (bar) | yi |
|---|---|---|---|---|---|---|---|
| methanol | 8.08097 | 1582.271 | 239.726 | 1.81 | 0.6 | 1.086 | 0.8424 |
| 1-propanol | 8.37895 | 1788.02 | 227.438 | 0.508 | 0.4 | 0.2032 | 0.1576 |

| | | | |
|---|---|---|---|
| BP pressure | 1.2892 | bar | |
| T | 80 | C | |
| | | K | |

$$y_i P = x_i P_i^{sat} \text{ or } K_i = \frac{y_i}{x_i} = \frac{P_i^{sat}}{P}$$

$$P = \sum x_i P_i^{sat} \text{ and } y_i = \frac{x_i P_i^{sat}}{P} = x_i K_i$$

$$\boxed{y_i P = x_i P_i^{sat} \text{ or } K_i = \frac{y_i}{x_i} = \frac{P_i^{sat}}{P} \quad P = \sum x_i P_i^{sat} \text{ and } y_i = \frac{x_i P_i^{sat}}{P} = x_i K_i}$$

3b

# Given xi, P, calculate bubble point temperature

| | A | B | C | Pi_sat (bar) | xi | Pi_sat*xi (bar) | yi |
|---|---|---|---|---|---|---|---|
| methanol | 8.08097 | 1582.271 | 239.726 | 1.81 | 0.6 | 1.086 | 0.8424 |
| 1-propanol | 8.37895 | 1788.02 | 227.438 | 0.508 | 0.4 | 0.2032 | 0.1576 |

| | | | |
|---|---|---|---|
| BP pressure | 1.2892 | bar | |
| T | 80 | c | |
| | 353.15 | | |

$P_1^{sat}(T)$

Iterate T until
P=$\sum x_i P_i^{sat}(T)$

# Given yi, T, calculate dew point pressure

| | A | B | C | Pi_sat (bar) | yi | yi/Pi_sat | xi |
|---|---|---|---|---|---|---|---|
| methanol | 8.08097 | 1582.271 | 239.726 | 1.81 | 0.6 | 0.331491713 | 0.2963 |
| 1-propanol | 8.37895 | 1788.02 | 227.438 | 0.508 | 0.4 | 0.787401575 | 0.7037 |

| | | |
|---|---|---|
| DP pressure | 0.89374028 | bar |
| T | 80 | c |

$$1 = \frac{y_1 P}{P_1^{sat}} + \frac{y_2 P}{P^{sat}}$$

$$K_i = \frac{y_i}{x_i} = \frac{P_i^{sat}(T)}{P}$$

$$P = \frac{}{\frac{y_1}{P_1^{s}}}$$

# Given yi, P, calculate dew point temperature

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Sheet1

Ready

60%