CHEE 210 Quiz #1

Date: Monday February 2, 2009

Please attempt all questions and be sure to include the units for each of your calculations. You have 1.5hrs. Also, have fun!

Question 1: [10 marks]

A coal power plant produces 500MW of power (equivalent to $4.32x10^7$ MJ/day of energy). If coal has a heating value of 27MJ/kg and contains 1.83kg CO_2/kg coal, and the coal power plant is 30% efficient:

a. How much CO_2 is released by the coal power plant per day? [5 marks]

b. How much CO_2 is released per MJ of energy produced by the coal power plant? [5 marks]

Question 2: [30 marks]

Note: For this question it is easiest if you keep your volumes in cm^3 and your pressures in bar, although not required.

A. With the help of the attached PV diagram for CO_2 (Figure 1), *calculate* using the van der Waals equation of state given in Table 1, the molar volume of the saturated liquid and the molar volume of the saturated vapor at 15^0C. The saturation pressure at 15^0C is 59bar and the critical point information for CO_2 is available in Table 2. [10 marks]

   (Only 1 guess is required for each volume but make sure you note down how you made your guess)

   Using the generalized density correlation for liquids (Figure 2), find the molar volume of the saturated liquid. Which value for the volume of the saturated liquid should be trusted? [5 marks]

B. In excel you find from the PV isotherm at 15^0C that Vr=24.25 at Pr=0.135. In addition, you have previously calculated the compressibility factor, Z=0.974 at Pr= 0.068. Using this information, calculate:

   a. The unknown compressibility factor at 15^0C and Pr=0.135 [10 marks]

   b. The second virial coefficient with respect to pressure, B' [5 marks]

Question 3: [30 marks]

Hydrogen gas for use in the Honda Clarity fuel cell car is produced at atmospheric pressure (1 atm or 1.01×10^5 Pa) and some unknown temperature but must be compressed to 350 atm (3.55×10^7 Pa) and 0^0C. It is known that the internal energy change is -1023 J/mol for the entire procedure. Multiple pathways are available for this procedure:

> **Pathway #1:** Isothermal compression to 350atm followed by isobaric cooling or heating to 0^0C
>
> **Pathway #2:** Adiabatic compression to 350atm and some unknown temperature followed by isobaric cooling or heating to 0^0C

The heat capacity at constant pressure (Cp) for hydrogen is 28.8 J/mol/K and is essentially constant over a wide range of temperatures.

A. For each of these two pathways, assume reversible, ideal gas behavior and:

   i. Calculate the initial temperature for the procedure [5 marks]

   ii. Calculate the heat and work required for each process *and* each pathway. Which pathway requires the least amount of work? [10 marks]

   iii. Sketch each pathway in a PV *and* PT diagram [10 marks]

B. You now realize that hydrogen likely does not behave like an ideal gas at these high pressures. Using information provided in Table 1 and Table 2, what is the most appropriate equation of state to use for hydrogen and why? Quantify your answer. [5 marks]

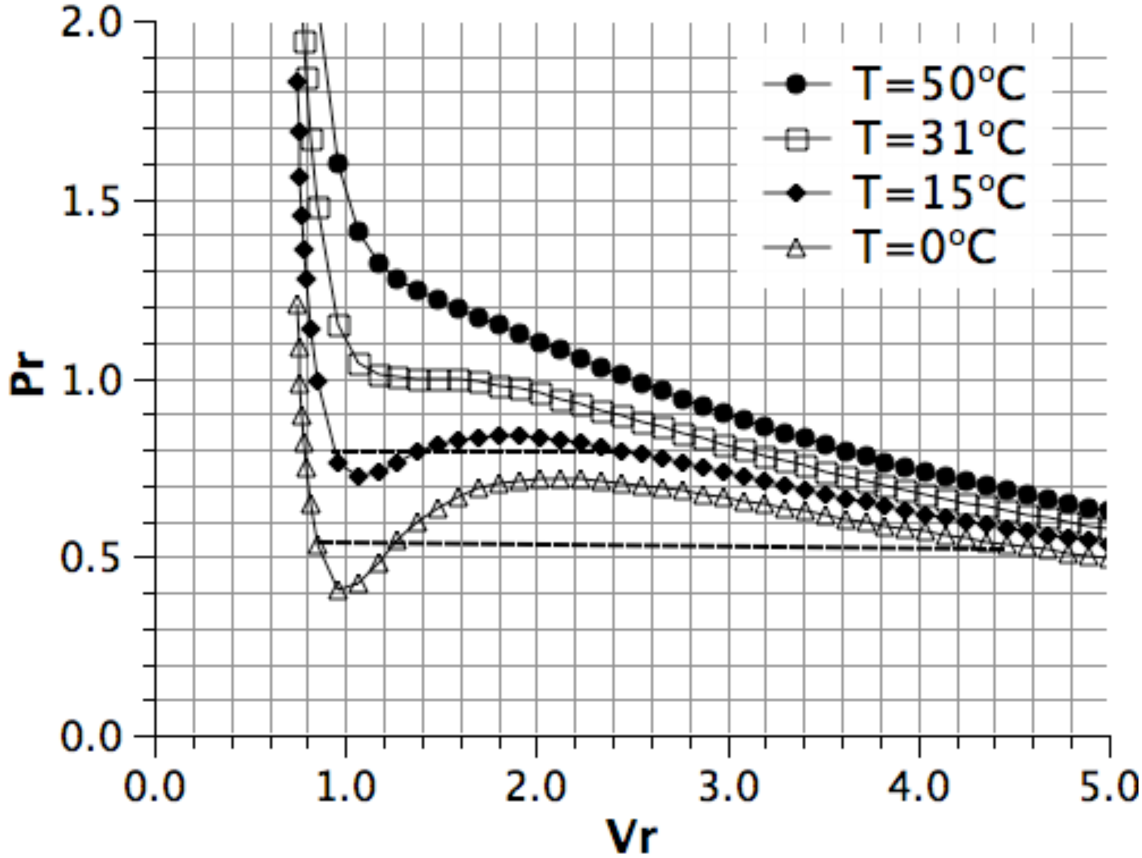


Figure 1. PV diagram for CO_2

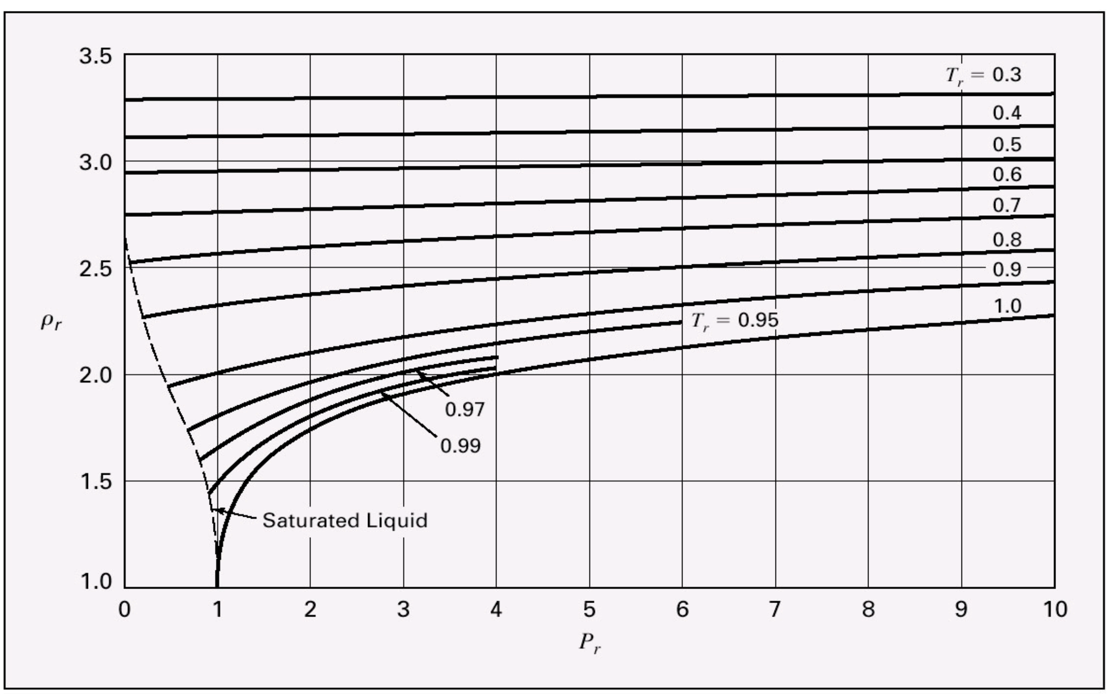


Figure 2. Generalized density correlation for liquids (Fig 3.16 in SVNA, 7th Ed)

Table 1. Parameter assignments for equations of state (Table 3.1 in SVNA, 7th Ed)

Eq. of State	$\alpha(T_r)$	σ	ϵ	Ω	Ψ	Z_c
vdW (1873)	1	0	0	1/8	27/64	3/8
RK (1949)	$T_r^{-1/2}$	1	0	0.08664	0.42748	1/3
SRK (1972)	$\alpha_{SRK}(T_r;\omega)^\dagger$	1	0	0.08664	0.42748	1/3
PR (1976)	$\alpha_{PR}(T_r;\omega)^\ddagger$	$1+\sqrt{2}$	$1-\sqrt{2}$	0.07780	0.45724	0.30740

$^\dagger\alpha_{SRK}(T_r;\ \omega) = \left[1 + (0.480 + 1.574\,\omega - 0.176\,\omega^2)\left(1 - T_r^{1/2}\right)\right]^2$

$^\ddagger\alpha_{PR}(T_r;\ \omega) = \left[1 + (0.37464 + 1.54226\,\omega - 0.26992\,\omega^2)\left(1 - T_r^{1/2}\right)\right]^2$

$$P = \frac{RT}{V-b} - \frac{a(T)}{(V-\epsilon b)(V+\sigma b)}$$

$$b = \Omega\frac{RT_C}{P_C}$$

$$a(T) = \Psi\frac{\alpha(T_r)R^2T_c^2}{P_c}$$

Table 2. Characteristic properties of pure species

	Molar mass	ω	Tc (K)	Pc (bar)	Zc	Vc ($cm^3\ mol^{-1}$)	Tn (K)
Carbon dioxide (CO_2)	44.010	0.224	304.2	73.83	0.274	93.4	
Hydrogen (H_2)	2.016	-0.216	33.19	13.13	0.305	64.1	20.4

Some helpful constants/conversions:

R = 83.14 cm^3 bar mol^{-1} K^{-1}
R = 82.06 cm^3 atm mol^{-1} K^{-1}
R = 8.314 J mol^{-1} K^{-1}

1 atm = 101325 Pa

Question 1

a) $\frac{4.32\times10^7 \text{ MJ}}{\text{day}} \times \frac{\text{Kg coal}}{27 \text{ MJ}} \times \frac{1.83 \text{ Kg } CO_2}{\text{Kg coal}} = 2.928\times10^6 \frac{\text{Kg } CO_2}{\text{day}}$

But this would be at 100% efficiency.

So actual usage $= \frac{2.928\times10^6}{0.3} = 9.76\times10^6 \frac{\text{Kg } CO_2}{\text{day}}$

b) $9.76\times10^6 \frac{\text{Kg } CO_2}{\text{day}} \times \frac{\text{day}}{4.32\times10^7 \text{ MJ}} = 0.23 \frac{\text{Kg } CO_2}{\text{MJ}}$ ~~energy~~

Question 2

A) $P = \frac{RT}{V-b} - \frac{a}{V^2}$

$T_c = 304.2\text{K}$ $P_c = 73.83 \text{ bar}$ $V_c = 93.4 \text{ cm}^3/\text{mol}$

$b = \Omega \frac{RT_c}{P_c} = \frac{1}{8} \times \frac{83.14\times304.2}{73.83} = 42.82 \text{ cm}^3/\text{mol}$

$a(T) = \Psi\alpha(T_r) \times \frac{R^2 \times T_c^2}{P_c} = \frac{27}{64} \times \frac{83.14^2 \times 304.2^2}{73.83} = 3655016.8 \text{ cm}^6\text{bar}/\text{mol}^2$

Values for V_{guess}:

From graph: $V_{liq}^{sat} \simeq 0.95\times V_c = 88.73 \text{ cm}^3/\text{mol}$

From graph: $V_{gas}^{sat} \simeq 2.5\times V_c = 233.5 \text{ cm}^3/\text{mol}$

} these values used as guess values

For V_{liq}^{sat}

V_{guess}	P	
88.73 cm³/mol	57 bar	iteration #1 (close enough to 59 bar)

For V_{vap}^{sat}

V_{guess}	P	
233.5 cm³/mol	58.5 bar	iteration #1 (close enough to 59 bar)

∴ from vDW EOS: $V_{liq}^{sat} = 88.73\ cm^3/mol$

$V_{vap}^{sat} = 233.5\ cm^3/mol$

Using generalized density correlation:

$$T_r = \frac{15+273}{304.2} = 0.95$$

From graph $\rho_r = 1.75$

$$\rho_r = \frac{V_c}{V} \qquad V = \frac{V_c}{\rho_r} = 53.37\ cm^3/mol$$

Trust the generalized correlations because they are experimental data.

B) a) $$Z = \frac{V_{real}}{V_{ideal}}$$

$V_{real} = 24.25 \times 93.4 = 2264.95\ cm^3/mol$

$V_{real} = \frac{RT}{P} = \frac{83.14 \times (15+273)}{0.135 \times 73.83} = 2402\ cm^3/mol$

$$Z = \frac{2264}{2402} = 0.943$$

b) $$\frac{dZ}{dP} = B' \quad \therefore \quad \frac{Z_2 - Z_1}{P_2 - P_1} = B' = \frac{0.943 - 0.974}{0.135 \times 73.83 - 0.068 \times 73.83} = -0.0063\ bar^{-1}$$

Question 3

$P_1 = 1 atm$ $P_2 = 350 atm$

$T_1 = ?$ $T_2 = 273 K$

$\Delta U = -1023 J/mol$

A) i) $\Delta U = C_v(T_2 - T_1)$ $C_v = C_p - R$

$\Delta U = -1023 = (28.8 - 8.314)(273 - T_1)$

$T_1 = 322.9 K = 50°C$

ii) Pathway # 1

isothermal compression to 350 atm

$Q = -RT \ln\left(\frac{P_2}{P_1}\right) = -8.314 \times 322.9 \times \ln\left(\frac{350}{1}\right) = -15727.9 J/mol$

$W = -Q = 15727.9 J/mol$

isobaric cooling to 273 K

$Q = C_p(T_2 - T_1) = 28.8(273 - 322.9) = -1438 J/mol$

$W = -R(T_2 - T_1) = -8.314(273 - 322.9) = 415 J/mol$

for pathway

$Q_{pathway} = -15727.9 - 1438 = -17166 J/mol$

$W_{pathway} = 15727.9 + 415 = 16143 J/mol$

Pathway #2

Adiabatic compression to 350 atm and T = ?

$$\frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{\frac{R}{C_P}} \qquad T_2 = 322.9 \times \left(\frac{350}{1}\right)^{\frac{8.314}{28.8}} = 1752\,K$$

$Q = 0$

$$W = C_V \Delta T = (28.8 - 8.314)(1752 - 322.9) = 29277\ J/mol$$

Isobaric cooling

$$Q = C_P(T_2 - T_1) = 28.8(273 - 1752) = -42589.4\ J/mol$$

$$W = -R(T_2 - T_1) = -8.314(273 - 1752) = 12294.7\ J/mol$$

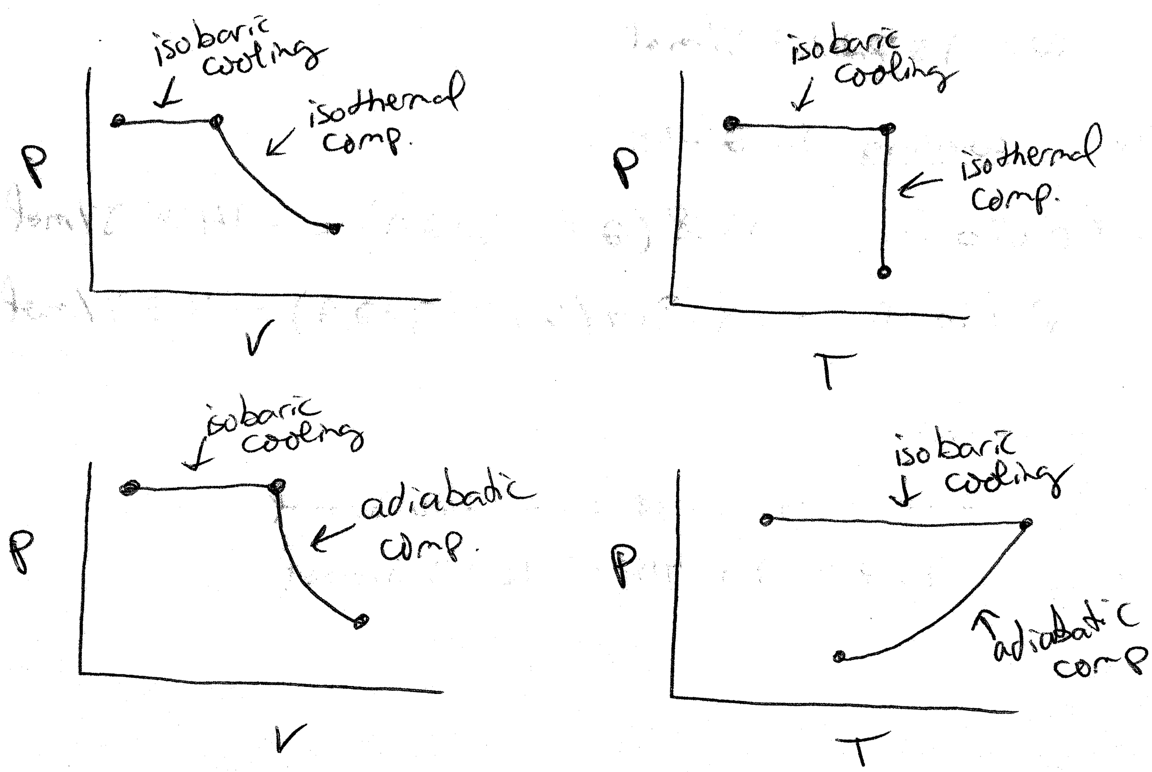
for pathway

$$Q_{pathway} = 0 - 42589.4 = -42589.4\ J/mol$$

$$W_{pathway} = 29277 + 12294.7 = 41573\ J/mol$$

∴ Pathway #1 requires less work

iii)



B. Best equation is Peng-Robinson because

Z_c (H_2) = 0.305

Z_c predicted by PR = 0.307

because PR accounts for molecular structure through ω