South Dakota School of Mines and Technology
Department of Materials Metallurgical Engineering

MET 320 HQ 3 Dec. 1, 2005

SEE DATA SHEET AT END OF EXAM - NO CALCULATORS – CLOSED BOOK AND NOTES
If a problem seems to be in error, state the trouble, state an assumed correction, and proceed.

1. Write the Big 6 Equations.

$$\mu_i = \mu_i^o + RT \ln p_i$$
$$\mu_i = \mu_i^o + RT \ln(p_i \gamma_i) - - or \ln(f_i)$$
$$\mu_i = \mu_i^o + RT \ln x_i$$
$$\mu_i = \mu_i^o + RT \ln(x_i \gamma_i) - - or \ln(a_i)$$
$$\mu_i = \mu_i^o + RT \ln \left[i\right]_i$$
$$\mu_i = \mu_i^o + RT \ln(\left[i\right]_i \gamma_i) - - or \ln(a_i)$$

2. Short answer:
   a) What is the difference between ΔG and ΔGº?
   The super script "o" means "when every reactant and product is in its standard state"

   b) What is the relative partial molar heat of mixing for an Ideal solution?
   Zero

   c) What is the name of the ThermoCalc program module that lists values of ΔS°, ΔH°, and ΔG° for an entered reaction at user-defined temperature intervals?
   TAB

3. Estimate the volume of 100 moles of NH_3 at 445 K (1.1*Tcritical) and 223 atm (2*Pcritical)? See Figure 8.4 Law of Corresponding States: z = 0.4

$$V = \frac{znRT}{P} = \frac{0.4 * 100 * 0.08205 * 445}{223} Liters$$ **Actual Solution:** 6.41 ℒ

4. Estimate the temperature required to raise the vapor pressure of water to 100 mmHg if it is known that the vapor pressure of water vapor above water at 22 °C is 20 mmHg.

Clasius-Clapeyron Eq.

$$\ln\left[\frac{p_2}{p_1}\right] = -\frac{\Delta H^o_{Vap}}{R}\left[\frac{1}{T_2} - \frac{1}{T_1}\right]$$
$$\ln\left[\frac{100}{20}\right] = -\frac{4320}{8.31}\left[\frac{1}{(273+T_2)} - \frac{1}{(273+22)}\right]$$

T_2 is in °C **Actual Solution:** 51.6 °C

5. Cu in a liquid Ag-Cu solution having a composition of $x_{Cu} = 0.1$ at a temperature of 1423 K reacts with half a mole of O_2 at 12 atm to form pure, solid Cu_2O. Show how to calculate the Gibbs energy change for this process.

Data: $2Cu_{(l)} + 0.5\ O_{2(g)} = Cu_2O_{(s)}$ $\Delta G^\circ = -195{,}000 - 7.12T\ln T + 143T$ J/gmole

$\Delta G = \Delta G^\circ + RT\ln(Q)$

$Q = \frac{a_{Cu_2O}}{a_{Cu}^2 p_{O_2}^{0.5}} = \frac{1}{0.26_{Cu}^2 12_{O_2}^{0.5}}$ **Actual Solution:** $\Delta G = \Delta G^\circ + RT \ln Q$

T, K	ΔG°, J/gfw	Q	ΔG, J/gfw
1423	-65,073	4.27	-47,906

6. Initially there are 5 moles of SO_2, 3 moles of O_2, and 1 mole of SO_3 in a reactor kept at a constant pressure or 2 atm and constant temperature. Setup the calculation to determine the equilibrium number of moles of each gas. All the species are gaseous.

1. $2SO_2 + O_2 = 2SO_3$ $K_{EQ} = 1.8$

2. Let x = moles of O_2 reacted

3. Mole balance to Equilibrium

i	Moles		
i	N_{init}	N_{Final}	p_i
SO_2	5	5-2x	$\frac{5-2x}{9-x}2$
O_2	3	3-x	$\frac{3-x}{9-x}2$
SO_3	1	1+2x	$\frac{1+2x}{9-x}2$
Total	9	9-x	2

4. $$K_{EQ} = \frac{\left[\frac{1+2x}{9-x}2\right]^2}{\left[\frac{5-2x}{9-x}2\right]^2\left[\frac{3-x}{9-x}2\right]} = \frac{[1+2x]^2}{[5-2x]^2\left[\frac{3-x}{9-x}2\right]}$$

5. Solve for x. Note $-0.5 \le x \le 2.5$. Otherwise a mole value becomes negative.

Actual Solution: by Microsoft Excel Goal Seek®

	x	Q
	0.965	1.800
i	**Final**	**p_i**
SO_2	**3.069**	**0.764**
O_2	**2.035**	**0.506**
SO_3	**2.931**	**0.730**
Total	**8.035**	**2.000**

DATA:

$H_2O_{(s)} = H_2O_{(l)}$	$\Delta H^\circ = 6{,}028$ J/gmole
$H_2O_{(l)} = H_2O_{(g)}$	$\Delta H^\circ = 43{,}267$ J/gmole
$2\,Cu(l) + 0.5\,O_2(g) = Cu_2O(s)$	$\Delta G^\circ = -195{,}000 - 7.12T\ln T + 143T$ J/gmole
$Cu_2O(s) = Cu_2O(l)$	$\Delta G^\circ = 13{,}580 - 9.0\,T$ J/gmole

Activity data for liquid
<u>Ag-Cu Alloys at 1423 K</u>

X_{Cu}	a_{Cu}
0.0	0.000
0.1	0.260
0.2	0.422
0.3	0.535
0.4	0.616
0.5	0.679
0.6	0.731
0.7	0.782
0.8	0.841
0.9	0.912
1.0	1.000

Table 8.1 The critical states, van der Waals constants, and values of Z at the critical points for several gases

Gas	T_{cr}, K	P_{cr}, atm	V_{cr}, cm³/mole	a, $\frac{l^2\cdot atm}{mole^2}$	b, liters/mole	Z_{cr}
He	5.3	2.26	57.6	0.0341	0.0237	0.299
H_2	33.3	12.8	65.0	0.2461	0.0267	0.304
N_2	126.1	33.5	90.0	1.39	0.0391	0.292
CO	134.0	35.0	90.0	1.49	0.0399	0.295
O_2	153.4	49.7	74.4	1.36	0.0318	0.293
CO_2	304.2	73.0	95.7	3.59	0.0427	0.280
NH_3	405.6	111.5	72.4	4.17	0.0371	0.243
H_2O	647.2	217.7	45.0	5.46	0.0305	0.184

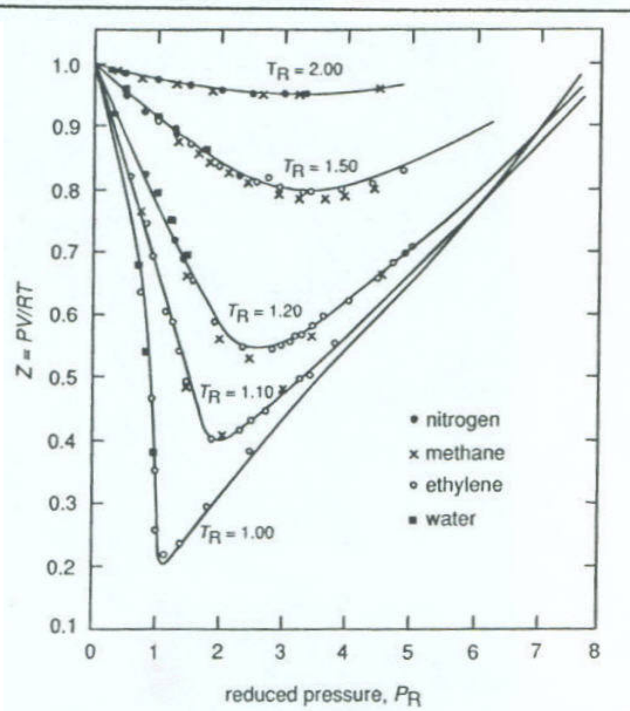

Figure 8.4 The variations of the compressibility factors of several gases with reduced pressure at several reduced temperatures