Quiz 8
Chemical Engineering Thermodynamics
March 10, 2016

8.14. A 1 m^3 isolated chamber with rigid walls is divided into two compartments of equal volume. The partition permits transfer of heat. One side contains a nonideal gas at 5 MPa and 300 K and the other side contains a perfect vacuum. The partition is ruptured, and after sufficient time for the system to reach equilibrium, the temperature and pressure are uniform throughout the system. The objective of the problem statements below is to find the final *T* and *P*.

The gas follows the equation of state

$$\frac{PV}{RT} = 1 + \left(b - \frac{a}{T}\right)\frac{P}{RT}$$

where $b = 20$ cm³/mole; $a = 40{,}000$ cm³K/mole; and $C_P = 41.84 + 0.084T$(K) J/mol-K.

a. Set up and simplify the energy balance and entropy balance for this problem.

b. Derive formulas for the departure functions required to solve the problem.

c. Determine the final *P* and *T*.

For part "c" calculate the needed equation(s) and parameter(s).

d. Give a series of steps necessary to solve for T_f and P_f using Solver® in Excel®.

e. What are the values for T_f and P_f if the gas were an ideal gas? (These should be your starting values for Solver® in part "d".)

R = 8.314 J/mole-K = 8.314 cm³ MPa/mole-K

$$\frac{(U - U^{ig})}{RT} = \int_0^{\rho} -T\left[\frac{\partial Z}{\partial T}\right]_{\rho}\frac{d\rho}{\rho} \qquad 8.22$$

$$\frac{(S - S^{ig})}{R} = \int_0^{\rho}\left[-T\left[\frac{\partial Z}{\partial T}\right] - (Z-1)\right]\frac{d\rho}{\rho} + \ln Z \qquad 8.23$$

$$\frac{(H - H^{ig})}{RT} = \int_0^{\rho} -T\left[\frac{\partial Z}{\partial T}\right]_{\rho}\frac{d\rho}{\rho} + Z - 1 \qquad 8.24$$

$$\frac{(A - A^{ig})}{RT} = \int_0^{\rho}\frac{(Z-1)}{\rho}d\rho - \ln Z \qquad 8.25$$

$$\frac{(G - G^{ig})}{RT} = \int_0^{\rho}\frac{(Z-1)}{\rho}d\rho + (Z-1) - \ln Z \qquad 8.26$$

$$\left(\frac{H - H^{ig}}{RT}\right) = -\int_0^{P} T\left(\frac{\partial Z}{\partial T}\right)_P\frac{dP}{P} \qquad 8.29$$

$$\left(\frac{S - S^{ig}}{R}\right) = -\int_0^{P}\left[(Z-1) + T\left(\frac{\partial Z}{\partial T}\right)_P\right]\frac{dP}{P} \qquad 8.30$$

$$H = U + PV \Rightarrow \frac{H - H^{ig}}{RT} = \frac{U - U^{ig}}{RT} + \frac{PV - RT}{RT} = \frac{U - U^{ig}}{RT} + Z - 1 \qquad 8.20$$

$$A = U - TS \Rightarrow \frac{A - A^{ig}}{RT} = \frac{U - U^{ig}}{RT} - \frac{S - S^{ig}}{R}$$

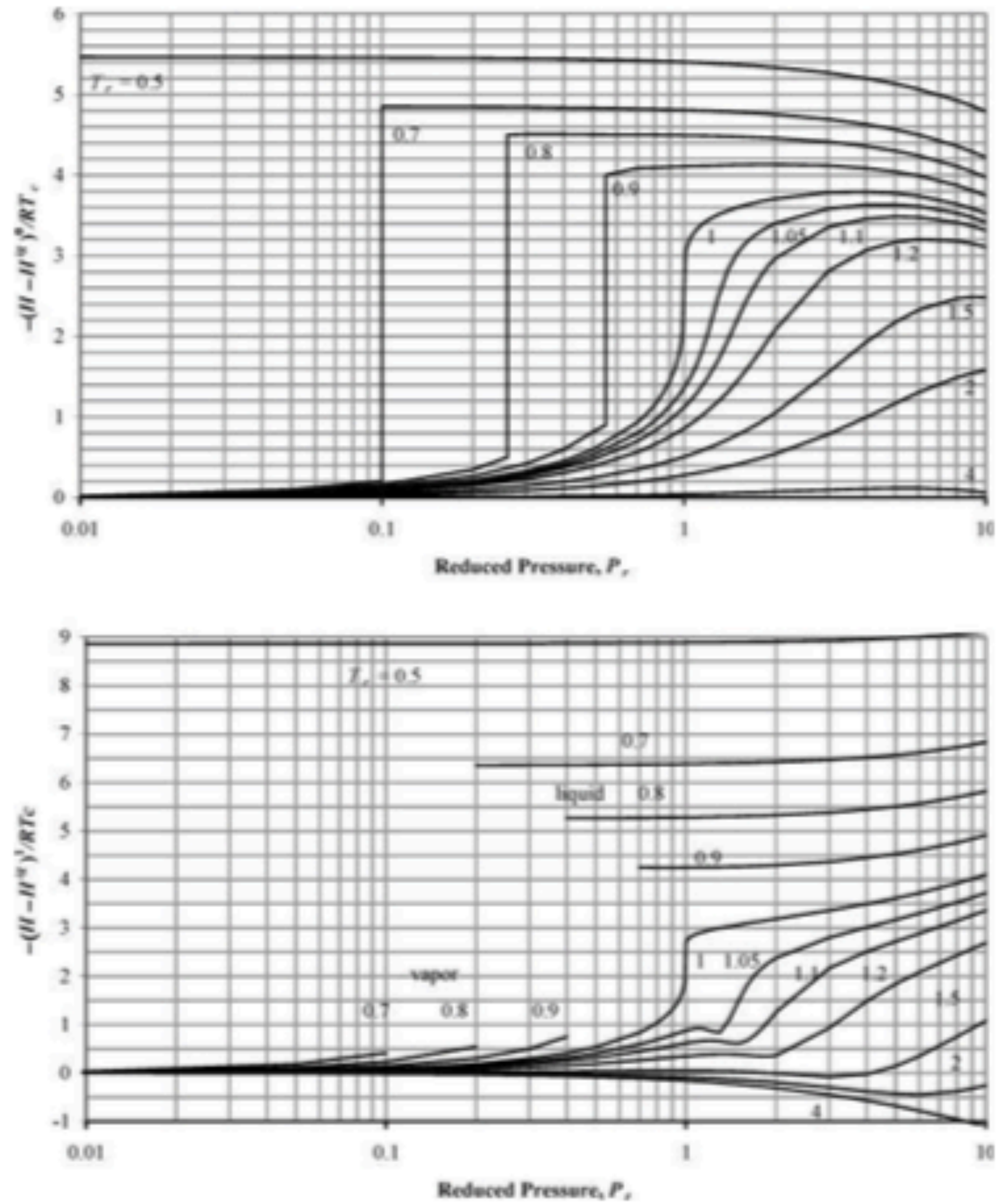

Figure 8.7. Generalized charts for estimating $(H - H^{ig})/RT_c$ using the Lee-Kesler equation of state. $(H - H^{ig})^0/RT_c$ uses $\omega = 0.0$, and $(H - H^{ig})^1/RT_c$ is the correction factor for a hypothetical compound with $\omega = 1.0$. Divide by reduced temperature to obtain the enthalpy departure function.

ANSWERS: **Quiz 8**
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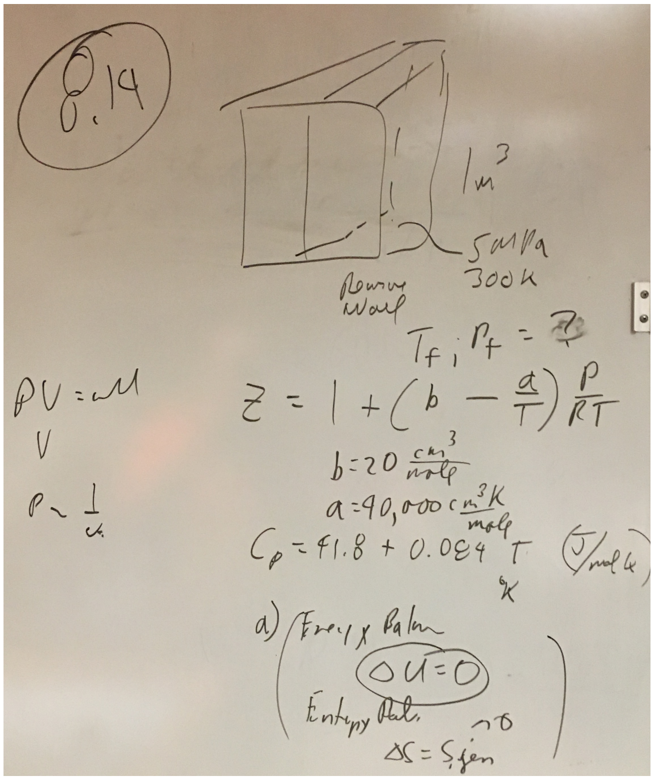

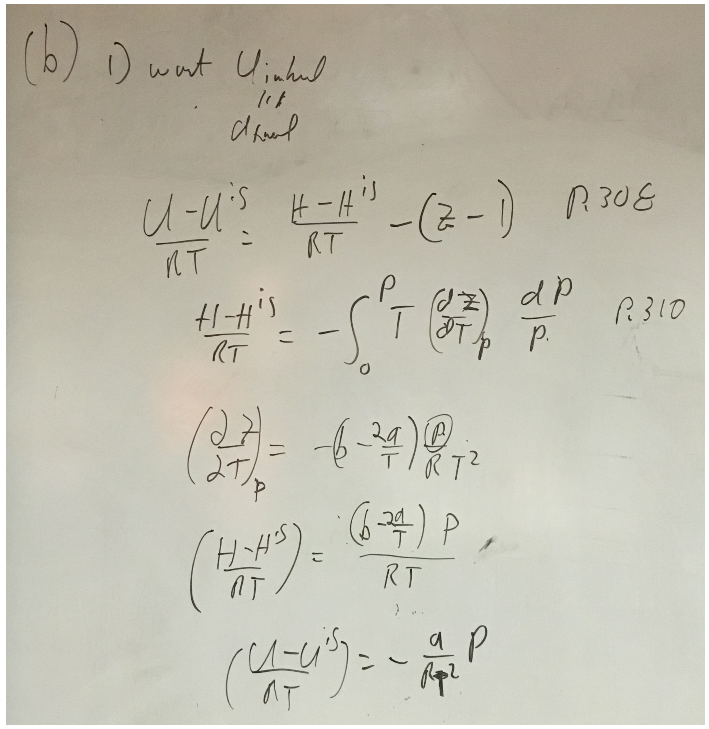

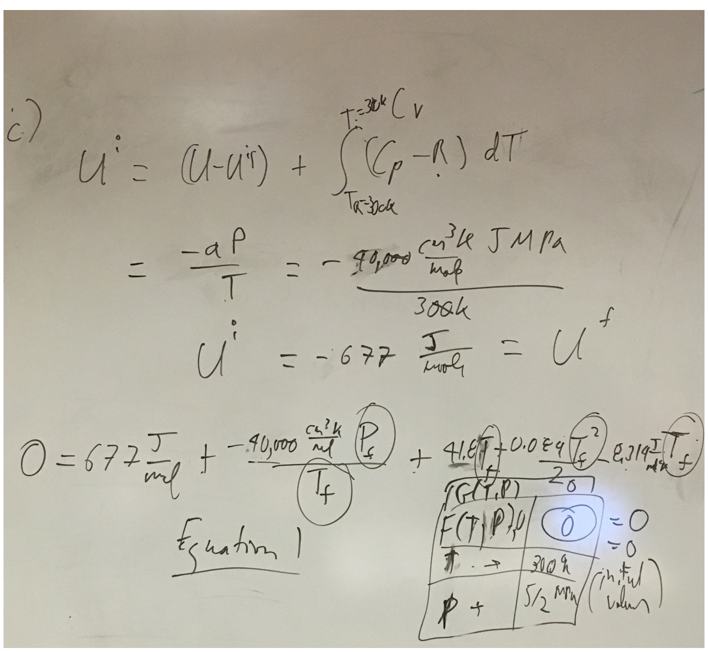

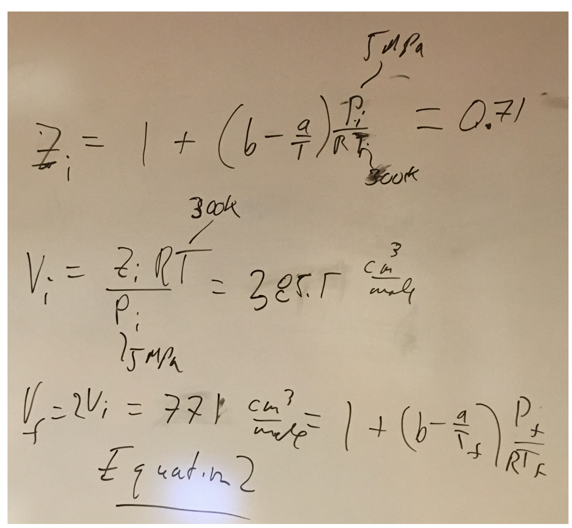

Initial guess for ideal gas would be T_f = 300K and P_f = 5MPa/2.

3.14) An 1-m^3 isolated chamber with rigid walls is divided into two…

a) Energy balance

$\Delta U = 0$

Entropy balance

$\Delta \underline{S} = \Delta \underline{S}_{gen}$

b) Need departure function for U. First get departure for H and use H = U + PV

$$\frac{H-H^{ig}}{RT} - Z + 1 = \frac{U-U^{ig}}{RT}$$

$$Z = 1 + \frac{bP}{RT} - \frac{aP}{RT^2}$$

$$-T\left(\frac{\partial Z}{\partial T}\right)_P = \frac{bT}{RT^2} - \frac{2aPT}{RT^3}$$

$$\frac{H-H^{ig}}{RT} = \int_0^P \left(\frac{bP}{RT} - \frac{2aP}{RT^2}\right)\frac{dP}{P} = \frac{bP}{RT} - \frac{2aP}{RT^2}$$

$$1 - Z = -\left(b - \frac{a}{T}\right)\frac{P}{RT}$$

$$U - U^{ig} = \frac{RT}{RT}\left[\left(bP - \frac{2aP}{T}\right) - bP + \frac{aP}{T}\right]$$

$$U - U^{ig} = -\frac{aP}{T}$$

c) Set $U^{ig}_R = 0$, set $T_R = 300$ K and $P_R = 2$ MPa

$U^i = \left(U - U^{ig}\right)^i + \int_{T_R}^{T^i} (C_P - R)\,dT$ = -40000(5)/300 = -667 J/mol

$U^f = \left(U - U^{ig}\right)^f + \int_{T_R}^{T^f} (C_P - R)\,dT = U^i$ = -40000(P)/(T) + 33.53 (T -300) + 0.042 (T^2 - 300^2) = -667 J/mol

Z^i = 0.773, $V^i = ZRT/P$ = 0.773(8.314)(300)/5 = 385.5cm^3/mol

$V^f = \frac{RT}{P} + \left(b - \frac{a}{T}\right) = 2V^i$ = 771 cm^3/mol

Programming in Excel and solving,

Solve two equations and two unknowns.

obj 1= -40000(P)/(T) + 33.53 (T -300) + 0.042 (T^2 - 300^2) +667

obj 2 = 8.314T/P + b-a/T -771

Solver gives T = 295 K, P = 2.76 MPa

	final	initial
P	2.766503	5
T	295.0177	300
V	771.0133	385.5067
Z	0.869631	0.772806
U		-666.6667

obj 1	-2.36E-09
obj 2	-2.25E-07