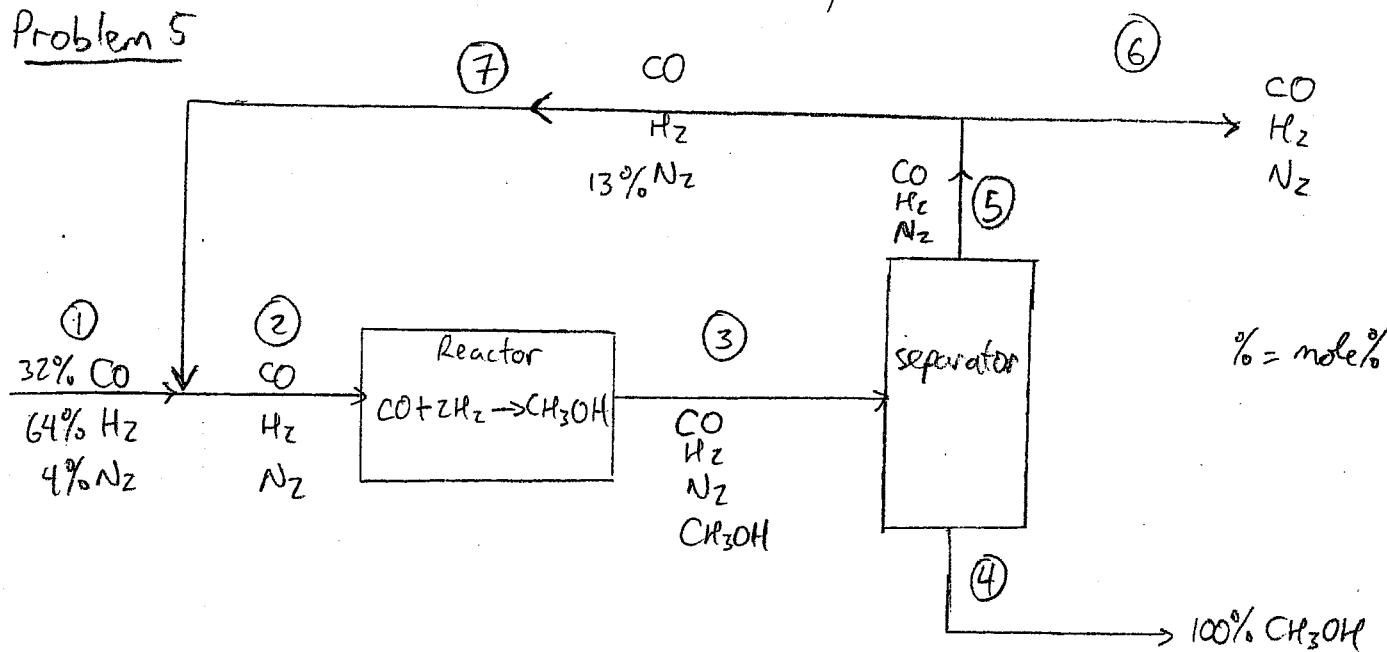


10.213

Spring 2002

Problem Set B

Solution

Problem 5

First, we draw the diagram and label the streams and all known information

Nomenclature:  $F_i$  = flow rate of stream  $i$  (mol/hr)

$x_{a,i}$  = mole % of species  $a$  in stream  $i$ , e.g.  $x_{N_2,7}=0.13$

$F_{a,i}$  = flow rate of species  $a$  in stream  $i$  =  $F_i \cdot x_{a,i}$

We are given that:  $\frac{F_7}{F_1} = \frac{\text{mole recycle}}{\text{mole fresh feed}} = \frac{5}{1}$

Since we are not given a basis, let us choose one: let  $F_1 = 1 \text{ mol/hr}$

a) We want to find out production rate of CH<sub>3</sub>OH (= F<sub>4</sub>).

Performing atomic / element balance over the whole system:

=<sub>0</sub> for atom bal.

$$\begin{array}{lcl} \text{Atom} & \text{In (stream 1)} + \text{Gen} & = \text{Out (streams 4 and 6)} + \text{Acc}^{\text{steady state}} \\ \text{H:} & (2)(0.64)(1 \text{ mol/hr}) & = (4)(F_4) + (2)(F_{H_2,6}) \quad (\text{i}) \\ \text{C:} & (1)(0.32)(1 \text{ mol/hr}) & = (1)(F_4) + (1)(F_{CO,6}) \quad (\text{ii}) \\ \text{N:} & (2)(0.04)(1 \text{ mol/hr}) & = \quad (2)(F_{N_2,6}) \quad (\text{iii}) \\ \text{O:} & (1)(0.32)(1 \text{ mol/hr}) & = (1)(F_4) + (1)(F_{CO,6}) \quad (\text{iv}) \end{array}$$

(1)

We have 4 equations and 4 unknowns:  $F_4$ ;  $F_{CO,6}$ ;  $F_{H_2,6}$ ;  $F_{N_2,6}$   
 But eq (ii) is the same as eq (iv)! This is because C and O  
 always stay together in our process  $\Rightarrow$  when there is C, there is O.  
 (We would still lack one equation if we do a species balance instead).  
 We do have one more piece of information:

$$X_{N_2,6} = 0.13 \quad (v)$$

Why? Because the compositions of streams 5, 6, and 7 must be the same  
 we are told  $X_{N_2,7} = 13\% \Rightarrow X_{N_2,6} = 13\%$  too. This means:

$$X_{N_2,6} = \frac{F_{N_2,6}}{F_G} = \frac{F_{N_2,6}}{F_{CO,6} + F_{H_2,6} + F_{N_2,6}} = 0.13$$

$$\Rightarrow F_{N_2,6} = 0.13 (F_{CO,6} + F_{H_2,6} + F_{N_2,6}) \quad (vi)$$

So we have 4 unknowns in 4 equations. Rearranging the terms:

$$\begin{aligned} (i): \quad 4F_4 + 2F_{H_2,6} &= 1.28 \text{ mol/hr} \\ (ii): \quad F_4 + F_{CO,6} &= 0.32 \text{ mol/hr} \\ (iii): \quad 2F_{N_2,6} &= 0.08 \text{ mol/hr} \\ (vi): \quad 0.13F_{H_2,6} + 0.13F_{CO,6} - 0.87F_{N_2,6} &= 0 \end{aligned} \quad \left. \begin{array}{l} 4 \text{ unknowns} \\ 4 \text{ independent} \\ \text{eqns} \end{array} \right\}$$

Solving the 4 equations (by hand or your favorite program):

$$F_{H_2,6} = 0.178 \text{ mol/hr} \quad F_{N_2,6} = 0.040 \text{ mol/hr}$$

$$F_{CO,6} = 0.089 \text{ mol/hr} \quad F_4 = 0.231 \text{ mol/hr}$$

$$\text{So production rate of } CH_3OH = F_4 = \boxed{0.231 \text{ mol/hr}} \quad (\text{ans})$$

(for basis of 1 mol/hr feed)

Note: There are many ways to solve this problem. All of them, however, will require using the information that  $X_{N_2,7} = 13\%$

b) We have solved for the composition of the purge gas in the previous problem:

$$\begin{array}{l} F_{He,6} = 0.178 \text{ mol/hr} \\ F_{CO,6} = 0.089 \text{ mol/hr} \\ F_{N_2,6} = 0.040 \text{ mol/hr} \end{array} \quad ] - F_6 = \boxed{0.307 \text{ mol/hr}}$$

$X_{He,6} = 58\%$
$X_{CO,6} = 29\%$
$X_{N_2,6} = 13\%$

c) Overall conversion =  $\frac{\text{mole reacted over entire process}}{\text{mole fed into entire process}} = \frac{\text{mole in} - \text{mole out}}{\text{mole in}}$

$$= \frac{F_{CO,1} - F_{CO,6}}{F_{CO,1}} = \frac{0.32 \text{ mol/hr} - 0.089 \text{ mol/hr}}{0.32 \text{ mol/hr}} = 72.1\%$$

Single-pass conversion =  $\frac{\text{mole reacted in reactor}}{\text{mole fed into reactor}} = \frac{\text{mole into reactor} - \text{mole out reactor}}{\text{mole into reactor}}$

Single-pass conv. =  $\frac{F_{CO,2} - F_{CO,3}}{F_{CO,2}}$  Let's find  $F_{CO,2}$  and  $F_{CO,3}$

$$F_7 = 5 F_1 \text{ (given)} \quad F_7 = 5(1 \text{ mol/hr}) = 5 \text{ mol/hr}$$

$$F_{CO,7} = X_{CO,7} \cdot F_7 = X_{CO,6} \cdot F_7 = 1.45 \text{ mol/hr}$$

CO balance over "joint":  $F_{CO,1} + F_{CO,7} = F_{CO,2} \quad (\text{no rxn})$

$$F_{CO,2} = 0.32 \text{ mol/hr} + 1.45 \text{ mol/hr} = 1.77 \frac{\text{mol}}{\text{hr}}$$

CO balance over "split":  $F_{CO,5} = F_{CO,6} + F_{CO,7} \quad (\text{no rxn})$

$$= (0.089 + 1.45) \text{ mol/hr} = 1.539 \frac{\text{mol}}{\text{hr}}$$

CO balance over separator:  $F_{CO,3} = F_{CO,5} = 1.539 \text{ mol/hr}$

Finally: single pass conversion =  $\frac{F_{CO,2} - F_{CO,3}}{F_{CO,2}} = \frac{(1.77 - 1.539) \text{ mol/hr}}{1.77 \text{ mol/hr}} = 13.1\%$

Conversion: overall = 72.1%  
single pass = 13.1%

const

- again many ways to get to the ans. ③

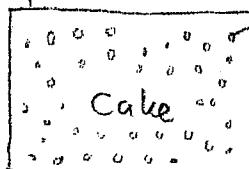
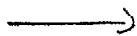
## Problem 6

System: cake (with baking soda inside)



$$V_1^t = 500 \text{ mL}$$

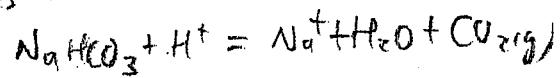
$$T_1 = 25^\circ\text{C}$$



$$V_2^t = 2,000 \text{ mL}$$

$$T_2 = 350^\circ\text{F}$$

bubbles



$\rightarrow$  see note at the end about  
"increasing fourfold"

1) Estimate M<sub>NaHCO<sub>3</sub></sub> added if bubbles contain 100% CO<sub>2</sub>.

Assume: - reaction is complete; all CO<sub>2</sub> goes into bubbles.

- without NaHCO<sub>3</sub> added, cake volume increases 11%

extrinsic - process is at P = 1 atm (constant); ideal gas

$$\Delta V^t = V_2^t - V_1^t = 1500 \text{ mL}; \text{ but } (11\% \times 500 \text{ mL}) = 55 \text{ mL} \text{ is not from bubbles.}$$

$$\text{So } V_{\text{bubbles}}^t = 1500 \text{ mL} - 55 \text{ mL} = 1445 \text{ mL}$$

$$\text{Ideal gas: } PV^t = nRT \quad T = 350^\circ\text{F} = 176.7^\circ\text{C} = 449.8 \text{ K}$$

$$n_{\text{bubble gas}} = \frac{PV^t}{RT} = \frac{(1 \text{ atm})(1445 \text{ mL})}{87.06 \frac{\text{mL atm}}{\text{mol K}} \cdot 449.8 \text{ K}} = 0.039 \text{ mol}$$

$$n_{\text{bubble gas}} = n_{\text{CO}_2} \xrightarrow{\text{stoichiometry}} n_{\text{NaHCO}_3, \text{reacted}} = 0.039 \text{ mol}$$

$$M_{\text{NaHCO}_3} = 0.039 \text{ mol} \times (23 + 1 + 12 + 3 \times 16) \frac{\text{g}}{\text{mol}} = \boxed{3.28 \text{ g}} \text{ ans.}$$

2) What if bubbles are only 60% CO<sub>2</sub>?

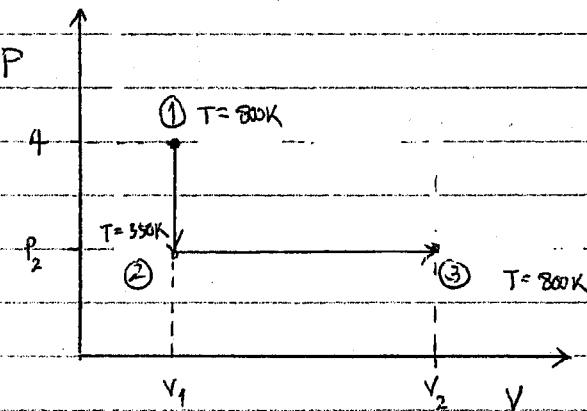
$$n_{\text{CO}_2} = 0.6 n_{\text{bubble gas}} = (0.6)(0.039 \text{ mol}) = 0.0234 \text{ mol}$$

$$M_{\text{NaHCO}_3} = 0.0234 \text{ mol} \times (23 + 1 + 12 + 3 \times 16) \frac{\text{g}}{\text{mol}} = \boxed{1.97 \text{ g}} \text{ ans.}$$

Note: If you chose "increase fourfold" to mean  $\Delta V^t = 2000 \text{ mL}$ ,  
the answers will be 4.41 g and 2.65 g

## Problem 7

Two-step process:



Assuming the gas is ideal, we can use  $PV^t = nRT$  to calculate P, V, or T of state ①, ②, and ③

\* remember, the values of P, V, T are not path dependent

$$\textcircled{1} \quad T = 800\text{ K}, \quad P = 4 \text{ bar} \quad ; \quad V^t = \frac{nRT}{P} = \frac{1 \times R \times 800}{4 \times 10^5}$$

$$V_1 = 2 \times 10^{-3} R \text{ m}^3$$

$$\textcircled{2} \quad T = 350 \text{ K}, \quad V = V_1 = 2 \times 10^{-3} R \text{ m}^3$$

$$P = \frac{nRT}{V^t} = \frac{1 \times R \times 350}{2 \times 10^{-3} R} = 1.75 \times 10^5 \text{ Pa} = 1.75 \text{ bar}$$

$$\textcircled{3} \quad P = P_2 = 1.75 \text{ bar} \quad T = 800 \text{ K}$$

$$V^t = \frac{nRT}{P} = \frac{1 \times R \times 800}{1.75 \times 10^5} = 4.57 \times 10^{-3} R \text{ m}^3$$

Assuming mechanical reversibility

$$W = - \int P dV^t = -n \int_{V_i}^{V_f} P dV$$

for a constant volume process From ①  $\rightarrow$  ②

$$dV^t = dV = 0$$

$$W_{\text{step 1}} = 0$$

for a constant pressure process

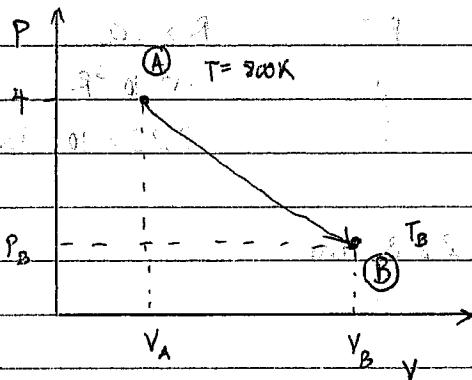
$$\begin{aligned} W &= -nP \int_{V_i}^{V_f} dV = -nP(V_f - V_i) \\ &= -P(V_f^t - V_i^t) \quad \text{as } n \text{ is constant} \\ &\quad (\text{closed system}) \end{aligned}$$

$$\begin{aligned} W_{\text{step 2}} &= -P_2(V_2 - V_1) = -1.75 \times 10^5 (4.57 \times 10^{-3} R - 2 \times 10^{-3} R) \\ &= -450 R \text{ J} \end{aligned}$$

-ve sign as the gas expands and do work  
on the surroundings.

For a single step isothermal expansion:

T is constant in isothermal process



$$T_B = T_A = 800 \text{ K}$$

$$W = -n \int P dV$$

$$\text{For ideal gas } PV = RT \quad \therefore P = \frac{RT}{V}$$

$$W = -n \int \frac{RT}{V} dV$$

T is constant  $\leftarrow$  remember W is path dependent, here the path we chose is the constant T path

$$W = -nRT \int_{V_A}^{V_B} \frac{1}{V} dV$$

$$W = -nRT \ln \left( \frac{V_B}{V_A} \right)$$

we know that  $T = 800 \text{ K}$

$$V_A = 2 \times 10^{-3} \text{ m}^3$$

and we need W to be  $-450 \text{ J}$

$$-450 \text{ J} = -1 \times R \times 800 \times \ln \left( \frac{V_B}{2 \times 10^{-3} \text{ m}^3} \right)$$

$$\ln \left( \frac{V_B}{2 \times 10^{-3} \text{ m}^3} \right) = 0.5625$$

$$V_B = 3.57 \times 10^{-3} R \text{ m}^3/\text{mol}$$

From ideal gas EOS i.e.  $PV = RT$

$$\begin{aligned} P &= \frac{RT}{V} = \frac{R \times 800}{3.57 \times 10^{-3} R} \\ &= 2.23 \times 10^5 \text{ Pa} \end{aligned}$$

∴ Final pressure is 2.23 bar

### Problem 8

a) At all times the pressure in the cylinder equals the weight of the elevator

i.e. the piston moves by reversible expansion

$$P = \frac{F}{A} = \frac{4000 \times 9.81}{2.5} = 15696 \text{ Pa}$$

b) This is a constant pressure process

Initial condition (1)  $T = 293 \text{ K}$   $V = 25 \text{ m}^3$

Final condition (2)  $T = ?$   $V = 25 + (2.5 \times 3)$   
 $= 32.5 \text{ m}^3$

as the gas is ideal, we can calculate its final temperature from

$$PV^t = nRT$$

$$PV_1^t = nRT_1 \rightarrow \frac{P}{nR} = \frac{T_1}{V_1^t}$$

$$PV_2^t = nRT_2 \rightarrow \frac{P}{nR} = \frac{T_2}{V_2^t}$$

$\uparrow$  constant

$$\therefore \frac{T_1}{V_1^t} = \frac{T_2}{V_2^t}$$

$$T_2 = \frac{V_2^t}{V_1^t} T_1 = \frac{32.5}{25} \times 293 = 380.9 \text{ K}$$

$$\text{also } n = \frac{PV_2^t}{RT_2} = \frac{15696 \times 32.5}{8.314 \times 380.9} = 161 \text{ moles}$$

for a constant pressure process  $Q = n\Delta H = n \int_{T_1}^{T_2} C_p dT$

$$Q = n C_p (T_2 - T_1) \quad \text{as } n \text{ is constant}$$

$$= 161 \times 30 \times (380.9 - 293)$$

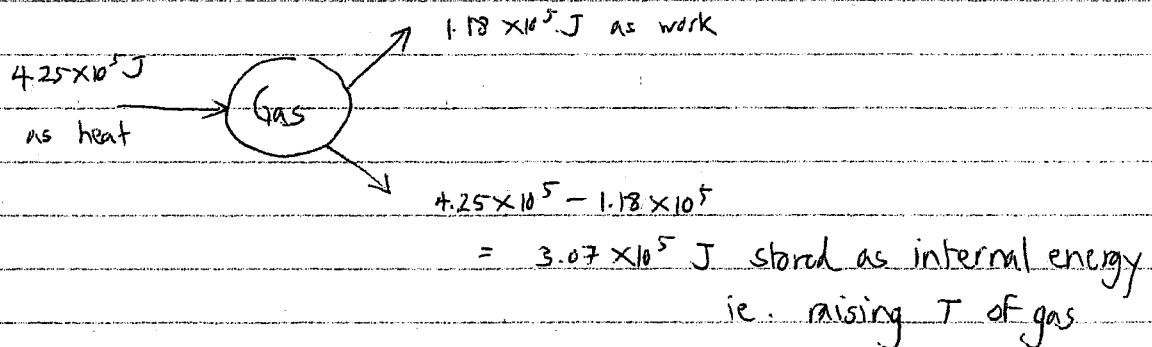
$$= 4.25 \times 10^5 \text{ J}$$

(i) for a constant pressure process

$$W = -n \int_{V_1}^{V_2} P dV = -nP(V_2 - V_1) = -P(V_2^t - V_1^t)$$

$$= -15696 \times (32.5 - 25)$$

$$= -1.18 \times 10^5 \text{ J}$$



$$\therefore \frac{1.18 \times 10^5}{4.25 \times 10^5} \times 100 = 28\% \text{ is used to do work}$$

and 72% to raise its temperature

d) During lowering process both P and T remain constant, we simply reduce the gas volume by venting away some of the gas

$$PV^t = nRT$$

$$\frac{P}{RT} = \frac{n}{V^t} = \text{constant}$$

$$\frac{n_{\text{initial}}}{V^t_{\text{initial}}} = \frac{n_{\text{final}}}{V^t_{\text{final}}}$$

$$\frac{161}{32.5} = \frac{n_{\text{final}}}{25}$$

$$\therefore n_{\text{final}} = 124 \text{ moles}$$

$$\therefore \text{vent } 161 - 124 = 37 \text{ moles}$$

e) this is not an efficient process both in terms of energy and time