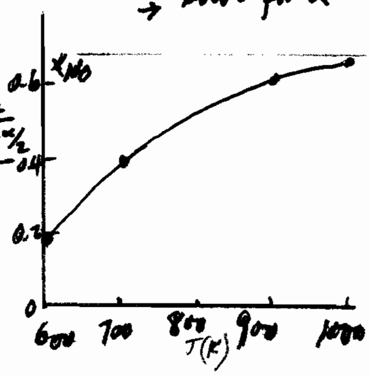
2.615 HW #3 Solution

(1) $NO + \frac{1}{2}O_2 \rightleftharpoons NO_2$ say dissociation coeff α

mole: α, $\frac{\alpha}{2}$, $(1-\alpha)$ ⇒ elemental balance is satisfied (add to 1 mol N, 2 mol O)

$$\frac{X_{NO_2}}{X_{NO}\sqrt{X_{O_2}}}\underbrace{\left(\frac{p}{p_0}\right)}_{=1}^{1-1-\frac{1}{2}} = 10^{K_{NO_2}-K_{NO}-\underbrace{\frac{K_{O_2}}{2}}_{=0}} \quad \text{or} \quad \frac{1-\alpha}{\alpha\sqrt{\frac{\alpha}{2}}}\left(1+\frac{\alpha}{2}\right)^{1/2} = 10^{K_{NO_2}-K_{NO}} \rightarrow \text{solve for } \alpha$$

T	$K_p(T)$ NO	NO_2	$K_{NO_2}-K_{NO}$	$10^{K_{NO_2}-K_{NO}}$	α	$x_{NO}=\frac{\alpha}{1+\alpha/2}$
600	-7.210	-6.111	+1.099	12.560	.21	.19
700	-6.086	-5.714	+0.345	2.213	.502	.401
900	-4.587	-5.185	-0.598	0.2523	.878	.610
1000	-4.062	-5.000	-0.938	0.1153	.939	.639
					Asymptotic	.6667



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(2) (Problem 3-8)

→ reactor →

CO	3%
O_2	7%
N_2	74%
CO_2	6%
H_2O	10%

Input concentration n_i (mol/cc)

$n_i = \frac{N_i}{V} = \frac{N_i}{N}\frac{N}{V} = x_i\frac{p}{RT}$; $\frac{p}{RT} = \frac{1.013\times10^5}{8314\times10^3} = 1.22\times10^{-2}$

$n_{CO} = 3\times10^{-2}\times1.22\times10^{-2} = 3.66\times10^{-4}\ \text{kmol/m}^3 = \underline{\underline{3.66\times10^{-7}\ \text{mole/cc}}}$

$n_{O_2} = 7\times10^{-2}\times1.22\times10^{-2} = 8.53\times10^{-4}\ \text{kmol/m}^3 = \underline{\underline{8.53\times10^{-7}\ \text{mole/cc}}}$

$$\frac{d[CO]}{dt} = -4.3\times10^{11}[CO][O_2]^{1/4}\exp\left(-\frac{E}{RT}\right)$$

$$= -4.3\times10^{11}\times3.66\times10^{-7}\times(8.53\times10^{-7})^{1/4}\exp\left(-\frac{2\times10^4}{10^3}\right) = \underline{\underline{-9.86\times10^{-6}\ \text{mol/cc/sec}}}$$

Input mixture: total C atom = .09 mole, O atom = .29 mole } per 1 mole of original mixture (assume N_2 and H_2O do not dissociate)

$CO + \frac{1}{2}O_2 \rightleftharpoons CO_2$
a mole b mole c mole } C atom balance $a+c = .09$; O atom balance $a+2b+2c = .29$

equilibrium $\frac{x_{CO_2}}{x_{CO}\sqrt{x_{O_2}}}\underbrace{\left(\frac{p}{p_0}\right)^{-1/2}}_{=1} = 10^{10.2} \Rightarrow \frac{c}{a\sqrt{b}}\sqrt{a+b+c+\overset{N_2}{.74}+\overset{H_2O}{.10}} = 10^{10.2}$

for the last equation to be true, $c \gg a$. ⇒ $c \simeq .09$; $b = \frac{.29-2c}{2} = .055$

and $a = c\sqrt{c+.84}/\sqrt{b}\times10^{10.2} = 2.34\times10^{-11}$

$n_{CO} = x_{CO}\frac{p}{RT} = \frac{2.34\times10^{-11}}{.055+.09+.84}\times\frac{1.013\times10^5}{8314\times10^3} = 2.89\times10^{-13}\ \text{kmol/m}^3 = \underline{\underline{2.89\times10^{-16}\ \text{mol/cc}}} \simeq 0$

Time to reach equilibrium

$$\simeq \frac{[CO]-[CO]_{eq}}{-\frac{d[CO]}{dt}} \simeq \frac{3.66\times10^{-7}}{9.86\times10^{-6}} = 3.7\times10^{-2}\ s = \underline{\underline{37\ ms}}$$

3) (Problem 4.1)

(a) Stoichiometric combustion $C_2H_6 + 3\frac{1}{2}(O_2 + 3.773N_2) \rightarrow 2CO_2 + 3H_2O + 3.773\times3.5N_2$ (30 gm; $3.5\times4.773\times28.96 = 483.79$ gm)

$\Rightarrow (A/F)_s = 16.13$; Actual A/F $= 7/0.48$; $\phi = \frac{16.13}{7/.48} = 1.11$

Using the notation in table 4-3: $y = 3$; $\varepsilon = \frac{4}{4+y} = \frac{4}{7}$; $\phi = 1.11$; $\psi = 3.773$.

Assume the burned gas is frozen at 1740K, then $k_{water\ gas} = 3.5$ and eq. (4.6) may be solved for the CO mole value c: $(k-1)c^2 - c\{k[2(\phi-1)+\varepsilon\phi] + 2(1-\varepsilon\phi)\} + 2k\varepsilon\phi(\phi-1) = 0$

or $2.5c^2 - c\{3.5[2\times.11 + \frac{4}{7}\times1.11] + 2(1-\frac{4}{7}\times1.11)\} + 2\times3.5\times\frac{4}{7}\times1.11\times0.11 = 0 \Rightarrow c = \underline{0.15}$

(The other root is discarded because it will give a negative CO_2 mole value.)

		mole/mole	mole fractions
CO_2	$\varepsilon\phi - c$	0.48	0.090
H_2O	$2(1-\varepsilon\phi)+c$	0.88	0.164
CO	c	0.15	0.028
H_2	$2(\phi-1)-c$	0.07	0.013
N_2	ψ	3.773	0.705
total	$(2-\varepsilon)\phi+\psi$	5.35	1

(b) $(C_2H_5OH) + 3(O_2 + 3.773N_2) \rightarrow 2CO_2 + 3H_2O + 3\times3.773N_2$

$(A/F)_s = \underline{9.01}$; $(A/F) = \frac{7}{0.48} = 14.58 \Rightarrow \phi = \underline{0.62} < 1$ lean

So products are CO_2, H_2O and excess O_2, N_2 only.

$0.62(C_2H_5OH) + 3(O_2 + 3.773N_2) \rightarrow 1.24CO_2 + 1.86H_2O + 1.14O_2 + 11.32N_2$

$x_{CO_2} = \underline{7.97\%}$; $x_{H_2O} = \underline{12\%}$; $x_{O_2} = \underline{7.33\%}$; $x_{N_2} = \underline{72.8\%}$

(4) (Problem 4.9) — Elemental balance leads to the reaction equation: (per mole of product)

$$0.0164C_8H_{18} + 0.192(O_2 + 3.773N_2) \rightarrow 0.12CO_2 + 0.14H_2O + 0.01CO + 0.005H_2 + 0.7247N_2 + 0.0003C_8H_{18}$$

energy input (per mole of product)	energy unutilized in exhaust (per mole of product)		
C_8H_{18}	CO	H_2	C_8H_{18}
$= 0.0164\times114\times44.4 = 83.01$ MJ	$= 28\times.01\times10.1 = 2.83$ MJ	$0.005\times2\times120 = 1.2$ MJ	$0.0003\times114\times44.4 = 1.52$ MJ
(%) 100%	total 6.7% → { 3.4%	1.45%	1.83%