HW 3 solution

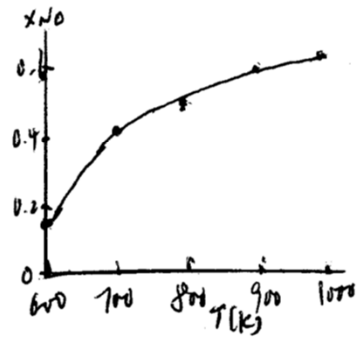
(1) $NO + \frac{1}{2} O_2 \rightleftharpoons NO_2$; total 1 mol of N and 2 mole of O

	NO	O_2	NO_2
moles	a	b	c

; elemental balance $\left.\begin{array}{l} a+c=1 \\ a+2b+2c=2 \end{array}\right\} \Rightarrow$ $\begin{array}{l} c = 1-2b \\ a = 1-c = 2b \end{array}$

Equilibrium $\dfrac{\frac{c}{a+b+c}}{\frac{a}{a+b+c}\left(\frac{b}{a+b+c}\right)^{1/2}} = 10^{k_{p NO_2} - k_{NO} - \frac{k_{O_2}}{2}} \equiv k_p$ or $\dfrac{1-2b}{2b^{3/2}}(1+b)^{1/2} = k_p(T)$

T(K)	$\log k_p(T)$ NO	NO_2	$k_{NO_2} - k_{NO}$	$10^{k_{NO_2} - k_{NO}}$	b	x_{NO}
600	−7.210	−6.111	+1.099	12.56	0.1033	0.1892
700	−6.086	−5.714	+0.345	2.213	0.2511	0.4014
800	−5.243	−5.417	+0.174	1.493	0.2924	0.4525
900	−4.587	−5.185	−0.598	0.2523	0.4309	0.6100
1000	−4.062	−5.000	−0.938	0.1153	0.4694	0.6389



(2) (Problem 3-8)

$\longrightarrow$ reactor $\longrightarrow$

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

Input concentration n_i (mol/cc)

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

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

$n_{O_2} = 7\times10^{-2}\times1.22\times10^{-2} = 8.53\times10^{-4}$ 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 $\left.\begin{array}{l} \text{C atom} = .09 \text{ mole} \\ \text{O atom} = .29 \text{ mole} \end{array}\right\}$ per 1 original mole of mixture (assume N_2 and H_2O do not dissociate)

$\left.\begin{array}{l} CO + \frac{1}{2}O_2 \rightleftharpoons CO_2 \\ \text{a mole b mole c mole} \end{array}\right\}$ $\begin{array}{l} \text{C atom balance} \quad a+c = .09 \\ \text{O atom balance} \quad a+2b+2c = .29 \end{array}$

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, $c \gg a$. $\Rightarrow c \simeq .09$; $b = \frac{.29-2c}{2} = .055$

$a = \left(\frac{c}{\sqrt{b}}\sqrt{b+c+0.84}\right)/10^{10.2} = \frac{0.09}{\sqrt{0.055}}\frac{\sqrt{0.09+0.055+0.84}}{10^{10.2}} = 2.40\times10^{-11}$

$n_{CO} = x_{CO}\frac{p}{RT} = \frac{2.4\times10^{-11}}{(0.09+0.055+0.84)}\times\frac{1.013\times10^5}{8314\times10^3} = 2.97\times10^{-13}$ kmol/m^3 = $\underline{2.97\times10^{-16} \text{ mol/cc}}$
$\simeq 0$ small

Time to reach equilibrium

$\tau = \frac{[CO]-[CO]_{eq}}{\left.\frac{d[CO]}{dt}\right|_0} = \frac{(3.66\times10^{-7} - \overset{\simeq 0}{\cancel{3\times10^{-16}}})}{9.86\times10^{-6}} = 3.7\times10^{-2}\text{ s} - \underline{\underline{37 \text{ ms}}}$

Problem could be solved easily using the computer program "exhaust_comp" on the web.

3) (Problem 4.1)

30 gm $3.5 \times 4.773 \times 28.96 = 483.79$ gm

(a) Stoichiometric combustion $C_2H_6 + 3\frac{1}{2}(O_2 + 3.773N_2) \rightarrow 2CO_2 + 3H_2O + 3.773 \times 3.5 N_2$

$\Rightarrow (A/F)_s = 16.13$; 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 $K_{\text{water gas}} = 3.5$ 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 $2.5c^2 - c\{3.5[2 \times .11 + \frac{4}{7} \times 1.11] + 2(1 - \frac{4}{7} \times 1.11)\} + 2 \times 3.5 \times \frac{4}{7} \times 1.11 \times 0.11 = 0 \Rightarrow c = \underline{\underline{0.15}}$

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

(b) $(C_2H_5OH) + 3(O_2 + 3.773N_2) \rightarrow 2CO_2 + 3H_2O + 3 \times 3.773 N_2$

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

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

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

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

		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

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

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

<u>energy input</u> (per mole of product) | <u>energy unutilized in exhaust</u> (per mole of product)

	C_8H_{18}	CO	H_2	C_8H_{18}
	$= 0.0164 \times 114 \times 44.4 = 83.01$ MJ	$= 28 \times .01 \times 10.1 = 2.83$ MJ	$0.005 \times 2 \times 120 = 1.2$ MJ	$0.0003 \times 114 \times 44.4 = 1.52$ MJ
(%)	100%	total $\underline{\underline{6.7\%}} \rightarrow$ { $\underline{\underline{3.4\%}}$	$\underline{\underline{1.45\%}}$	$\underline{\underline{1.83\%}}$

Combustion inefficiency=6.7%; combustion efficiency=(100-6.7)%=93.3%
Inefficiency due to fuel in the exhaust = 1.83%

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2.61 Internal Combustion Engines
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