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4A13 – Combustion & I.C. Engines.

Cribs – 2016.

1) a) $$A + A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A + A^* \qquad (R1)$$

$$A^* \xrightarrow{k_3} P \qquad (R2)$$

(i) $$\frac{d[P]}{dt} = k_3 [A^*]$$

$$\frac{d[A^*]}{dt} = k_1 [A]^2 - k_2 [A][A^*] - k_3 [A^*]$$

$$= k_1 [A]^2 - \left[k_2 [A] + k_3\right] [A^*]$$

if $[A^*]$ is in steady state then $\frac{d[A^*]}{dt} = 0$

$$\Rightarrow [A^*] = \frac{k_1 [A]^2}{k_2 [A] + k_3}$$

$$\therefore \boxed{\frac{d[P]}{dt} = \frac{k_1 k_3 [A]^2}{k_2 [A] + k_3} = \frac{k_1 [A]^2}{\frac{k_2}{k_3}[A] + 1}}$$

(ii) In the high pressure limit rate of (R1) is larger than (R2) ie $k_2[A] \gg k_3$ or $\frac{k_2}{k_3}[A] \gg 1$

$$\Rightarrow \boxed{\frac{d[P]}{dt} = \frac{k_3 k_1}{k_2} [A]} \quad \text{This is } I^{st} \text{ order}$$

For the low pressure limit

Collisional reactions are slower compared to decay. ie $k_2[A] << k_3$

or $\frac{k_2}{k_3}[A] << 1$

$\Rightarrow \boxed{\frac{d[P]}{dt} = k_1[A]^2}$ This is 2^{nd} order.

(b) $CH_4 + \frac{2}{\phi}(O_2 + \frac{0.79}{0.21}N_2) \rightarrow a\,CO_2 + b\,CO + c\,H_2O + d\,H_2 + e\,N_2$

$\phi = 2$; $P = 5$ bar, $T = 1200K$

N atom balance: $2e = \frac{0.79}{0.21} \times 2 \Rightarrow \boxed{e = 3.7619}$

C atom balance: $a + b = 1 \Rightarrow a = 1 - b$

H atom : $c + d = 2 \Rightarrow d = 2 - c$

O atom : $2a + b + c = 2 \Rightarrow c = 2 - 2a - b$

$d = 2 - b$

4 unknowns & 3 eqns. $\Rightarrow \underline{\underline{c = b.}}$

4^{th} eqn. comes from Kp relation.

fuel rich combustion. So, consider water-gas shift reaction.

$CO + H_2O \rightleftharpoons CO_2 + H_2$

(3)

$$K_p = \frac{(p_{CO_2}/p)\,(p_{H_2}/p)}{(p_{CO}/p)\,(p_{H_2O}/p)} = \frac{X_{CO_2}\,X_{H_2}}{X_{CO}\,X_{H_2O}}$$

$$= \frac{n_{CO_2}\,n_{H_2}}{n_{CO}\,n_{H_2O}} = \frac{ad}{bc} = \exp(-0.311)$$

from the data book.

$$\frac{(1-b)(2-b)}{b^2} = 0.7327$$

Solving for $b = 0.7117$ and 10.5116

This isn't meaningful Solution because a & $d < 0$.

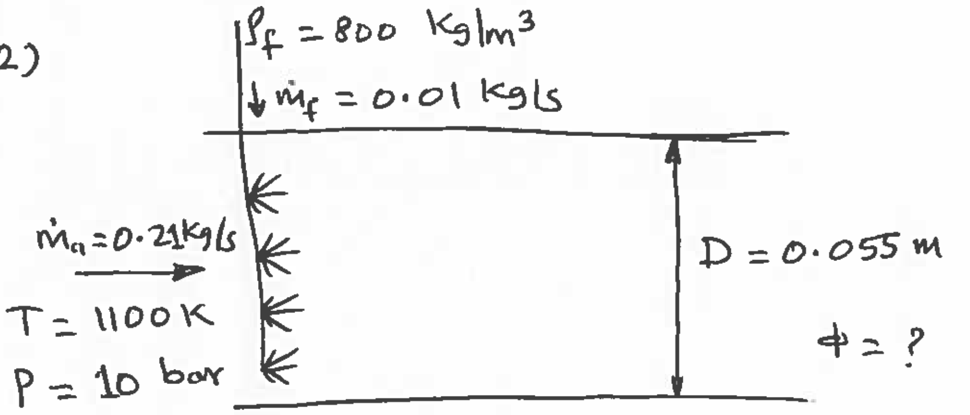
$$\Rightarrow \quad a = 0.2883$$
$$b = 0.7117$$
$$c = 0.7117$$
$$d = 1.2883$$
$$e = 3.7619$$
$$\text{total} = 6.7619$$

$$\Rightarrow \quad X_{CO_2} = 0.0426$$
$$X_{CO} = 0.1053$$
$$X_{H_2O} = 0.1053$$
$$X_{H_2} = 0.1905$$
$$X_{N_2} = 0.5563$$
$$\Sigma = 1.00$$

This is the volumetric Composition @ $T = 1200K$, $\phi = 2.0$. $p = 5bar$

Change in pressure wouldn't affect this composition.

(2)



$d_{in} = 60 \times 10^{-6}\ m; \quad B = 8 \times 10^{-7}\ m^2/s$

(a)

$$\phi = \frac{(\dot{m}_f/\dot{m}_{air})}{(\dot{m}_f/\dot{m}_a)_{st}}$$

$$C_{12}H_{26} + a\left(O_2 + \frac{0.79}{0.21} N_2\right) \longrightarrow 12\,CO_2 + 13\,H_2O + \frac{0.79}{0.21}\,a\,N_2$$

O atom balance $\Rightarrow$ $\boxed{a = \frac{37}{2}}$

$$\left(\frac{\dot{m}_f}{\dot{m}_a}\right)_{st} = \frac{(12 \times 12 + 26 \times 1)}{\frac{37}{2}\left(32 + \frac{0.79}{0.21} \times 28\right)} = 0.0669$$

$$\phi = \frac{(0.01/0.21)}{0.0669} = 0.7118 \qquad \boxed{\phi = 0.7118}$$

(b)

$d_{in} = 60 \times 10^{-6}\ m$

$$m = \rho_f \frac{4}{3}\pi\left(\frac{d}{2}\right)^3$$

$$\frac{dm}{dt} = -\dot{m}'' A = \frac{-\rho_f B}{4d} 4\pi\left(\frac{d}{2}\right)^2$$

$$\rho_f \frac{4}{3}\pi\left(\frac{d}{2}\right)^2 \frac{3}{2}\frac{dd}{dt} = \frac{-\rho_f B}{4d} 4\pi \frac{d^2}{4}$$

$$\Rightarrow \frac{dd}{dt} = -\frac{B}{2d}$$

$$\int_0^t dt \Rightarrow d^2(t) = d^2(0) - Bt$$

$$\boxed{d^2 = d_{in}^2 - Bt}$$

@ t_{evap} $d = 0$

$$\therefore t_{evap} = \frac{d_{in}^2}{B} = \frac{(60 \times 10^{-6})^2}{8 \times 10^{-7}} = 4.5 \times 10^{-3}\ s$$

$$L_{evap} = U t_{evap} = 4.5 \times 10^{-3}\ U$$

U - comes from mass conservation

$$\therefore \dot{m} = \rho U A \Rightarrow U = (\dot{m}/\rho A)$$

$$A = \frac{\pi}{4} D^2 = \frac{\pi}{4} \times (0.055)^2 = 2.3758 \times 10^{-3}\ m^2$$

To find mixture density ρ

$$C_{12}H_{26} + \underbrace{\cancel{\frac{37}{2\times 0.7118}}}_{\sim 26}\left(O_2 + \frac{0.79}{0.21}N_2\right)$$

$$\therefore x_f = \frac{1}{\left(1+26+26\,\frac{0.79}{0.21}\right)} = 0.008$$

$$x_{O_2} = \frac{26}{\left(1+26+26\,\frac{0.79}{0.21}\right)} = 0.2083$$

$$x_{N_2} = 1-(x_f + x_{O_2}) = 0.7837$$

$$MW_{mix} = \sum x_i W_i = 0.008\times 170 + 0.2083\times 32 + 28\times 0.7837$$

$$= 29.969$$

$$\therefore \rho = \frac{P\,MW_{mix}}{RT} = \frac{10\times 10^5 \times 29.969}{8314\times 1100} = 3.2769\ \mathrm{kg/m^3}$$

$$\therefore U = \frac{(0.01+0.21)}{3.2769\times 2.3758\times 10^{-3}} = 28.26\ \mathrm{m/s}$$

$$\therefore L_{evap} = 28.26\times 4.5\times 10^{-3} = 0.127\ \mathrm{m}$$

$$\boxed{L_{evap} = 0.127 = 12.7\ \mathrm{cm}}$$

(c) $T_{a,bio} = 1.1\, T_{a,f}$ $\qquad T_{a,f} = T_a = 15000\ K$

$T = 1100K$

$$\tau_{ign} \sim e^{(T_a/T)}$$

$$\Rightarrow \frac{\tau_{ign,bio}}{\tau_{ign,f}} = \frac{e^{(T_{a,bio}/T)}}{e^{(T_{a,f}/T)}} = e^{(0.1 T_a/T)} = 3.91$$

$$L_{ign,bio} = U\tau_{ign,bio} = U\tau_{ign,f}\ 3.91$$

$$L_{ign,bio} = 3.9\, L_{ign,f} \Rightarrow \boxed{L_{ign,bio} \approx 4\, L_{ign,f}}$$

Ignition length for the bio-fuel is about 4 times longer than for $C_{12}H_{26}$.

This implies that the ignition occurs outside the Combustor, which is undesirable. This will destroy the high pressure turbine. This can be avoided by either

1) increasing the combustor length – which is impractical

2) increasing the air temperature substantially.

Q3

i) Shift from gasoline to diesel driven by CO2/fuel economy (FE) regulatory structure. Manufacturers are fined significant amounts of money if their fleet average CO2/FE exceeds set levels – in the EU for example this is presently €95 per gram CO2/km exceedance on the standard drive cycle. Like-for-like performance diesel engines are significantly more efficient as they are unthrottled, run lean and have a higher compression ratio.

ii) Electric vehicles are attractive to the vehicle manufacturers as they are incentivised by the regulatory authorities via a significantly beneficial effect on CO2 exceedance fines.

iii) For gasoline engines, reducing noxious emissions to the regulatory levels is (compared to diesel engines, cheap and effective). This is because nearly all gasoline engines run at stoichiometry ("lambda 1") and at this condition simultaneous oxidation of unburnt hydrocarbons (uHCs) and carbon monoxide (CO), and reduction of oxides of nitrogen (NOx) is possible. Particle matter (PM) is usually at levels that do not require aftertreatment.

iv) For diesel engines, as well as the need to reduce uHCs, CO and NOx, PM also has to be dealt with. With respect to NOx the issues are however very much more severe than with the gasoline engine. Diesel engines generally run lean of stoichiometric, but the reduction of NOx requires (in practice) chemically reducing reactions. Two methods of performing this function have become established.

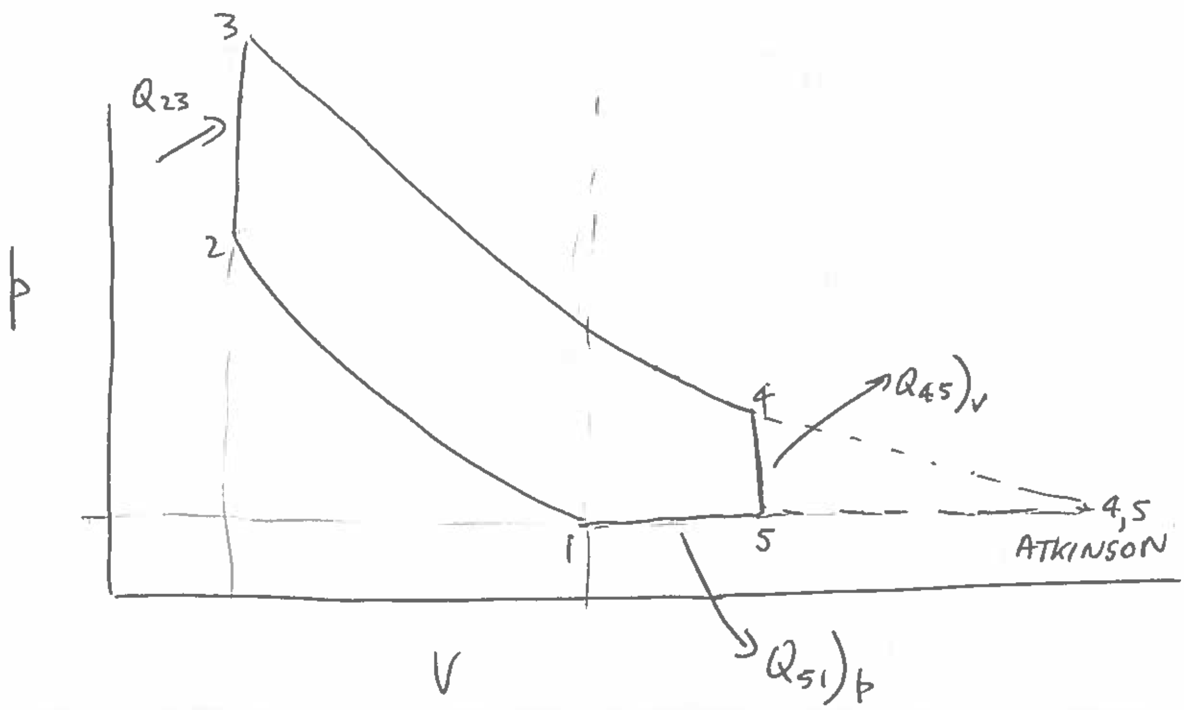
a. One is so-called SCR (selective catalytic reactor) system, where via urea injection, other complicated hardware and a complicated sequence of reactions, the NOx is effectively removed.

b. The other is the so-called LNT (Lean NOx Trap) system, where the trap consists of a monolith coated with compounds that can store NOx during normal lean running, and also catalytic material that can convert the stored NOx to benign products, via reducing reactions, during occasional rich running of the engine. The LNT system is significantly cheaper than the SCR method, but effective operation is much more sensitive to exhaust temperature and poisoning.

catalyst ?

Soln

a)



b)

$$\eta = 1 - \frac{Q_{out}}{Q_{in}} = 1 - \frac{Q_{45} + Q_{51}}{Q_{23}}$$

Where

$$Q_{23} = mc_v(T_3 - T_2)$$

$$Q_{45} = mc_v(T_4 - T_5)$$

$$Q_{51} = mc_p(T_5 - T_1)$$

So $\eta = 1 - \dfrac{c_v(T_4 - T_5) + c_p(T_5 - T_1)}{c_v(T_3 - T_2)}$

Working round the cycle:-

1 – 2 $T_2 = T_1 r_c^{\gamma-1}$ (isentropic compression)

2 – 3 $T_3 = T_2 + \theta T_1 = T_1\left(r_c^{\gamma-1} + \theta\right)$ (constant volume heat addition)

5 – 1 $T_5 = \dfrac{V_5}{V_1}T_1 = \dfrac{r_e}{r_c}T_1$ (constant pressure heat rejection)

4 – 5 $T_4 = \dfrac{T_5}{r_e^{\gamma-1}} = T_1\left(\dfrac{\theta + r_c^{\gamma-1}}{r_e^{\gamma-1}}\right)$ (constant-volume heat rejection)

Substituting into the relationship for efficiency

$$\eta = 1-\frac{c_v(T_4-T_5)+c_p(T_5-T_1)}{c_v(T_3-T_2)} = 1-\frac{1}{r_e^{\gamma-1}}-\frac{1}{\theta}\left(\frac{r_e}{r_c}\left(\left(\frac{r_e}{r_c}\right)^{-\gamma}-1+\gamma\right)-\gamma\right)$$

For $r_e = r_c$

$$\eta = 1-\frac{1}{r_e^{\gamma-1}}-\frac{1}{\theta}(1-1+\gamma-\gamma) = 1-\frac{1}{r_e^{\gamma-1}}$$, the normal Otto cycle expression.

c) For the Atkinson cycle, we have $T_4 = T_5$

So $T_1\left(\frac{r_e}{r_c}\right) = T_1\left(\frac{\theta + r_c^{\gamma-1}}{r_e^{\theta-1}}\right)$

Or

$r_e^{\gamma} = r_c\theta + r_c^{\gamma}$ or $r_e = \left(r_c\theta + r_c^{\gamma}\right)^{\frac{1}{\gamma}}$

$$\eta_{Atkinson} = 1-\frac{Q_{51}}{Q_{23}} = 1-\frac{c_p\left(T_1\left(\frac{r_e}{r_c}\right)-T_1\right)}{c_v\theta T_1} = 1-\frac{\gamma(r_e-r_c)}{\theta r_c} = 1-\frac{\gamma(r_e-r_c)}{\left(r_e^{\gamma}-r_c^{\gamma}\right)}$$

$$r_e = \left(10*11+10^{1.4}\right)^{\frac{1}{1.4}} = 33.26$$

And

$$\eta_{Atkinson} = 1-\frac{1.4(33.26-10)}{\left(33.26^{1.4}-10^{1.4}\right)} = 70.4\%$$

$$\eta_{otto} = 1-\frac{1}{r_c^{\gamma-1}} = 1-\frac{1}{10^{0.4}} = 60.2\%$$

Comments.

The absolute efficiencies are wildly optimistic, of course. The Atkinson cycle engine with an expansion ration 3.3 time the compression ratio would be very bulky – and frictional losses would be greater too. The mechanical realisation is expensive too. The use of variable valve timing to achieve something of the same effect is more realistic.