4A13 - Combustion & Engines.

B 1.

$$A \xrightarrow{k_1} D \qquad (R1)$$

$$A + D \xrightarrow{k_2} \alpha D + \text{Product} \qquad (R2)$$

$$D \xrightarrow{k_w} \text{Product} \qquad (R3)$$

$$D + M \xrightarrow{k_g} M + \text{Product} \qquad (R4)$$

a) (R1) is chain initiation as it produces radical

(R2) is chain branching if $\alpha > 1$
chain carrier if $\alpha = 1$
chain termination if $\alpha = 0$

(R3) is wall termination - high energy molecule colliding with the vessel wall looses energy and becomes a stable molecule.

(R4) is gas phase termination reaction, a collision partner is required for gas phase termination but not for wall termination.

(b) $$\frac{d[D]}{dt} = k_1[A] + (\alpha - 1) k_2 [A][D] - k_w [D] - k_g [D][M]$$

(c) for steady state

$$\frac{d[D]}{dt} = 0 \Rightarrow [D] = \frac{k_1 [A]}{(1-\alpha) k_2 [A] + k_w + k_g [M]}$$

to have finite $[D]$

$$(1-\alpha) k_2 [A] + k_w + k_g [M] > 0$$

Rearranging this gives

$$\boxed{\alpha < 1 + \frac{k_w + k_g [M]}{k_2 [A]}}$$ as required

(d) under chemical explosion $[D] \to \infty$ or becomes very large.

$$\Rightarrow (1-\alpha) k_2 [A] + k_w + k_g [M] = 0$$

$$\Rightarrow \alpha = 1 + \frac{k_w + k_g [M]}{k_2 [A]}$$

In the early stages k_i's, $[M]$ and $[A]$ are constant, implying that $[D]$ will grow exponentially only if $\alpha > 1$.

Thus, the condition for the chemical explosion is

$$\boxed{\alpha \geqslant 1 + \frac{k_w + k_g[M]}{k_2[A]}}$$

(e) The above condition can be written as

$$\alpha \geqslant 1 + \frac{k_g[M]}{k_2[A]}\left\{\frac{k_w}{k_g[M]} + 1\right\}$$

if $k_w << k_g[M]$, then

$$\boxed{\alpha \geqslant 1 + \frac{k_g[M]}{k_2[A]}}$$

as required.

2) $T = 1400\,K$, $\phi = 3.0$, Fuel $C_4H_{10}O$

(a) No, because the chemical kinetics play dominant role in the reaction zones.

(b)

$$C_4H_{10}O + \frac{a}{\phi}\left(O_2 + \frac{0.79}{0.21}N_2\right)$$

$$\rightarrow b_1 CO_2 + b_2 CO + b_3 H_2O$$

$$+ b_4 H_2 + b_5 N_2$$

$$b_5 = \frac{a}{\phi}\frac{0.79}{0.21}$$ Since N_2 is taken to be inert

for Stoichiometry, $\phi = 1$

$$C_4H_{10}O + a\left(O_2 + \frac{0.79}{0.21}N_2\right)$$

$$\longrightarrow 4CO_2 + 5H_2O + a\frac{0.79}{0.21}N_2$$

O-atom balance gives $\boxed{a = 6}$

for $\phi = 3$

C-atom balance gives

$$b_1 + b_2 = 4 \Rightarrow b_2 = 4 - b_1$$

$$H : \quad 2b_3 + 2b_4 = 10 \quad \Rightarrow \quad b_3 + b_4 = 5$$

$$\Rightarrow \quad b_4 = 5 - b_3$$

$$O : \quad 2b_1 + b_2 + b_3 = 5$$

$$\Rightarrow \quad b_1 + b_3 = 1 \quad \Rightarrow \quad b_3 = 1 - b_1$$

$$\& \quad b_4 = 4 + b_1$$

Now we have 4 unknowns & 3 equations.

$\Rightarrow$ Need 1 K_p relation.

Since the combustion is fuel rich, consider the water-gas shift reaction

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

$$K_p = \frac{(p_{CO_2}/p_0)\,(p_{H_2}/p_0)}{(p_{CO}/p_0)\,(p_{H_2O}/p_0)} = \frac{b_1\, b_4}{b_2\, b_3}\,\frac{(p/p_0)^2}{(p/p_0)^2}$$

$$= \frac{b_1\,(4+b_1)}{(4-b_1)\,(1-b_1)} = 0\ 4644$$

Since $\ln(K_p) = -0.767$ for $T = 1400\,K$ for Rxn 8 in the data book

$$\Rightarrow \quad 0.5356\, b_1^2 + 6.322\, b_1 - 1.8576 = 0$$

$$\Rightarrow \quad \boxed{b_1 = 0.2869}$$

$\leftarrow$ taking the +ve root since moles can't be negative

$b_1 = 0.2869$

$b_2 = 3.7131$

$b_3 = 0.7131$

$b_4 = 4.2869$

$b_5 = 7.5238$

$\text{Sum} = 16.5238$

mole fractions are

$X_{CO_2} = \frac{b_1}{\text{Sum}} = 0.0174$

$X_{CO} = 0.2247$

$X_{H_2O} = 0.0432$

$X_{H_2} = 0.2594$

$X_{N_2} = 0.4553$

$\text{Sum} = 1.0000$

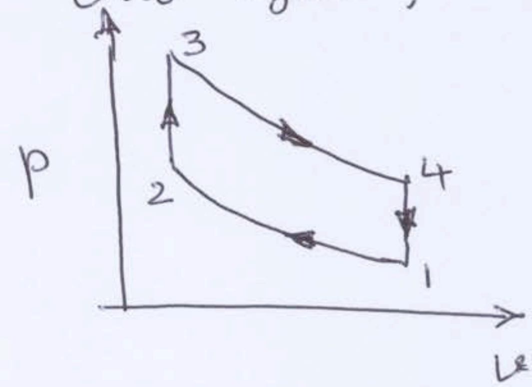
(c) NO, because the sum of the mole number is zero for the Kp relation.
(No pressure dependence appear in the Kp relation for the water-gas shift reaction)

(d) H_2 Yield can be increased by shifting the water-gas shift reaction to the right. This can be achieved by adding (spraying) water vapour into the reactor.

$CO + H_2O \rightleftharpoons CO_2 + H_2$

$H_2O \uparrow \Rightarrow H_2 \uparrow$ by Le-Chartelier principle.

3) ideal Otto cycle ; $\gamma = 1.4$



(a) $2-3$ is constant volume combustion

$$\Rightarrow m\, C_v (T_3 - T_2) = m_f\, Q$$

$$\Rightarrow (T_3 - T_2) = \Delta T = \frac{m_f}{m}\frac{Q}{C_v}$$

$$\frac{m_f}{m} = \frac{m_f}{m_a}\frac{m_a}{m}$$

but $m = m_f + m_a + m_r$

$$\Rightarrow 1 = \frac{m_f}{m} + \frac{m_a}{m} + \frac{m_r}{m}$$

$$\Rightarrow \frac{m_a}{m} = \left(1 - x_r - \frac{m_f}{m}\right)$$

Now; $\dfrac{m_f}{m} = \dfrac{m_f}{m_a}(1 - x_r)$ $\quad \Rightarrow \dfrac{m_a}{m} = (1 - x_r)$

$\because \dfrac{m_f}{m} << x_r$

$$\therefore \boxed{\Delta T = \frac{m_f}{m_a}\frac{Q(1-x_r)}{C_v}}$$ as required.

(b) Burnt gas temperature is

$$T_3 = T_2 + \Delta T$$

for isentropic compression $\dfrac{T_2}{T_1} = r_c^{\gamma - 1} = 9^{0.4} = 2.408$

$$\therefore T_2 = 722.4\ \text{K} \simeq \underline{\underline{722\ \text{K}}}$$

for case A

$$T_{3A} = T_2 + 2100 = 2822\ K$$

$$\frac{\Delta T_B}{\Delta T_A} = \frac{(m_f/m_a)_B}{(m_f/m_a)_A}\,\frac{(1-x_r)_B}{(1-x_r)_A}$$

Both cases are at Stoichiometric conditions

$$\Rightarrow \left(\frac{m_f}{m_a}\right)_B = \left(\frac{m_f}{m_a}\right)_A$$

$$\therefore\ \frac{\Delta T_B}{\Delta T_A} = \frac{(1-x_r)_B}{(1-x_r)_A} = \frac{0.7}{0.9} = 0.778$$

$$\Delta T_B = 1633.8 \Rightarrow \boxed{T_{3,B} = 2355.8 = 2356\ K.}$$

(c) Thermal efficiency for ideal Otto cycle is

$$\eta_{th} = 1 - \frac{1}{r^{\gamma-1}} = 1 - 9^{-0.4} = 0.585$$

No change between cases A & B.

(d) $W_{net} = \eta_{th} m_f Q = \eta_{th} m C_v \Delta T$

$$\frac{W_{net,B}}{W_{net,A}} = \frac{\Delta T_B}{\Delta T_A} = \frac{(1-x_r)_B}{(1-x_r)_A} \quad \text{from part (b)}$$

$$= 0.778$$

% Change in indicated work is

$$100\left(\frac{W_{net,A} - W_{net,B}}{W_{net,A}}\right) = \left(1 - \frac{W_{net,B}}{W_{net,A}}\right) 100$$

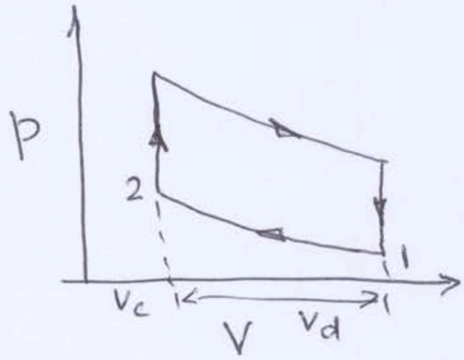
$$\Rightarrow 1 - 0.778 = \underline{\underline{22.2\ \%}}$$

22.2 % drop in the net work in Case B with respect to A

or 28.5 % increase in the Case A with respect to B

(e) The mass in the cylinder must be increased by using turbo or Super charging.

4) ideal cycle:



$$r = \frac{V_d + V_c}{V_c} = \frac{V_1}{V_2}$$

$$V_1 = V_d + V_c$$

$$r = \frac{V_d}{V_c} + 1 \implies \frac{V_d}{V_c} = (r-1)$$

(a) $$\text{imep} = \frac{W}{V_d} = \frac{\eta m_f Q}{V_d} = \frac{\eta m q^*}{V_d} \; ; \; q^* = \frac{m_f Q}{m}$$

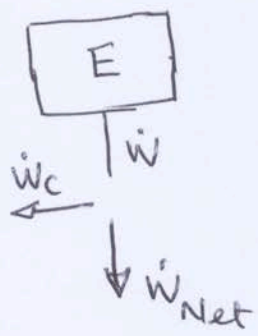
Q – LCH for fuel.

$$m = \rho_1 V_1 = \rho_1 (V_d + V_c)$$

$$\therefore \frac{m}{V_d} = \rho_1 \left(1 + \frac{V_c}{V_d}\right) = \rho_1 \left(\frac{r}{r-1}\right)$$

$$\therefore \boxed{\text{imep} = \eta q^* \rho_1 \left(\frac{r}{r-1}\right)} \quad \text{as required.}$$

(b) (i)



$$\frac{\dot{W}'_{Net}}{\dot{W}} = \frac{\dot{W}' - \dot{W}_c}{\dot{W}}$$

$$= \frac{\dot{m}' w' - \dot{m}'_a w_c}{\dot{m} w}$$

Prime indicates the supercharged engine.

$$\Rightarrow \frac{\dot{W}'_{net}}{\dot{W}} = \frac{\dot{m}'}{\dot{m}} \underbrace{\frac{w'}{w}}_{\approx 1} - \underbrace{\frac{\dot{m}'_a}{\dot{m}}}_{\left(\frac{\dot{m}'_a}{\dot{m}'} \frac{\dot{m}'}{\dot{m}}\right)} \frac{w_c}{w}$$

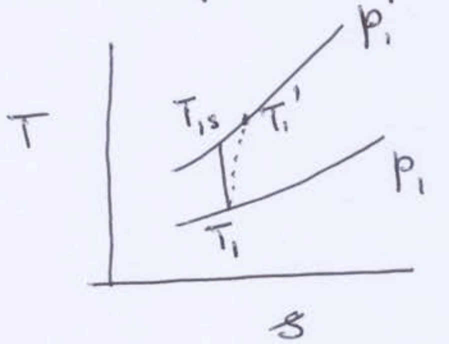
≈ 1 Since engine specific work is unchanged

$\frac{\dot{m}'_a}{\dot{m}'} \approx 1$ Since $\dot{m}'_f << \dot{m}'_a$

$$\Rightarrow \boxed{\frac{\dot{W}'_{net}}{\dot{W}} = \frac{\dot{m}'}{\dot{m}} - \frac{\dot{m}'}{\dot{m}} \frac{w_c}{w}} \quad \text{--- } (1)$$

but $\frac{\dot{m}'}{\dot{m}} = \frac{\rho'_1}{\rho_1}$ Since V_d is the same.

for the supercharger: $r_c = \frac{p'_1}{p_1}$



$$\eta_c = \frac{T_{1s} - T_1}{T'_1 - T_1} = \frac{T_{1s}/T_1 - 1}{T'_1/T_1 - 1}$$

$$\Rightarrow \frac{T'_1}{T_1} = 1 + \frac{\left(T_{1s}/T_1 - 1\right)}{\eta_c}$$

for isentropic compression: $\frac{T_{1s}}{T_1} = \left(\frac{p'_1}{p_1}\right)^{\frac{\gamma-1}{\gamma}} = r_c^{\left(\frac{\gamma-1}{\gamma}\right)}$

$$\text{So, } \frac{T'_1}{T_1} = 1 + \frac{r_c^{\left(\frac{\gamma-1}{\gamma}\right)} - 1}{\eta_c}$$

$$= (1 + f) \quad \text{where } f \equiv \frac{r_c^{\frac{\gamma-1}{\gamma}} - 1}{\eta_c}$$

$$\therefore \quad \frac{\rho_1'}{\rho_1} = \frac{p_1'}{p_1}\,\frac{T_1}{T_1'}$$

$$= \frac{r_c}{(1+f)} = \frac{\dot{m}'}{\dot{m}} \qquad \text{—— (2)}$$

also $$w_c = \frac{c_p(T_{1s} - T_1)}{\eta_c} = \frac{c_p T_1}{\eta_c}\left(\frac{T_{1s}}{T_1} - 1\right)$$

$$= c_p T_1 \, \frac{\left(r_c^{\frac{\gamma-1}{\gamma}} - 1\right)}{\eta_c} = c_p T_1 \, f$$

$$\therefore \quad \frac{w_c}{w} = \frac{c_p T_1}{\eta q^*}\, f = b f \qquad \text{—— (3)}$$

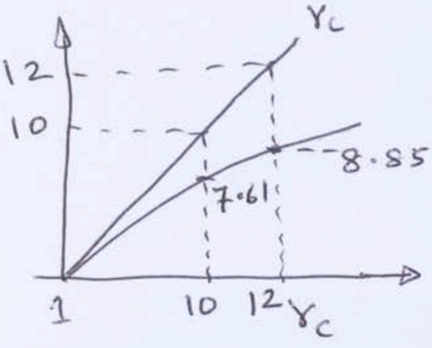
Hence $$\frac{\dot{W}_{net}'}{\dot{W}} = \frac{\dot{m}'}{\dot{m}}\left(1 - \frac{w_c}{w}\right)$$ from (1)

$$\Rightarrow \quad \boxed{\frac{\dot{W}_{net}'}{\dot{W}} = r_c\left(\frac{1 - bf}{1+f}\right)}$$ after using (2) & (3)

as required.

(ii) Putting $b = 0.1$, $\eta_c = 0.7$ $\gamma = 1.4$ in the above equation gives

$$\frac{\dot{W}_{net}'}{\dot{W}} = r_c\left(\frac{8 - r_c^{0.29}}{6 + r_c^{0.29}}\right) \Rightarrow$$



(c) $$\eta' = \frac{\dot{W}'_{net}}{\dot{m}'_f Q} = \frac{\dot{m}' w' - \dot{m}'_a w_c}{\dot{m}'_f Q}$$

$$= \frac{\eta q^*}{q^*} - \underbrace{\frac{\dot{m}'_a}{\dot{m}'}}_{\approx 1 \text{ since } \dot{m}'_f \ll \dot{m}'_a}\left(\frac{\dot{m}'}{\dot{m}'_f Q}\right) w_c$$

$$\Rightarrow \quad \eta' = \eta - \frac{c_p T_1 f}{q^*}$$ since $w_c = c_p T_1 f$
See Eq. 3

Hence $$\boxed{\eta' = \eta - \frac{c_p T_1}{q^*} \frac{\left(r_c^{\frac{\gamma-1}{\gamma}} - 1\right)}{\eta_c}}$$ as required

(d) The supercharger is used to provide additional power when required, despite a compromise on the overall efficiency.