4A13 - Combustion & Engines

Cribs - 2025 .

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 $\frac{d[A^*]}{dt} = 0$

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

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

25%

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

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

For the low pressure limit

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

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

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

25%

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

$\phi = 2$; $P = 5$ 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. $\Rightarrow \underline{\underline{c = b.}}$

4th eqn. comes from K_p 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.

50%

(a) (i) First order (unimolecular) reactions

$$A \rightarrow b_1P_1 + b_2P_2 + \cdots$$

(ii) Second order or bimolecular reactions

$$R_1 + R_2 \rightarrow b_1P_1 + b_2P_2 + \cdots$$

(iii) Third order or trimolecular reactions

$$R_1 + R_2 + R_3 \rightarrow b_1P_1 + b_2P_2 + \cdots$$

5%

(b) Chain reactions are classified as follows.

(i) Chain initiation - forms an unstable/excited molecule or atom

$$H_2 + O_2 \rightarrow 2OH$$

$$H_2 + M \rightarrow H + H + M$$

(ii) Chain Propagation: number of unstable/excited species remain constant

$$OH + H_2 \rightarrow H_2O + H; \quad CO + OH \rightarrow CO_2 + H$$

(iii) Chain branching: number of unstable/excited species increases

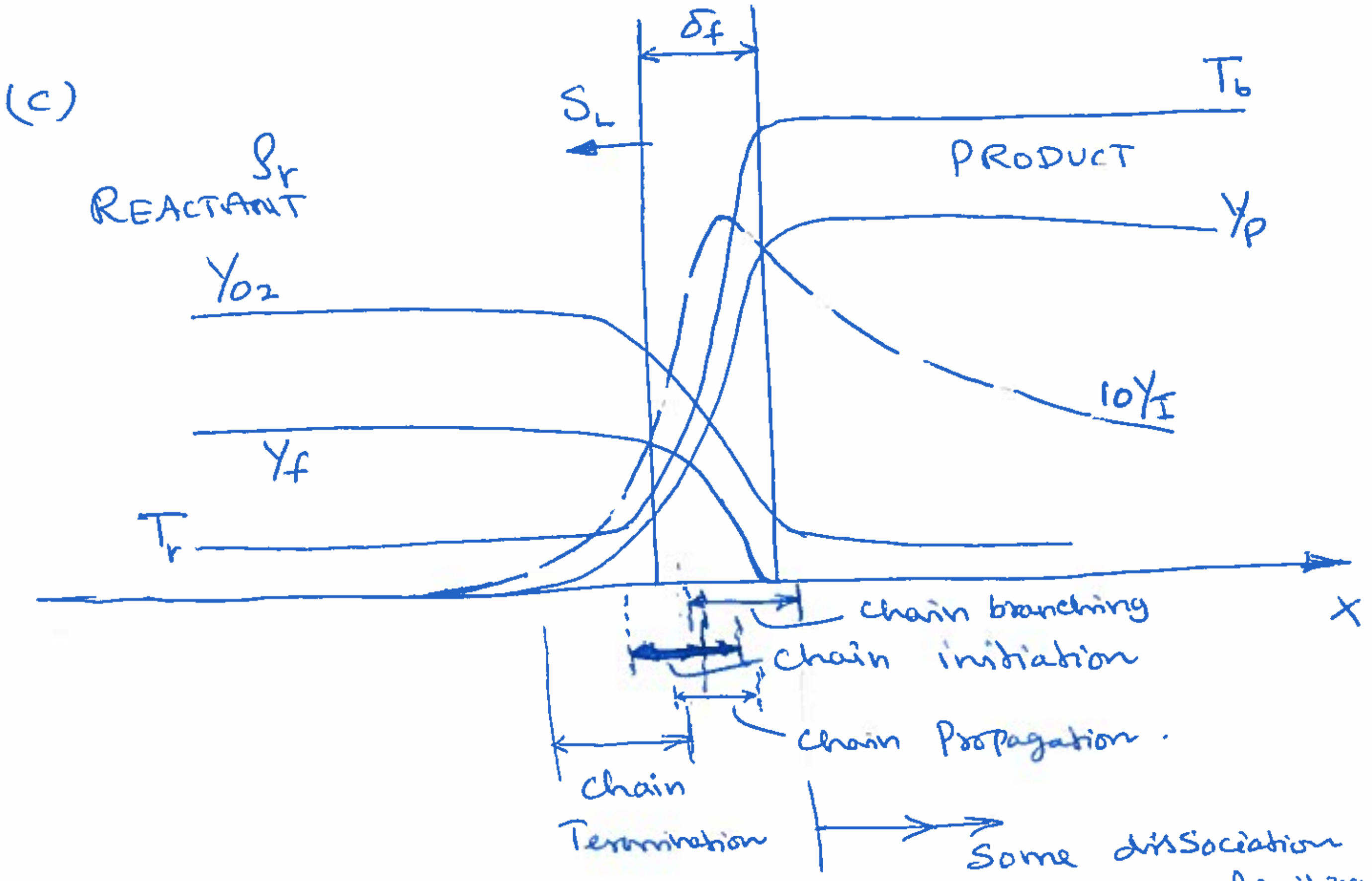
$$H + O_2 \rightarrow OH + O; \quad CH + O_2 \rightarrow CHO + O$$

(iv) Chain termination: number of unstable species produced is zero. This reaction consumes unstable/excited species

$H + H + M \rightarrow H_2 + M$; $H + OH + M \rightarrow H_2O + M$

10%

(c)



Chain initiation!
attacks fuel molecule

Chain propagation & branching: have high T_a

⇒ They occur is high T regions.

Chain termination: - usually have low T_a or $E_a \approx 0$, ~~⇒~~ but will involve radicals & intermediate species. Thus these reactions occur in the upstream edge (side) of the flame as shown above.

20%

(d) Balancing the convective heat flux across the flame and the reactive heat flux

$$\lambda \frac{(T_b - T_r)}{\delta_f} \approx \dot{\omega} H \delta_f$$

H - heat of combustion $= c_p (T_b - T_r)$

$$\Rightarrow \boxed{\delta_f \approx \left(\frac{\lambda}{c_p \dot{\omega}}\right)^{1/2}}$$

Reactive mass flux $\approx$ Convective mass flux into the flame

$$\dot{\omega} \delta_f \approx \rho_r S_l$$

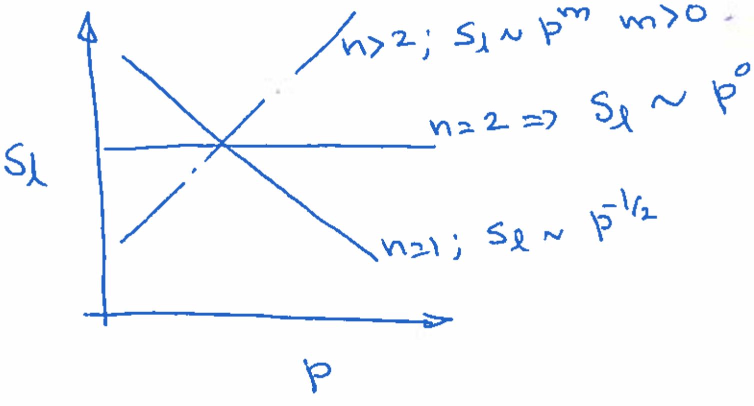
$$\Rightarrow S_l \approx \frac{1}{\rho_r} \sqrt{\frac{\dot{\omega} \lambda}{c_p}} \Rightarrow \boxed{S_l \approx \sqrt{\frac{\lambda \dot{\omega}}{\rho_r^2 c_p}}}$$

25%

(e) $$\dot{\omega} = p^n Y_r A_f \exp\left(-\frac{T_a}{T_f}\right)$$

$$\rho_r = \frac{p}{R T_r}$$

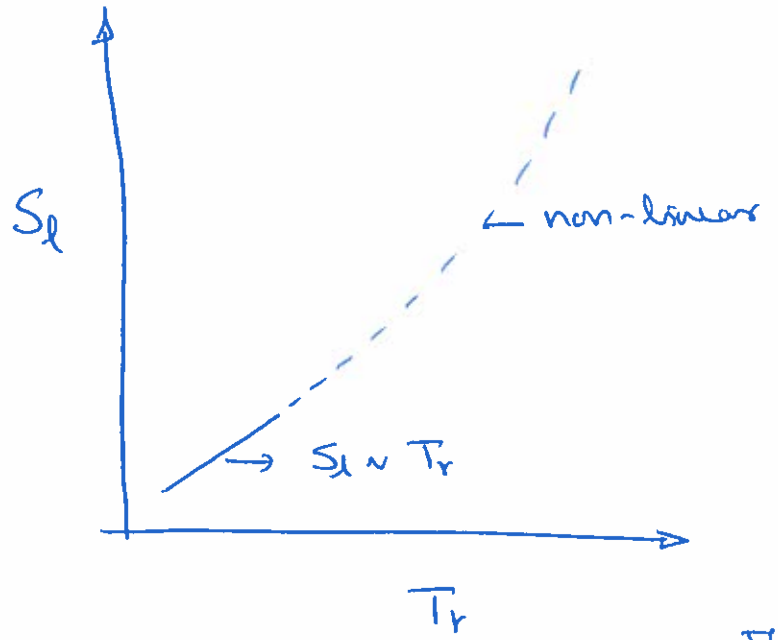
$$\Rightarrow S_l = \sqrt{\frac{\lambda}{c_p} A_f Y_r R^2} \; T_r \; p^{\frac{n-2}{2}} \exp\left(-\frac{T_a}{2T_f}\right)$$



p dependence of S_l depends on the overall order of the reaction.

experiments shows that $S \sim p^{-1/2}$ typically, for bimolecular reactions.

at high p $S_l \sim p^m$. $m>0$.



As $T_r \uparrow$ $T_b \uparrow$

for small T_r the increase in T_b is small and thus the linear term will dominate.

For large increase in T_r the exponential term dominates.

These behaviours are supported well by experimental observations.

$$\phi = \frac{(Y_f/Y_{air})_{act}}{(Y_f/Y_{air})_{stoi}} \qquad (Y_f = Y_r)$$

$\Rightarrow$ as $\phi \uparrow$ $Y_f \uparrow$ $\Rightarrow$ $S_l \uparrow$ because $S_l \sim \sqrt{Y_f}$

as per the above equation, only if every other quantities remain constant.

But $T_b \uparrow$ as $Y_f \uparrow$ (or $\phi \uparrow$). So, the behaviour of S_l with ϕ is the compound effects of Y_f, T_b, and A_f in the equation written above. Thus, the general behaviour of S_l with ϕ is that S_l increases with ϕ. Since the above reaction rate expression is valid for lean mixture, the variation of S_l with ϕ for $\phi > 1$ isn't represented.

40%

⑬

(a) (i) $\dot{Q} = 15\,kW$, $\dot{m}_a / \dot{m}_f = 100$, $Q_{LCV} = 120\ MJ/kg$, $\rho_{H_2} = 0.082\,kg/m$

$\rho_a = 1.17\ kg/m^3$, $d = 1\,mm$

$$\dot{m}_{H_2} = \frac{\dot{Q}}{Q_{LCV}} = \frac{15}{120 \times 10^3} = 1.25 \times 10^{-4}\ kg/s$$

5 nozzles and 2 fuel ports in each

$$\therefore\ \dot{m}_j = \frac{\dot{m}_{H_2}}{10} = 1.25 \times 10^{-5}\ kg/s$$

$$U_j = \frac{\dot{m}_j}{\rho_{H_2} A_j} = \frac{1.25 \times 10^{-5}}{0.082 \times \pi \left(\frac{0.001^2}{4}\right)} = 194.091\ m/s$$

$$\dot{m}_a = \dot{m}_{H_2} \times 100 = 1.25 \times 10^{-2}\ kg/s$$

$$\therefore\ \dot{m}_{cf} = \frac{\dot{m}_a}{5} = 2.5 \times 10^{-3}\ kg/s$$

$$U_{cf} = \frac{\dot{m}_{cf}}{\rho_a A_{cf}} = \frac{2.5 \times 10^{-3}}{1.17 \times \pi \left(\frac{0.0075^2}{4}\right)} = 48.366\ m/s$$

$$J = \frac{\rho_j U_j^2}{\rho_{cf} U_{cf}^2} = \frac{0.082 \times 194.091^2}{1.17 \times 48.366^2} = 1.1289$$

$$\frac{y}{J^{1/2} d} = 1.6 \left(\frac{x}{J^{1/2} d}\right)^{1/3} \Rightarrow y = (1.1289)^{1/2} \times 0.001 \times 1.6 \times \left(\frac{7.5 d}{(1.1289)^{1/2} d}\right)^{1/3}$$

$$y = 3.261 \times 10^{-3} \simeq 3.26\ mm$$

25%

(ii) $\rho_{NH_3} = 0.69\ kg/m^3$, $Q_{LCV} = 18.6\ MJ/kg$, $\dot{m}_a / \dot{m}_f = 7.5$

$$\dot{m}_{NH_3} = \frac{\dot{Q}}{Q_{LCV}} = \frac{15}{18.6 \times 10^3} = 8.0645 \times 10^{-4}\ kg/s \Rightarrow \dot{m}_j = 8.0645 \times 10^{-5}\ kg/s$$

$$U_j = \frac{\dot{m}_j}{\rho_{NH_3} A_j} = \frac{8.0645\times10^{-5}}{0.69\times\pi\left(\frac{0.001^2}{4}\right)} = 148.812 \text{ m/s}$$

$$\dot{m}_a = 7.5\times\dot{m}_{NH_3} = 6.048\times10^{-3} \Rightarrow \dot{m}_{cf} = 1.2097\times10^{-3} \text{ kg/s}$$

$$U_{cf} = \frac{\dot{m}_{cf}}{\rho_a A_{cf}} = \frac{1.2097\times10^{-3}}{1.17\times\pi\left(\frac{0.0075^2}{4}\right)} = 23.403 \text{ m/s}$$

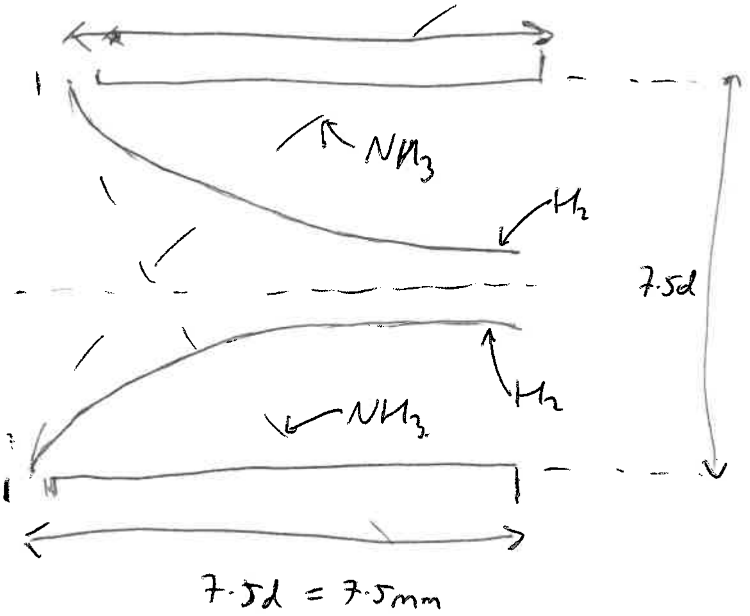
$$J = \frac{\rho_j U_j^2}{\rho_{cf} U_{cf}^2} = \frac{0.69\times148.812^2}{1.17\times23.403^2} = 23.845$$

$$\Rightarrow y = (23.845)^{1/2}\times0.001\times1.6\times\left(\frac{7.5\cancel{d}}{(23.845)^{1/2}\cancel{d}}\right)^{1/3}$$

$$y = 9.0145\times10^{-3} \approx 9.01 \text{ mm}$$

25%

(iii) The jet trajectories do not intersect with H_2, but they do with NH_3. This is due to the higher momentum flux ratio of NH_3.



Since the fuel jets interact with NH_3, mixing will be enhanced and more premixed mixture enters the chamber.

To prevent this, more holes or increased hole diameter can reduce the momentum flux ratio.

When using H_2, we want to avoid having a more premixed mixture as flashback can occur due to higher flame speed. Insufficient mixing can cause hotspots and enhanced NO_x formation. The tests demonstrate it is challenging to use the same geometry when using different fuels.

20%

(b) The Damkohler number is

$$Da = \frac{\text{physical or flow time scale}, \tau_f}{\text{chemical time scale}, \tau_c} = \frac{L/U_b}{\delta_L/S_L}$$

τ_c can also be ν/S_L^2.

τ_f uses a length scale based on the combustor length (L). The bulk velocity represent the velocity at the exit of the nozzle. (U_b)

δ_L is the laminar flame thickness and S_L is the laminar flame speed.

For stability, $Da > Da_{cr}$ (critical value) for a flame to exist.

S_L for H_2 is more than an order of magnitude higher than for NH_3. Also, δ_L is smaller for H_2. Chemical time scales are therefore much smaller for H_2, which causes the Da number to increase. Higher values of U_b are possible for H_2.

$$\frac{Da_{,H_2}}{Da_{,NH_3}} = C = \frac{L/U_{b,H_2}}{L/U_{b,NH_3}} \times \frac{\tau_{c,NH_3}}{\tau_{c,H_2}} = \frac{U_{b,NH_3}\,\tau_{c,NH_3}}{U_{b,H_2}\,\tau_{c,H_2}}$$

For crude estimate, take $U_b \approx U_4$. (from part (a))

$$\Rightarrow \frac{\tau_{c,NH_3}}{\tau_{c,H_2}} = C\,\frac{U_{b,H_2}}{U_{b,NH_3}} = 2.067\,C.$$

30%

We expect $\tau_{c,NH_3}/\tau_{c,H_2} > U_{b,H_2}/U_{b,NH_3}$ (possibly more than an order of magnitude) and therefore $C > 1$. Using different fuels leads to challenges with scaling Da, since the Reynolds number should be considered.

④

(a) Diesel engines have higher compression ratios and therefore a higher efficiency.

They compress mostly air, rather than a fuel-air mixture in SI engines, during the compression stroke, which brings the cycle nearer to the ideal cycle.

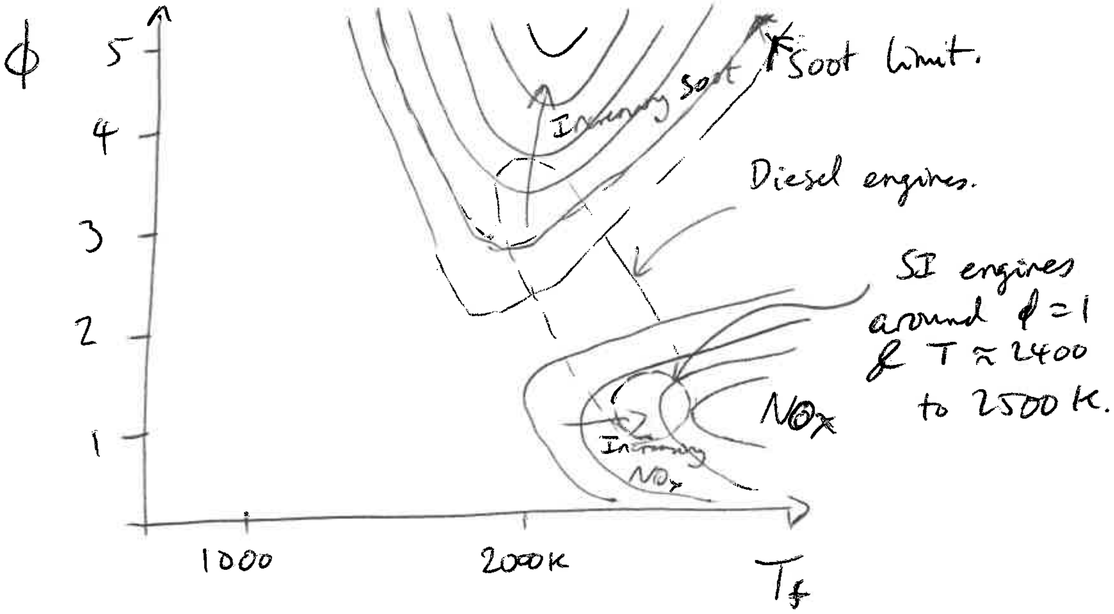
Diesel engines can run at part load by reducing the amount of fuel injected rather than through throttling. Therefore, the losses due to throttling at part loads are eliminated.

For SI engines, combustion is initiated by a spark at top dead centre, where the fuel-air mixture have already been mixed. Therefore, the fuel must be resistant to autoignition.

For diesel engines, the fuel must be easy to ignite as there is no spark and the fuel is injected, when the air has been compressed, close to top dead centre.

25%

(b)



Main features: (1) Soot level increases as ϕ increases at around 2000K.

(2) NOx level increases with ϕ around 1 and lean mixtures. It starts to form from around 1800K, but increases with T. Also forms with longer residence times.

25%

(c)(i) Intake: The valves and port orientation influence the direction of the inlet flow. The major patterns of bulk motion are swirl and tumble, which have high levels of turbulence. For swirl, the vortex is aligned with the cylinder axis and for tumble, the vortex is normal to the cylinder axis.

Compression: From start to the end of the stroke (BDC to TDC), the swirl vortex will survive compression and the tumble vortex produces turbulence close to TDC. A piston with a bowl can also produce 'squish' during compression close to TDC, as mass is displaced into the piston bowl. The bowl controls how swirl and tumble evolve during the compression stroke. The bowl can also augment swirl as the radius decreases.

Power: The level of turbulence intensity u' influences the speed of flame propagation from the ignition kernel. In general, turbulence aids flame propagation and a characteristic speed of propagation, the turbulent flame speed S_T, increases with turbulence intensity ($S_T \propto u'$). During the power stroke, the overall effect of combustion causes the turbulence to decay towards BDC.

Exhaust: Hot products leave the cylinder when the valve opens. The valve timing affects trapped exhaust products (internal EGR) and the pressure difference across the valve. The flow velocity across the valve must not be close to choked flow to reduce losses.

40%

(ii) The piston shape and valve placement vary significantly depending on the application (eg. small diesel engines vs. large marine engines).

For small diesel engines, 'squish' augments swirl and helps mix fuel spray with air.

For large diesel engines, the flow and turbulence are relatively mild to maximise volumetric efficiency. Too much swirl will increase heat losses to the walls and cause the volumetric efficiency to decrease.

10%