

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



(ii) Second order or bimolecular reactions



(iii) Third order or trimolecular reactions



(b) Chain reactions are classified as follows.

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



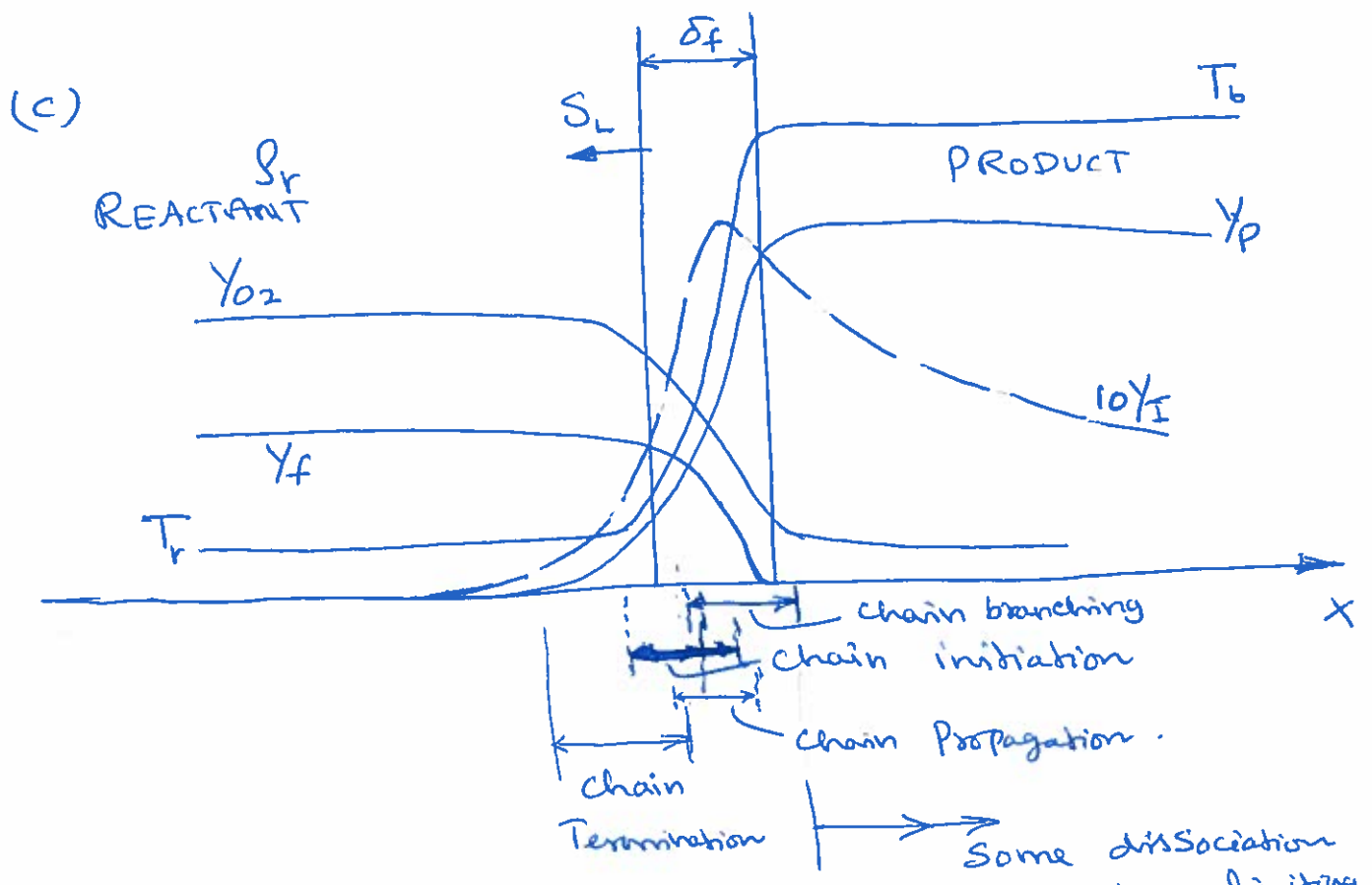
(ii) chain Propagation: number of unstable/excited species remain constant



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



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



Some dissociation reaction limiting the maximum temperature.

Chain initiation: attacks fuel molecule

Chain Propagation & branching: have high T_a
 \Rightarrow They occur in 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.

(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
= $c_p (T_b - T_r)$

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

Reactive mass flux \approx Convective mass flux into the flame

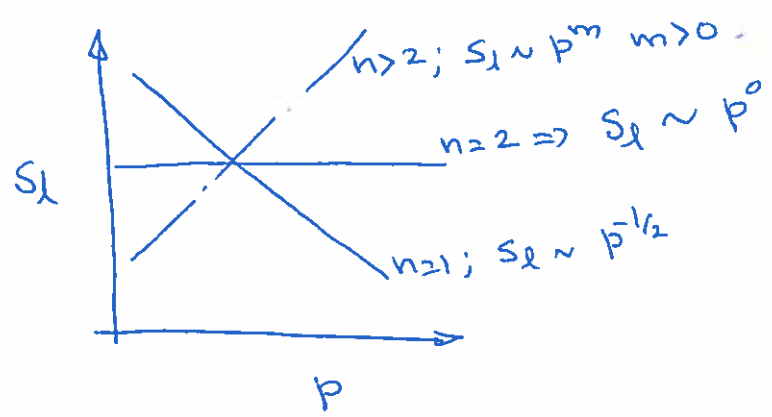
$$\dot{\omega} \delta_f \approx \rho_r S_L$$

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

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

$$\rho_r = \frac{p}{RT_r}$$

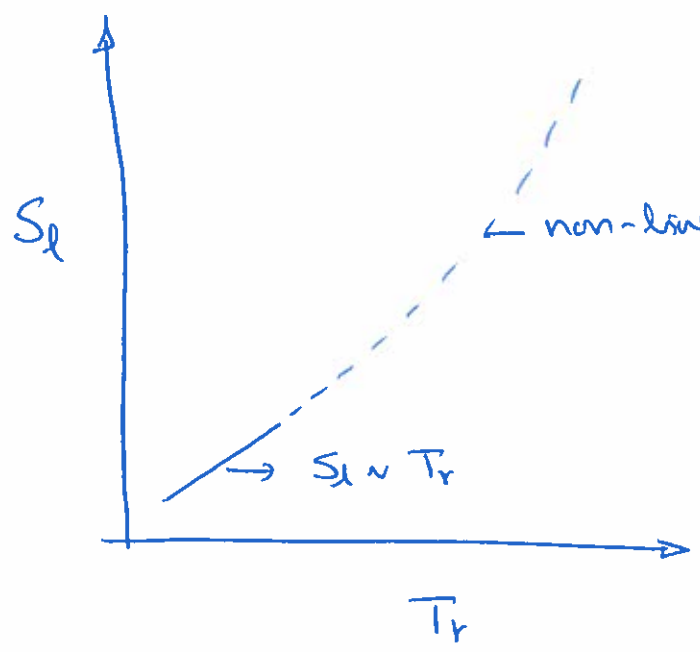
$$\Rightarrow S_L = \sqrt{\frac{\lambda}{c_p} A_f Y_r R^2} T_r p^{\frac{n-2}{2}} \exp\left(-\frac{T_a}{2T_f}\right)$$



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

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

at high p $S_L \sim p^m$ bimolecular reactions. $m > 0$.



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.

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

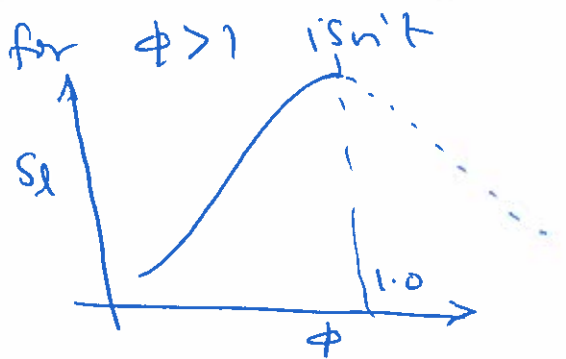
\Rightarrow as $\phi \uparrow$ $Y_f \uparrow \Rightarrow S_L \uparrow$ because $S_L \sim \sqrt{Y_f}$

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

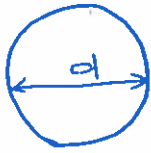
But $T_b \uparrow$ as $Y_f \uparrow$ (or $\phi \uparrow$). So, the behaviour of S_L with ϕ is the compound effects of

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 small for lean mixture, the variation of S_L with ϕ for $\phi > 1$ isn't represented.



2)



$N_2, 1 \text{ bar}$
 $T_a = 700 \text{ K}$

$\Rightarrow Y_{f, \infty} = 0$

(a) $-\frac{dm_e}{dt} = A \dot{m}''$

$m_e = \frac{4}{3} \pi \left(\frac{d}{2}\right)^3 \rho_l = \frac{\pi}{6} d^3 \rho_l$

$A = \pi d^2$

$\frac{\pi}{6} d^3 \rho_l \frac{dd}{dt} = - \pi d^2 \frac{\beta}{4d}$

$\Rightarrow 2d \frac{dd}{dt} = -\beta \Rightarrow \boxed{d^2 = d_0^2 - \beta t}$

(b) $d = 0$ when the droplet is fully evaporated.

$\Rightarrow t_v = \frac{d_0^2}{\beta} = \frac{\rho_l d_0^2}{8 \rho D \ln\left(\frac{1 - Y_{f, \infty}}{1 - Y_{f, 0}}\right)}$

$\therefore Y_{f, \infty} = 0 \Rightarrow \boxed{t_v = \frac{\rho_l d_0^2}{8 \rho D \ln\left(\frac{1}{1 - Y_{f, 0}}\right)}}$

(c) $\dot{q}'' = 2 \lambda \frac{(T_a - T_s)}{d}$

energy flux at the surface: heat conduction = ^{evapo.} heat flux.

$A \dot{q}'' = A \dot{m}'' h_{fg} \Rightarrow \dot{q}'' = \dot{m}'' h_{fg}$

$2 \lambda \frac{(T_a - T_s)}{d} = \frac{\rho_l \beta}{4d} h_{fg}$

$$\Rightarrow \beta = \frac{\rho \lambda (T_a - T_s)}{\rho_l h_{fg}} = \frac{8 \rho D}{\rho_l} \ln \left(\frac{1}{1 - Y_{f,0}} \right) \quad (6)$$

$$\Rightarrow \ln \left(\frac{1}{1 - Y_{f,0}} \right) = \frac{\lambda (T_a - T_s)}{\rho D h_{fg}}$$

$$Le = \frac{\alpha}{D} = \frac{\lambda}{\rho c_p D} = 1 \Rightarrow \frac{\lambda}{\rho D} = c_p$$

$$\therefore \ln \left(\frac{1}{1 - Y_{f,0}} \right) = c_p \frac{(T_a - T_s)}{h_{fg}}$$

$$\Rightarrow \boxed{Y_{f,0} = 1 - \exp \left[-c_p \frac{(T_a - T_s)}{h_{fg}} \right]} \text{ as required.}$$

(d) $\rho_l = 750 \text{ kg/m}^3$ $c_p = 1.075 \text{ kJ/kg-K}$

$D = 1.78 \times 10^{-5} \text{ m}^2/\text{s}$ $h_{fg} = 256 \text{ kJ/kg}$ $T_s = 490 \text{ K}$

$d_0 = 20 \times 10^{-6} \text{ m}$

$$Y_{f,0} = 1 - \exp \left[-\frac{1.075}{256} \times (700 - 490) \right] = 0.58598$$

$$\ln \left(\frac{1}{1 - Y_{f,0}} \right) = 0.8818$$

$$\therefore t_v = \frac{750 \times (20 \times 10^{-6})^2}{8 \times 1.78 \times 10^{-5} \times 8 \times 0.8818} = \frac{2.389 \times 10^{-4}}{8} \text{ s}$$

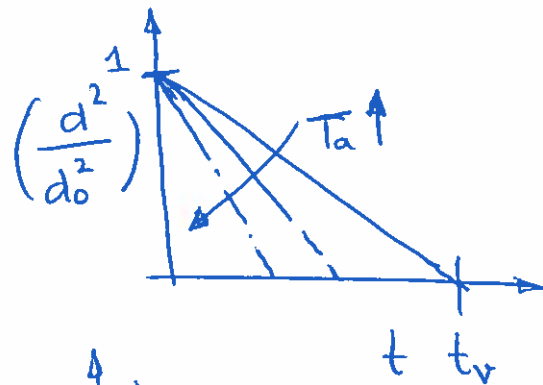
$\rho \approx$ density of N_2 @ 1 bar & 700 K

$$\rho = \frac{1 \times 10^5 \times 28}{8.314 \times 10^3 \times 700} = 0.481 \text{ kg/m}^3$$

$\therefore t_v = 4.967 \times 10^{-3} \text{ s} \approx \underline{\underline{5 \text{ ms}}}$

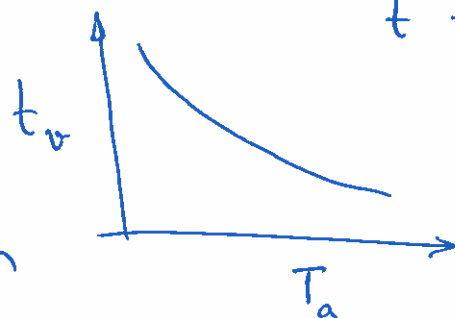
if $T_a \uparrow \quad Y_{f,0} \uparrow \Rightarrow t_v \downarrow$

$d_0 \downarrow \quad t_v \downarrow$



with Pressure!

As $p \uparrow \quad \rho \uparrow \Rightarrow t_v \downarrow$
if everything else remain const.



But T_s depends on p , also h_{fg} decreases with p increasing.
(Saturation temperature or boiling point)

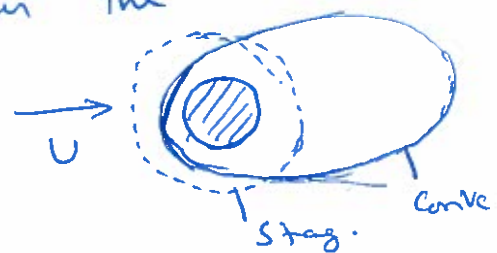
Thus, the effect of ~~changing~~ changing p on t_v is highly non-linear, but t_v generally decreases as $p \uparrow$

(e) If there is convective flow then the heat flux at the droplet surface is through convective mechanism

$\& \text{ thus } \dot{q}'' = h(T_a - T_s)$

h - comes from Nusselt Correlations. $\& t_v \downarrow$ in convective flow.

The rest of the analysis remains the same.



$Y_f = \text{const.}$
iso-surface.

4A13 Final Exam - Crib

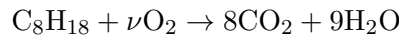
Q3. Residual and EGR

(a) Constant volume combustion [25%]

$$\begin{aligned}
 x_r &= \frac{m_r}{m} = \frac{m_r}{m_a + m_f + m_r} \\
 m c_v \Delta T &= m_f Q \\
 \frac{m}{m_a} c_v \Delta T &= \frac{m_f}{m_a} Q \\
 \frac{m}{m_a} &= 1 + \frac{1}{AFR} + \frac{m_r}{m_a} = 1 + \frac{1}{AFR} + \frac{m_r}{m} \frac{m}{m_a} \\
 \frac{m}{m_a} (1 - x_r) &= 1 + \frac{1}{AFR} \\
 \frac{m}{m_a} &= \left(1 + \frac{1}{AFR}\right) \left(\frac{1}{1 - x_r}\right) \\
 \left(1 + \frac{1}{AFR}\right) \left(\frac{1}{1 - x_r}\right) c_v \Delta T &= \frac{1}{AFR} Q \\
 \frac{c_v \Delta T}{Q} &= \frac{1 - x_r}{1 + AFR}
 \end{aligned}$$

(b) [30%]

Iso-octane C_8H_{18}



$$W_i = 8 \times 12 + 18 = 114 \text{ g/mol}$$

$$W_a = 29 \text{ g/mol}$$

$$\nu = 8 + 18/4 = 12.5$$

$$AFR_s = \frac{\nu}{0.21} \frac{W_a}{W_i} = \frac{12.5}{0.21} \frac{29}{117} = 15.1$$

$$\Delta T_A = \frac{Q}{c_v} \frac{1 - x_r}{1 + AFR} = \frac{51 \times 10^6 \text{ J/kg}}{1500 \text{ J/kgK}} \frac{1 - 0.1}{1 + 15.1} = 1900K$$

This is an upper estimate, considering that (i) dissociation would lower the temperature, and (ii) the c_v of the burned gases is higher than that of the fresh mixture.

Assuming adiabatic compression:

$$T_2 = r^{\gamma-1} T_1 = 9^{0.4} \times 300K = 722K$$

$$T_3 = 2622 \text{ K}$$

(c) [25%] Case B:

The addition of EGR changes primarily the residual fraction in the mixture. Assuming that no other factors are changed, we have :

$$\frac{\Delta T_B}{\Delta T_A} = \frac{1 - x_{r,B}}{1 - x_{r,A}} = \frac{1 - 0.3}{1 - 0.1} = 0.77$$

$$\text{imep} = \eta m_f Q = \eta \frac{m_f}{m_a} Q \frac{m_a}{m} = \eta Q m \frac{1 - x_r}{1 + AFR}$$

Assuming that the thermal conversion efficiency, volumetric efficiency, initial density and AFR are unaffected between cases A and B, we have:

$$\frac{\text{imep}_B}{\text{imep}_A} = \frac{1 - x_{r,B}}{1 - x_{r,A}} = 0.77$$

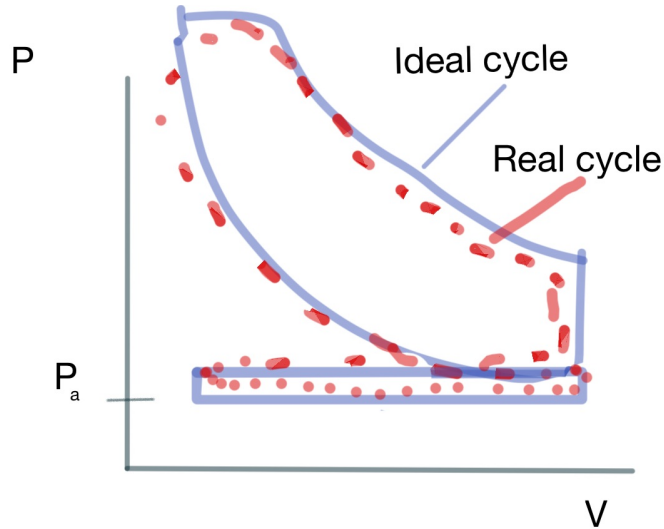
However, EGR can change volumetric efficiency, initial density and combustion timing, which may have an effect on the overall work rate.

(d) [10%] The same power and imep can be restored by supercharging or turbocharging the mixture.

(e) [10%] EGR lowers the peak temperature by virtue of mixture dilution, as well as the higher specific heat capacity of the residual gases. This leads to a drastic reduction in nitric oxides which are formed at high temperatures. EGR can also increase efficiency by aiding load control without pumping losses, even if the indicated work may be lower due to the lower specific heat ratio of the resulting burned mixture. Excessive EGR beyond 30% causes misfires and higher carbon monoxide and hydrocarbon emissions.

(a) [20%]

The ideal cycle assumes adiabatic compression and expansion, instantaneous heat addition at constant volume or pressure, and instantaneous lossless gas exchanges. The real cycle is subject to heat losses, finite rate of heat release over a range of crankangles, pressures and volumes, and finite time and lossy flow exchange processes.



(b) [20%]

Solving for the cycle:

$$T_2 = T_1 r^{\gamma-1}$$

Energy conservation constant volume 2-3a:

$$Q_{23a} = U_{3a} - U_2 = mc_v(T_{3a} - T_2) = \beta \frac{Q}{m}$$

$$\frac{T_{3a}}{T_1} - \frac{T_2}{T_1} = \beta \frac{Q}{mc_v T_1} = \beta q$$

Energy conservation constant pressure 3a-3b:

$$Q_{23a} = U_{3b} - U_{3a} + W_{3a3b} = m[c_v(T_{3b} - T_{3a}) + p_3(V_{3b} - V_{3a})]$$

$$= c_p(T_{3b} - T_{3a}) = (1 - \beta) \frac{Q}{m}$$

$$(T_{3b} - T_{3a}) = (1 - \beta) \frac{Q}{mc_p T_1}$$

$$\frac{T_{3a}}{T_1} \left(\frac{T_{3b}}{T_{3a}} - 1 \right) = \frac{1 - \beta}{\gamma} q$$

$$\frac{T_{3a}}{T_1} (\alpha r - 1) = \frac{1 - \beta}{\gamma} q$$

But

$$\frac{T_{3a}}{T_1} = \beta q + r^{\gamma-1}$$

So that

$$(\beta q + r^{\gamma-1})(\alpha r - 1) = \frac{1 - \beta}{\gamma} q$$

Solving for α , we have:

$$\alpha = \left[\frac{1 - \beta}{\gamma} \frac{q}{\beta q + r^{\gamma-1} + 1} \frac{1}{r} \right]$$

Q.E.D.

(c) [20%]

$$W_g = \oint \delta W = - \oint \delta Q = Q_{2-3a} + Q_{3a-3bQ} + Q_{41} = Q + mc_v(T_4 - T_1)$$

Find T_4 :

$$\begin{aligned} \frac{T_4}{T_1} &= \frac{T_4}{T_{3b}} \frac{T_{3b}}{T_{3a}} \frac{T_{3a}}{T_1} = \left(\frac{v_4}{v_{3b}} \right)^{-(\gamma-1)} (\alpha r) \frac{T_{3a}}{T_1} \\ \frac{v_4}{v_{3b}} &= \frac{v_4}{v_1} \frac{v_1}{v_{3b}} = \frac{r}{\alpha r} = \frac{1}{\alpha} \\ \frac{T_4}{T_1} &= \alpha^{\gamma-1} (\alpha r) (\beta q + r^{\gamma-1}) \end{aligned}$$

$$\begin{aligned} \frac{W_g}{mc_v T_1} &= q - c_v \frac{T_4 - T_1}{c_v T_1} = q - \left(\frac{T_4}{T_1} - 1 \right) \\ &= q - \alpha^{\gamma} r (\beta q + r^{\gamma-1}) + 1 \\ w &= 1 + q - \beta q \alpha^{\gamma} r - (\alpha r)^{\gamma} \end{aligned}$$

(d) [20%]

Real cycles:

- heat and dissipation losses during compression and expansion: polytropic compression
- rate of combustion governed by finite rate of mixing and heat release: autoignition, followed by mixing controlled combustion – this means that the constant volume and constant pressure are only approximations to the real rate of heat release
- intake/exhaust valve opening process and gas exchange is not instantaneous, and depend on the pressure ratios between manifold and cylinder
- real gas effects: mixture properties are not constant, and depend on the amount of residual, temperature, and equivalence ratio via the specific heats of the real species

The limits to compression ratio in compression-ignition engines are set by a combination of noise and vibration, mechanical constraints, as well as achievable maximum efficiencies relatively to emissions control: maximum pressures lead to higher temperatures and higher NO_x.

(e) [20%]

- Turbocharging is *necessary* in compression-ignition engines to control load, as the equivalence ratio cannot go beyond about 0.7 without incurring unacceptably particulate matter high emission. This is in contrast with spark-ignition engines, in which the load control is typically provided by a throttle, which is not present in compression-ignition engines.
- Intercooling increases the density of the incoming mixture downstream of the compressor, allowing higher loads to be reached.
- Both turbocharging and intercooling can also be used in spark ignition engines, but the additional cost and weight is not as favourable in lighter weight spark ignition engines, which can have simple throttle load control.