

Student name: Solutions

1. In the boom tube lab, we measured the laminar flame speed of methane. We are thinking about using the tube to measure the laminar flame speed of gasoline.
 - a. (25 points) Calculate the expected value of the laminar flame speed of a stoichiometric mixture of isooctane and air initially at 25°C and 1 atm. Assume that the ignition temperature is 370°C and the adiabatic flame temperature is 2002°C. Assume the thermal diffusivity (α) is 2.26E-4 m²/s.

$$S_L = \left\{ \frac{\alpha (T_p - T_{ig}) \bar{r}}{(T_{ig} - T_r) [Fuel]_i} \right\}^{1/2}$$



$$X_{C_8H_{18}} = \frac{1}{1 + 12.5 \cdot 4.76} = 0.0165 \quad X_{O_2} = \frac{12.5}{1 + 12.5 \cdot 4.76} = 0.2066$$

$$[Fuel]_i = \frac{P x_i}{R T_i} = \frac{(101.3 \text{ kPa} \cdot 1000 \text{ Pa/kPa}) (0.0165)}{(8.314 \text{ m}^3 \text{ Pa/mol-K}) (298 \text{ K})} = 0.6758 \frac{\text{mol}}{\text{m}^3} = 6.76 \times 10^{-7} \frac{\text{mol}}{\text{cc}}$$

$$[O_2]_i = \frac{P x_i}{R T_i} = \frac{(101.3 \text{ kPa} \cdot 1000 \text{ Pa/kPa}) (0.2066)}{(8.314 \text{ m}^3 \text{ Pa/mol-K}) (298 \text{ K})} = 8.45 \frac{\text{mol}}{\text{m}^3} = 8.45 \times 10^{-6} \frac{\text{mol}}{\text{cc}}$$

$$\bar{r} = A_0 \exp\left(\frac{-E_a}{R T_{ave}}\right) \left(\frac{[Fuel]_i}{2}\right)^a \left(\frac{[O_2]_i}{2}\right)^b \quad T_{ave} = \frac{(2002 + 370)}{2} = 1186^\circ\text{C} = 1459 \text{ K}$$

$$A_0 = 4.6 \times 10^{11} \quad E_a/k = 15101 \text{ K} \quad a = 0.25 \quad b = 1.5$$

$$\bar{r} = 4.6 \times 10^{11} \cdot \exp\left(\frac{-15101 \text{ K}}{1459 \text{ K}}\right) \left(\frac{6.76 \times 10^{-7} \text{ mol/cc}}{2}\right)^{0.25} \left(\frac{8.45 \times 10^{-6} \text{ mol/cc}}{2}\right)^{1.5}$$

$$\bar{r} = 0.00308 \frac{\text{mol}}{\text{cc-s}} \cdot \frac{(100)^3 \text{ cm}^3}{\text{m}^3} = 3080.88 \frac{\text{mol}}{\text{m}^3 \text{ s}}$$

$$S_L = \left\{ \frac{2.26 \times 10^{-4} \text{ m}^2/\text{s} (2002 - 370) \text{ K} (3080.88 \text{ mol/m}^3 \text{ s})}{(370 - 25) \text{ K} \cdot 0.6758 \text{ mol/m}^3} \right\}^{1/2}$$

$$| S_L = 2.2 \text{ m/s} |$$

- b. (5 points) As you may recall, when operating the boom tube the flames occasionally propagate outside of the tube. If we want to stop this from occurring with a flame arrestor, what is the maximum mesh spacing we should choose?

mesh spacing = quench distance (d_0)

$$d_0 = 8 \frac{\alpha}{S_L}$$

$$\text{or } d_0 \approx \delta = S_L \cdot \frac{[\text{Fuel}]}{r}$$

$$d_0 = 8 \cdot \frac{2.26 \times 10^{-4} \text{ m}^2/\text{s}}{2.2 \text{ m/s}}$$

$$\text{or } d_0 = 2.2 \text{ m/s} \cdot \frac{6.76 \times 10^{-7} \text{ mol/cc}}{0.00308 \text{ mol/cc-s}}$$

$$d_0 = 8.72 \times 10^{-4} \text{ m} \\ \text{or } 0.82 \text{ mm}$$

$$d_0 = 4.83 \times 10^{-4} \text{ m} \\ \text{or } 0.48 \text{ mm}$$

- c. (5 points) Flame propagation in a gasoline engine occurs at an elevated pressure. To be able to experimentally measure the change in flame speed in such conditions, we are thinking about putting the boom tube in a pressure chamber so that we can vary the pressure. Is it worth it? For example, if we were to measure the flame speed in 10 atm, how big of a change would we see compared to 1 atm?

$$S_L \propto P^{\frac{(a+b)}{2} - 1}$$

for isooctane, $a = 0.25$
 $b = 1.5$

$$S_L \propto P^{\frac{(0.25+1.5)}{2} - 1}$$

$$S_L \propto P^{-0.125}$$

$$\frac{S_{L,1 \text{ atm}}}{S_{L,10 \text{ atm}}} \propto \left(\frac{1}{10}\right)^{-0.125}$$

$$\frac{S_{L,1 \text{ atm}}}{S_{L,10 \text{ atm}}} \propto 1.33$$

so it is a very small change.

$$S_{L,1 \text{ atm}} = S_{L,10 \text{ atm}} \cdot 1.33$$

$$S_{L,10 \text{ atm}} = 2.2 \text{ m/s} \cdot \frac{1}{1.33} = 1.65 \text{ m/s}$$

2. (15 points) The next generation of space vehicles to replace the Space Shuttle is being designed to operate with a sub-atmospheric pressure (about 0.5 atm) and an increased oxygen concentration (about 30%). How would the height of a jet-diffusion flame change, if it at all? Explain the individual effect of reduced pressure and increased oxygen concentration. Assume that the mass diffusivity (D) behaves like the thermal diffusivity (α).

Effect of pressure

if $D \sim \alpha = \frac{k}{\rho c}$ $\alpha \sim P^{-1}$ so $D \sim P^{-1}$

as the pressure \downarrow , D would \uparrow

$L_f \propto \frac{V_{jet} v_{jet}^2}{D}$ so if $D \uparrow$, $L_f \downarrow \Rightarrow$ if $P \downarrow$, $L_f \downarrow$

Effect of oxygen

physical argument:

Flame height \rightarrow "axial location where the surrounding fluid (air) reaches the centerline of the jet" pg. 5 \rightarrow Air reaches centerline by diffusion:

$m_k = -\rho D \frac{d\psi_k}{dx} \rightarrow$ diffusion is driven by the concentration gradient. As the $[O_2] \uparrow$, this gradient \uparrow , and diffusion \uparrow . the location where the fuel reaches the oxidizer would \therefore be at a lower height, $L_f \downarrow$

using correlation in book

$L_f = \frac{Q_{fuel} (T_{fuel}/T_f)}{4\pi D_{ox} \ln(1+1/s)} \left(\frac{T_{fuel}}{T_f} \right)^{0.67}$
 $S = \left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2} \right) \left(1 + \frac{X_{N_2}}{X_{O_2}} \right)$
 $\therefore \frac{0.9}{0.3} = 3.3$

so this term \downarrow but $\ln(1+1/s) \uparrow$

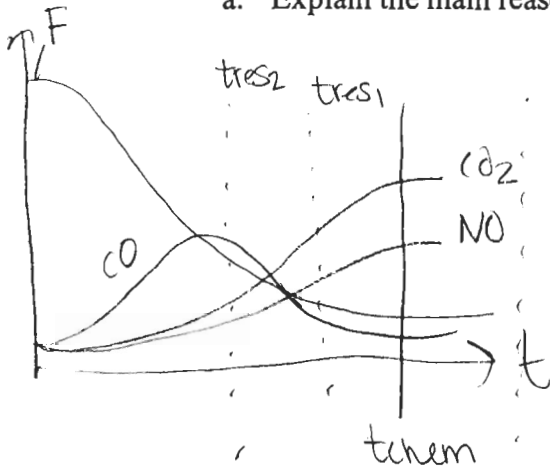
Also $T_f \uparrow$ as $[O_2] \uparrow$

Both terms in the denominator $\therefore L_f \downarrow$ as $[O_2] \uparrow$

or
 flame at $\phi = 1$. When $[O_2] \uparrow$, the fuel does not need to travel as far to find enough O_2 and $\therefore L_f \downarrow$.

3. (20 points) Measurements of the *exhaust* gases from an internal combustion engine show that increasing the engine speed RPM (by accelerating) beyond a certain value increases the concentration (emission) of CO but decreases the concentration of NO. These measurements are taken right at the exhaust port before catalyst.

a. Explain the main reason for the emission trend vs. RPM. (10 points)



As you \uparrow the RPM, the residence time \downarrow . As shown in the diagram, CO is formed early in the combustion process and NO is formed later. If you \uparrow the RPM to a high enough speed, your $t_{res} < t_{chem}$ and you'll end up at t_{res2} in the figure.

b. How would the emissions of pollutants change with RPM if the engine were cold? (5 points)

If the engine were cold, the $t_{chem} \uparrow$
 $t_{chem} = \frac{[F]}{\dot{r}}$ as $T \downarrow$, $\dot{r} \downarrow$ so $t_{chem} \uparrow$

The time scales on the above graph would be shortened so that the RPM where $t_{res} < t_{chem}$ would be lower and \therefore for a given RPM you'll be producing more CO and less NO than if it were warm.

Also, formation of NO is very temperature sensitive. As $T \downarrow$, $NO \downarrow$, so at a given RPM you'll produce less NO when the engine is cold (NO production takes time and temperature)

c. How would the emissions change if the air is enriched with oxygen? (5 points)

If the air is enriched with oxygen,

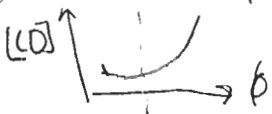
①
$$\dot{r} \uparrow : \dot{r} \propto [F]^a [O_2]^b \cdot \exp(-E_a/RT)$$
 if $[O_2] \uparrow$, $\dot{r} \uparrow$
 also if $[O_2] \uparrow$, $T_{ad} \uparrow$ so $\dot{r} \uparrow$
 $t_{chem} \propto \dot{r}^{-1}$ so if $\dot{r} \uparrow$, $t_{chem} \downarrow$

so you could go to a higher RPM before $t_{res} < t_{chem}$. so at a given RPM, you'll produce more NO and less CO.

②. Also, if $[O_2] \uparrow$, $T_{ad} \uparrow$ and because the production of NO is very temp sensitive, you'll produce more NO than if it were regular air.

(NO production takes time and temperature)

③ As $[O_2] \uparrow$, $\phi \downarrow$. More O_2 to oxidize $CO \rightarrow CO_2$
 For a given mass & oxidizer flow rate, $\phi \downarrow$ so $CO \downarrow$.



4. (30 points) You are given a new biofuel and need to figure out if it will cause your spark ignition engine to knock. At the beginning of the compression stroke, the stoichiometric fuel/air mixture is at 25°C and 1 atm. The mixture is then isentropically compressed with a volumetric compression ratio of 10. If the engine cooling system provides a convective heat transfer coefficient of 250 W/m²K, does the mixture autoignite? Assume that the surface area to volume ratio is 0.05 m⁻¹ and the engine coolant is at 97°C. The properties of the fuel are:

$E_a/R = 20,000\text{K}$ $Q_c = 1.81\text{ MJ/mol fuel}$ $a = 0.25$ $b = 1.5$
 $A_o = 2.1\text{E}9$ Stoichiometric reaction: Fuel + 6.5 * air → Products

The isentropic relations are:

$\left(\frac{T_2}{T_1}\right) = \left(\frac{V_1}{V_2}\right)^{k-1}$ $\left(\frac{P_2}{P_1}\right) = \left(\frac{V_1}{V_2}\right)^k$ where $k = 1.387$

$T_2 = (25+273)(10)^{0.387}$ $P_2 = 101.3(10)^{1.387}$
 $T_2 = 726.45\text{K}$ $P_2 = 2469.5\text{ kPa}$

Ignition occurs when $\dot{Q}_{loss} = \dot{Q}_{gen}$

$\dot{Q}_{loss} = hA(T - T_c) = 250 \frac{\text{W}}{\text{m}^2\text{K}} \cdot 0.05 \frac{\text{m}}{\text{m}} (726.47 - 370\text{K})$

$\dot{Q}_{loss} = 4455.8\text{ W/m}^3$

$\dot{Q}_{gen} = \dot{r} Q_c$ $\dot{r} = A_o \exp(-E_a/RT) X_f^a X_o^b \left(\frac{P}{RT}\right)^{a+b}$

$X_f = \frac{1}{1+6.5 \cdot 4.76} = 0.0313$ $X_o = \frac{6.5}{1+6.5 \cdot 4.76} = 0.2035$

$\dot{r} = 2.1 \times 10^9 \cdot \exp\left(-\frac{20,000}{726.47}\right) \cdot 0.0313^{0.25} \cdot 0.2035^{1.5}$

$\left[\frac{2469.5\text{ kPa} \cdot 1000\text{ Pa/kPa}}{8.314\text{ Pa}\cdot\text{m}^3/\text{mol}\cdot\text{K}} \cdot \frac{(100)^3\text{cm}^3}{\text{m}^3} \cdot 726.47\text{K} \right]^{0.25+1.5}$

$\dot{r} = 1.05 \times 10^{10}\text{ mol/cc}\cdot\text{s}$

$\dot{Q}_{gen} = 1.05 \times 10^{10}\text{ mol/cc}\cdot\text{s} \cdot \frac{(100)^3\text{cc}}{1\text{m}^3} \cdot 1.81 \times 10^6\text{ J/mol} = 196\text{ W/m}^3$

$\dot{Q}_{loss} > \dot{Q}_{gen}$ so no it won't autoignite