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Combustion Theory (M526)
First Semester
Time: 3 h .
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Assume any missing data.
Answer the following questions.

1) A- Define Fire Point, Combustion, Adiabatic flame temperature, Reaction mechanism, Auto Ignition Temperature, Flammability limits, and Stoichiometric air.

Fire Point: Minimum temperature at which liquid fuel produces sufficient vapors to form a flammable mixture with air that continuously supports combustion establishing flame instead of just flashing.

Combustion: is defined as the oxidation process providing heat and light. Chemically it is defined as the transformation of stored chemical bonds into heat that can be used in various ways throughout the combustion device

Adiabatic flame temperature is defined as the flame temperature achieved with the assumption of no work and no changes in kinetic or potential energy for the given reactants due to complete combustion; thus all liberated energy is absorbed by the products attaining its maximum temperature.

Reaction mechanism is the sequence of events at the molecular level that control the speed and outcome of a reaction.

Auto Ignition Temperature: The lowest temperature required to make the combustion self-sustained without any external aid.

Flammability limits, sometimes referred to as explosion limits are defined as the concentration range in which a flammable substance can produce a fire or explosion when an ignition source (such as a spark or open flame) is present.

Stoichiometric or theoretical air is the minimum amount of air supplies sufficient oxygen required for the complete combustion of all fuel elements.

B- Prove the relation used to compute the equilibrium constant:

$$
-\frac{\Delta G^{\circ}}{R_{u} T}=\ln \left[\frac{y_{C}^{v_{C}} y_{D}^{v_{D}}}{y_{A}^{\nu_{A}}} y_{B}^{v_{B}}\left(\frac{P}{P_{r e f}}\right)^{v_{C}+v_{D}-\nu_{A}-v_{B}}\right]=\ln K(T)
$$

For equilibrium the Gibbs function of this mixture must be a minimum. This yields

$$
\begin{aligned}
& (d G)_{T, P}=\sum\left(d G_{i}\right)_{T, P}=\sum\left(\bar{g}_{i} d N_{i}\right)_{T, P}=0 \\
& \bar{g}_{D} d N_{D}+\bar{g}_{C} d N_{C}+\bar{g}_{A} d N_{A}+\bar{g}_{B} d N_{B}=0
\end{aligned}
$$

Here $\bar{g}_{i}$ is the molar Gibbs function for component i (also called the chemical potential).

To find a relation among the dN 's, we select a corresponding stoichiometric reaction. Consider the theoretical reaction where:

In this case:

$$
\begin{gathered}
v_{A} A+v_{B} B \leftrightharpoons v_{C} C+v_{D} D \\
d n_{A}=-v_{A} d \varepsilon \& d n_{B}=-v_{B} d \varepsilon \\
d n_{C}=+v_{C} d \varepsilon \& d n_{D}=+v_{D} d \varepsilon
\end{gathered}
$$

Note:

- v's are the stoichiometric coefficient, but
- n's are the number of moles present
- Any decrease in moles of $A$ and $B$ there is an increase in $C$ and $D$ relative to the degree of reaction $\varepsilon$.
The change in Gibbs function can be expressed:
$d G_{T, P}=\left(v_{C} \bar{g}_{C}+v_{D} \bar{g}_{D}-v_{A} \bar{g}_{A}-v_{B} \bar{g}_{B}\right) d \varepsilon$
Where $\overline{\mathrm{g}}_{i}(T, P)=\overline{\mathrm{g}}_{i}^{\mathrm{s}}(T)+R_{u} T \ln \frac{y_{i} P}{P_{\text {ref }}}$
Then
$\Delta G_{T, P}^{*}=\left(v_{C} \bar{g}_{C}+v_{D} \bar{g}_{D}-v_{A} \bar{g}_{A}-v_{B} \bar{g}_{B}{ }^{\circ}\right)$
At equilibrium $d G_{T, p}=0$ then:
$0=\left(v_{C} \bar{g}_{C}+v_{D} \bar{g}_{D}-v_{A} \bar{g}_{A}-v_{B} \bar{g}_{B}\right)$
$0=v_{C}\left(\overline{\mathrm{~g}}_{c}+R_{u} T \ln \frac{y_{C} p}{p_{\text {ref }}}\right)+v_{D}\left(\overline{\mathrm{~g}}_{D}+R_{u} T \ln \frac{y_{D} P}{P_{\text {ref }}}\right)-v_{A}\left(\overline{\mathrm{~g}}_{A}+R_{u} T \ln \frac{y_{A} p}{p_{r e f}}\right)-v_{A}\left(\overline{\mathrm{~g}}_{A}+R_{u} T \ln \frac{y_{A} p}{P_{r e f}}\right)$
We can get:
$-\frac{\Delta G^{*}}{R_{u} T}=\ln \left[\frac{y_{C}^{v_{C}} y_{D}^{v_{D}}}{y_{A}^{v_{A}} y_{B}^{v_{B}}}\left(\frac{P}{P_{r e f}}\right)^{v_{C}+v_{D}-v_{A}-v_{B}}\right]=\ln K(T)$
where K is the equilibrium constant defined by:
$K(T)=\frac{y_{C}^{v_{C} C} y_{D}^{v_{D}}}{y_{A}^{v_{A}} y_{B}^{v_{B}}}\left(\frac{P}{P_{r e f}}\right)^{v_{C}+v_{D}-v_{A}-v_{B}}$

2) A- state the major resources of heat losses from the boiler.

- Stack losses will combine the sensible heat losses or dry gas losses and the latent heat losses. Sensible heat losses relate to the heat used to heat the combustion gases exiting the stack; the higher the volume and temperature of the flue gases the larger the dry gas heat losses. Latent heat losses are due to the water vapor in the flue gases (a large amount of energy is used as water evaporates).
- Skin/shell losses, which are the losses due to radiation from the boiler walls can be minimized with proper insulation and in general are relatively small.
- In coal and wood fired boilers, ash is normally a by-product of combustion that is collected in hoppers or ash collection areas; it is imperative that the amount of carbon left in those ashes is reduced to extremely small amounts given the resulting heat losses and the negative effects that carbon has in disposing of those ashes.


## B- How does the reaction rate differ from the equilibrium constant?

The rate of reaction differes from the equilibrium constant, as:

- The rate of a reaction is the change in concentration per unit time, whereas the rate constant is the proportionality constant relating the reaction rate to the concentrations of reactants.
- The rate constant remains constant throughout a reaction, regardless of the initial concentrations of the reactants, whereas the rate of a reaction changes with reactant concentration.
- The rate and the rate constant will have the same numerical values and units only if the reaction is zero-order.
- For reaction orders other than zero, the rate and rate constant are numerically equal only when the concentrations of all reactants are 1 M but, their units will be different.


## C- State different parameters affecting the fuel atomization and the main spray characteristics.

1- Fluid Properties Affecting the Spray Among a variety of factors affecting droplet size the fluid properties in particular its surface tension, viscosity, and density.
2- Operating conditions as the fluid exit velocity and the fluid pressure
3- Geometrical parameters as jet hole diameter, number of holes, and the hole thickness.
The main parameters to describe fuel spry include the spray cone angle, droplet sauter mean diameter and the size distribution.

## 3) A- Differentiate between premixed and diffusion flames

| parameter | premixed | diffusion |
| :--- | :--- | :--- |
| Mixing <br> reactants | Fuel and oxidizer are mixed <br> prior to the burner jet (before <br> combustion zone) | Fuel and oxidizer are introduced <br> separately into the combustion <br> zone |
| Motivation of <br> reaction | Rate of burning depends mainly <br> on the chemical kinetics of <br> reaction | Rate of burning depends mainly <br> on the mixing rate between fuel <br> and oxidizer |
| Flame front | There exists a flame zone <br> through which the fuel and air <br> react each with other at any <br> equivalence ratio within | There exists a flame front through <br> which the fuel and air react each <br> with other, where the equivalence <br> ratio is always equal unity. |


|  |  |  |
| :---: | :---: | :---: |
| Flame stabilit | Flame is unstable at the flammability limits if there is any fluctuation in velocity streams of incoming mixture (Blow-off or flash-back) | The stability of diffusion flames depends mainly on the flow velocity of fuel as well as the mixing rate between fuel and air |
| Stability chart |  |  |

B- What are the main factors affecting the burning velocity and the flame thickness?

First of all the burning velocity and the flame thickness are related each to other (according to the thermal theory of flames, $\delta$ is considered as the thickness of pre-heat zone) since $\delta=2 \alpha / S_{L}$ thus the flame thickness is inversely proportional to burning velocity.
There are two main groups of variables affecting the laminar burning velocity; chemical and physical variables. Chemical variable includes the fuel-oxidant ratio (or the equivalence ratio), fuel type (or the molecular structure of the fuel), and additives and fuel blending, while, the physical variable includes the ignition energy, initial temperature, and pressure.

1- Temperature: the laminar burning velocity has a strong temperature dependence with independence factor of about 2 . The general preheating of the unburned gas mixture effect on the burning velocity can be represented in the form of: $S_{L}=A+B\left(\frac{T_{u}}{T_{o}}\right)^{\alpha}$
2- Pressure: From the previous analysis $S_{L} \propto P^{(n-2) / 2}$, for a global reaction order of 2, burning velocity should be independent of pressure. It is found stated, in a similar manner, that both the diffusion and thermal theories of flame propagation predict the following form of pressure dependency: $S_{L} \propto P^{\beta}$ and $\beta$ vary from 0 to -0.5 for a monomolecular reaction.
3- Equivalence ration: Generally, the laminar burning velocity has its maximum value at slightly rich mixture and falls down to its minimum value at the flammability limits in like bell-shaped curve, which is approximately about the axis, give equivalence ratio at which the maximum burning velocity occurs.
4- Fuel type: Generally, as the straight chain length (indicating number of carbon atoms in the chain) for alkanes, alkenes, and alkynes increased, the laminar burning velocity decreased, this emphasis the effect of unsaturation: the burning velocity increases in the order alkanes<alkenes< alkynes. All saturated hydrocarbons (alkane or paraffin such as propane and butane) posses approximately the same maximum burning velocity independently of the number carbon atoms in the molecule.
5- Dilution: The influence of the inert gases (diluents) depends upon the heat capacity, diffusion constant and thermal conductivity of the gas. Generally, the diluents reduce the reaction rate and the flame temperature thus reducing the burning velocity. However, the additives have a chemical effect on the burning velocity; it may be another fuel, catalytic agent, or inhibitor.

If the flammability limits for hydrogen, gasoline, and methane are given, and are stored in a storage room has dimensions of 4 mx 4 mx 4 m . Calculate the amount of each fuel, in kg , that must leak or evaporate into the room to form a flammable mixture. Assume a temperature of $30^{\circ} \mathrm{C}$ and a pressure of 1 atm

|  | LFL | UFL | Molecular Weight kg/mol |
| :--- | :--- | :--- | :--- |
| Hydrogen: | $4.0 \%$ | $75 \%$ | 0.002 |
| Gasoline: | $1.3 \%$ | $7.2 \%$ | 0.106 |
| Methane: | $5.0 \%$ | $15.0 \%$ | 0.016 |

Solution: The room of given dimensions will have a total volume of $4 \times 4 \times 4=64 \mathrm{~m}^{3}$.
Hydrogen: The lower flammable limit is $4 \%$ by volume hydrogen in air. Thus, the hydrogen gas required to reach the LFL is
$(0.04)\left(64 \mathrm{~m}^{3}\right)=2.56 \mathrm{~m}^{3}$
The molar density of any ideal gas at 1 atm and $30^{\circ} \mathrm{C}=303 \mathrm{~K}$ is:

$$
\rho=\frac{P}{R_{g} T}=\frac{1 \mathrm{~atm}}{\left(8.2057 \times 10^{-5} \mathrm{~m}^{3} \mathrm{~atm} / \mathrm{mol} \mathrm{~K}\right)(303 \mathrm{~K})}=40.2 \mathrm{~mol} / \mathrm{m}^{3}
$$

The total amount of hydrogen at the LFL is
$\left(2.56 \mathrm{~m}^{3}\right)\left(40.2 \mathrm{~mol} / \mathrm{m}^{3}\right)=102.9 \mathrm{~mol}$
$102.9 \mathrm{~mol}=0.206 \mathrm{~kg}$

Thus only 0.206 kg of hydrogen needs to leak out in order to explode.
Gasoline: The LFL is $1.3 \%$. The total volume of gasoline vapor required to reach the LFL is $(0.013)\left(64 \mathrm{~m}^{3}\right)=0.832 \mathrm{~m}^{3}$ The total moles of gasoline in this vapor is
$\left(0.832 \mathrm{~m}^{3}\right)\left(40.2 \mathrm{~mol} / \mathrm{m}^{3}\right)=33.4 \mathrm{~mol}$
$33.4 \mathrm{~mol}=3.54 \mathrm{~kg}$
Methane: The LFL is $5.0 \%$. The total volume of gasoline vapor required to reach the LFL is $(0.05)\left(64 \mathrm{~m}^{3}\right)=3.2 \mathrm{~m}^{3}$ The total moles of methane in this vapor is
$\left(3.2 \mathrm{~m}^{3}\right)\left(40.2 \mathrm{~mol} / \mathrm{m}^{3}\right)=128.6 \mathrm{~mol}$
$128.6 \mathrm{~mol}=2.06 \mathrm{~kg}$
Discuss with the help of sketch the temperature, fuel, and oxygen distributions within the diffusion and premixed flames.
For diffusion flames: As the fuel flows along the flame axis, it diffuses radially outward, while the oxidizer (e.g., air) diffuses radially inward. The flame surface is nominally defined to exist where the fuel and oxidizer meet in stoichiometric proportions, i.e.,

Flame surface $\equiv$ Locus of Points where the equivalence ratio, $\Phi$, equals unity







For premixed flames:


State the methods that are used to hold and stabilize flames?
Several methods are employed to hold and stabilize flames:

1. Low-velocity bypass ports.
2. Refractory burner tiles.
3. Bluff-body flameholders.
4. Swirl or jet-induced recirculating flows.
5. Rapid increase in flow area creating recirculating separated flow.

## State the different regimes of turbulent flames?

Turbulent flames regimes are differentiated according to various length scales exist simultaneously in a turbulent relative to the smallest scale called the Kolmogorov microscale, $l_{\mathrm{K}}$, that represents the smallest eddies in the flow. At the other extreme of the length-scale spectrum is the integral scale, $l_{0}$, which characterizes the largest eddy sizes. The basic structure of a turbulent flame is governed by the relationships of $l_{\mathrm{K}}$ and $l o$ to the laminar flame thickness, $\delta_{\mathrm{L}}$ as follow:

Wrinkled laminar-flame: $\delta_{\mathrm{L}} \leq l_{\mathrm{K}}$
Flamelets-in-eddies: $l_{\mathrm{o}}>\delta_{\mathrm{L}}>l_{\mathrm{K}}$
Distributed-reaction: $\delta_{\mathrm{L}}>l_{\mathrm{o}}$

Consider the measurement of turbulent flame speeds. An air-fuel mixture passes through a 40 x 40 mm flow channel with a flame anchored at the channel exit along the top and bottom walls, as shown in the sketch below. Quartz sidewalls contain the flame beyond the exit, while the top and bottom are open to the laboratory. For a mean flow velocity of $68 \mathrm{~m} / \mathrm{s}$, the resulting wedge-shaped flame has an included angle of $13.5^{\circ}$ estimated from time-exposure photographs. Estimate the turbulent burning velocity at this condition. The properties of the unburned mixture are $\mathrm{T}=293 \mathrm{~K} . \mathrm{P}=1 \mathrm{~atm}$. and $\mathrm{MW}=29$ $\mathrm{kg} / \mathrm{kmol}$.


Solution: the turbulent burning velocity can be determined from
$S_{t}=\frac{\dot{m}}{\bar{A} \rho_{u}}$
The reactants flowrate is $\dot{m}=A_{\text {duct }} v_{\text {duct }} P_{u}=1.206 * 0.04^{2} * 68=0.131 \mathrm{~kg} / \mathrm{s}$
where the reactants density is estimated using the ideal-gas law.
From the flame geometry (wedge), we estimate the apparent flame area. $\bar{A}$, first by finding the length of the flame sheet. L:
$\frac{\mathrm{h} / 2}{L}=\sin \left(\frac{13.5}{2}\right)$ or $L=\frac{h / 2}{\sin 6.75}=0.17 \mathrm{~m}$
Then $\bar{A}=2 *$ width $*$ length $=2 * 0.04 * 0.17=0.0136 \mathrm{~m}^{2}$
The turbulent burning velocity is:
$S_{t}=\frac{\dot{m}}{\bar{A} \rho_{u}}=\frac{0.131}{0.0136}=8 \mathrm{~m} / \mathrm{s}$
Note that we have calculated a mean turbulent burning velocity for the entire flame.

