Faculty of Engineering and Technology
Department of Chemical Engineering
University Of Jordan

Chemical Engineering Principles 2
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Fuel and Combustion

Dr.-Ing. Zayed Al-Hamamre

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Fuels and Their Properties

- The use of heat generated by a combustion reaction to produce steam. which drives turbines to produce electricity.
- Fuels burned in power-plant furnaces may be solids, liquids, or gases. Some of the more common fuels are:

1. Solid fuels:

- Coal (a mixture of carbon, water, noncombustible ash, hydrocarbons, and sulfur),
- Coke (primarily carbon-the solid residue left after coal or petroleum is heated, driving off volatile substances and decomposing hydrocarbons),
- Oil shales (diverse fine-grained rocks, which contain refractory organic material that can be refined into fuels). Soluble bitumen fraction constitutes about 20% of this organic material, whereas the remainder exists as an insoluble kerogenand.
- To a small extent Wood, biomass and solid waste (garbage).

Fuels and Their Properties

2. Liquid fuels:

- hydrocarbons obtained by distilling crude oil (petroleum); also coal tars and shale oil.
- Alcohols obtained by fermenting grains.

3. Gaseous fuels:

- Natural gas (80% to 95% methane, the balance ethane, propane, and small quantities of other gases);
- Light hydrocarbons obtained from petroleum or coal treatment,
- Acetylene, and hydrogen (the latter two are relatively expensive to produce).

The heating value

- The heating value of a combustible material is the negative of the standard heat of combustion.

Fuels and Their Properties

- The **higher heating value** (or total heating value or gross heating value) is $-\Delta\hat{H}_c^o$ With $H_2O(l)$ as a combustion product,.
- The lower heating value (or net heating value) is the value based on H_2O (v) as a product.
- Since $\Delta\hat{H}_c^o$ is always negative, the heating value is positive.
- To calculate a lower heating value of a fuel from a higher heating value or vice versa, you must determine the moles of water produced when one mole of the fuel is burned.
  - If this quantity is designated n, then

$$HHV = LHV + n\,\Delta\hat{H}_v(H_2O,\ 25^\circ C)$$

Where $\Delta\hat{H}_v(H_2O,\ 25^\circ C)$ the heat of vaporization of water at 25°C is

$$\Delta\hat{H}_v(H_2O,\ 25^\circ C) = 44.013\ \text{kJ/mol} = 18{,}934\ \text{Btu/lb-mole}$$

- If a fuel contains a mixture of combustible substances, its heating value (lower or higher) is

Fuels and Their Properties

$$HV = \sum x_i (HV)_i$$

where $(HV)_i$ is the heating value of the ith combustible substance.

x_i is the mass fractions of the fuel components if the heating values are expressed in units of (energy)/(mass), or

x_i mole fractions if the dimensions of the heating values are (energy)/(mole).

Table 9.6-1 Typical Heating Values of Common Fuels

	Higher Heating Value	
Fuel	kJ/g	Btu/lb_m
Wood	17	7700
Soft coal	23	10,000
Hard coal	35	15,000
Fuel oil, gasoline	44	19,000
Natural gas	54	23,000
Hydrogen	143	61,000

Example Cont.

Example *Calculation of a Heating Value*

A natural gas contains 85% methane and 15% ethane by volume. The heats of combustion of methane and ethane at 25°C and 1 atm with water *vapor* as the assumed product are given below:

$$CH_4(g) + 2\,O_2(g) \rightarrow CO_2(g) + 2\,H_2O(v): \quad \Delta\hat{H}_c^\circ = -802 \text{ kJ/mol}$$

$$C_2H_6(g) + \tfrac{7}{2}O_2(g) \rightarrow 2\,CO_2(v) + 3\,H_2O(v): \quad \Delta\hat{H}_c^\circ = -1428 \text{ kJ/mol}$$

Calculate the higher heating value (kJ/g) of the natural gas.

Example Cont.

Adiabatic Flame Temperature

- When a fuel is burned,
  - A considerable amount of energy is released.
  - Some of this energy is transferred as heat through the reactor walls,
  - The remainder raises the temperature of the reaction products;
  - The less heat transferred, the higher the product temperature.
  - The highest achievable temperature is reached if the reactor is adiabatic and all of the energy released by the combustion goes to raise the temperature of the combustion products (**adiabatic flame temperature, T_{ad}**).
- In adiabatic reactor ,

$$\dot{Q} = 0$$

$$\Rightarrow \quad \Delta\dot{H}(T_{\text{ad}}) = 0$$

Adiabatic Flame Temperature

Suppose $\dot{n}_f$(mol/s) of a fuel species with heat of combustion $\Delta\hat{H}_c^\circ$ is burned completely with pure oxygen or air in a continuous adiabatic reactor. If the reference states of the molecular feed and product species are those used to determine $\Delta\hat{H}_c^\circ$, the enthalpy change from inlet to outlet is

$$\Delta\dot{H} = \dot{n}_f \Delta\hat{H}_c^\circ + \sum_{\text{out}} \dot{n}_i \hat{H}_i(T_{\text{ad}}) - \sum_{\text{in}} \dot{n}_i \hat{H}_i(T_{\text{feed}}) = 0$$

$$\Rightarrow \quad \sum_{\text{out}} \dot{n}_i \hat{H}_i(T_{\text{ad}}) = -\dot{n}_f \Delta\hat{H}_c^\circ + \sum_{\text{in}} \dot{n}_i \hat{H}_i(T_{\text{feed}})$$

Example *Calculation of an Adiabatic Flame Temperature*

Liquid methanol is to be burned with 100% excess air. The engineer designing the furnace must calculate the highest temperature that the furnace walls will have to withstand so that an appropriate material of construction can be chosen. Perform this calculation, assuming that the methanol is fed at 25°C and the air enters at 100°C.

Example Cont.

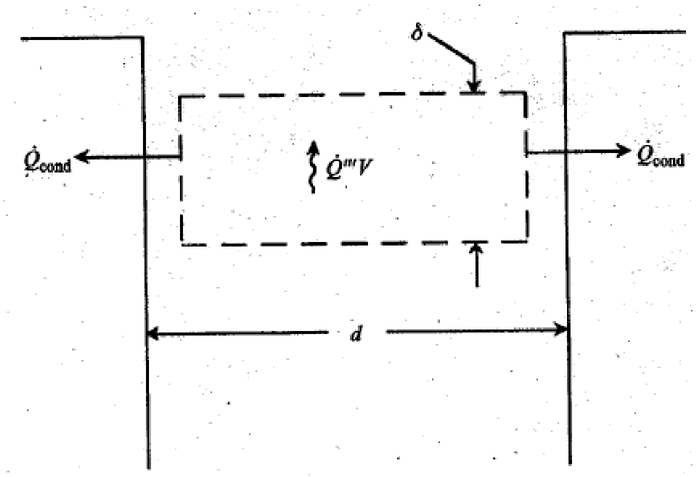
Example Cont.

Example Cont.

Example Cont.

Quenching, Flammability, and Ignition:

- Premixed flames get extinguished upon entering sufficiently small passageways.
- If the passageway is large enough flame will propagate through it.
- Quenching distance: critical diameter of a tube or critical distance between two flat plates through which a flame will not propagate (determined experimentally).



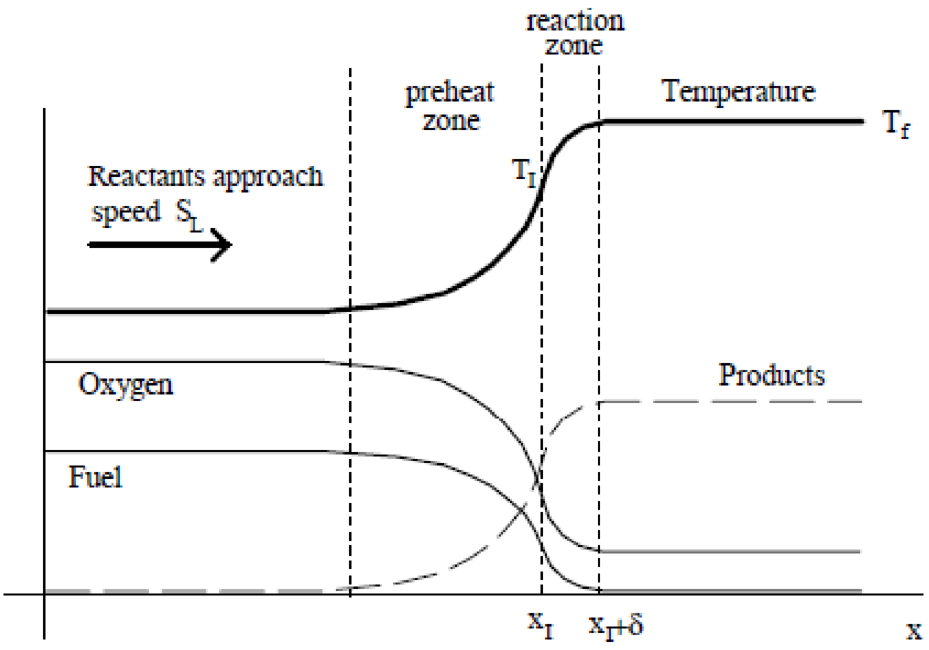
Flammability and Ignition

- ✓ Flashback: propagation of the flame back towards upstream of the burner.
- ✓ Flashback will happen if the reactant flow rate sustaining a laminar premixed flame is significantly reduced or shut-off and the passageways upstream of the flame are larger than the quenching distances.
- o Ignition will occur only if enough energy is added to the gas to heat a slab about as thick as a steady propagating laminar flame to the adiabatic flame temperature.
- o The rate of liberation of heat by chemical reactions inside the slab must approximately balance the rate of heat loss from the slab by thermal conduction.

Laminar Premixed Flames

- A flame is caused by a self-propagating exothermic reaction which is accompanied by a reaction zone.
- It will propagate through a stationary gas mixture at a characteristic velocity (*burning velocity).*
- For most hydrocarbon-air stoichiometric mixtures, this velocity is about 0.4 to 0.6 m/s.
- For hydrogen-air mixtures, this velocity is several meters per second.
- The velocity of this wave is controlled by the diffusion of heat and active radicals.
- For a flame burning in a mixture of gases of known pressure and composition, two characteristic properties may be defined and measured, the burning velocity and the flame temperature.
  - Flame temperature can be predicted from thermodynamic data, if we invoke the assumption of chemical equilibrium.
  - Various flame theories attempt to predict the laminar flame propagation from physical and chemical properties.

Laminar Premixed Flames

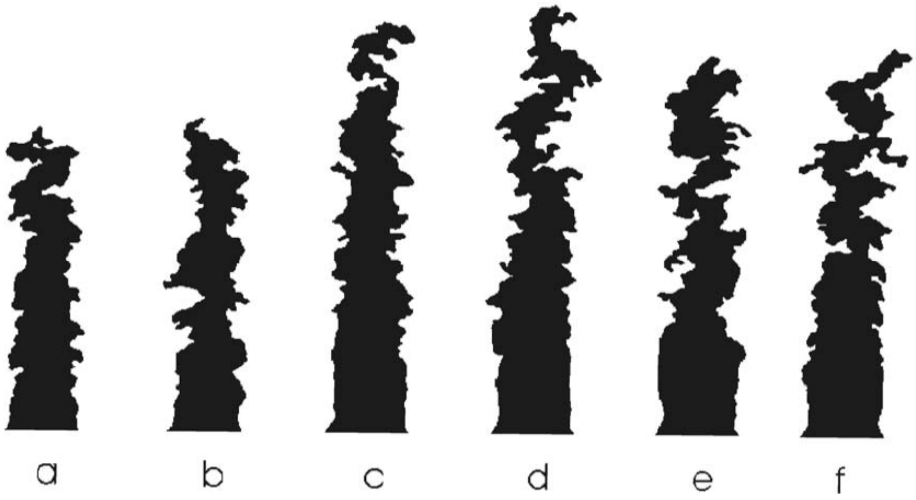


Laminar Premixed Flames

- Historically, there have been two approaches to formulating the laminar flame propagation in premixed gases:
    1. Thermal propagation: the mixture is heated by conduction to the point where the rate of reaction is sufficiently rapid to become self propagating.
    2. Diffusional propagation: diffusion of active species, such as atoms and radicals, from the reaction zone or the burned gas into the unreacted mixture causes reaction to occur.
- Reality: diffusion of heat and active radicals.

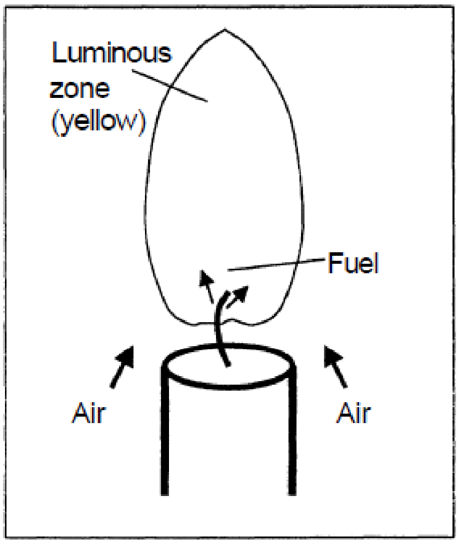
Turbulent Premixed Flames

- Structure of turbulent premixed flames;



Laminar diffusion flame

- Fuel and air are coming separately into the combustion area.
- Convection and diffusion to mix fuel and air.
- Then chemical reaction can take place



The candle flame as classical example of laminar diffusion flame

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Flammability Limits

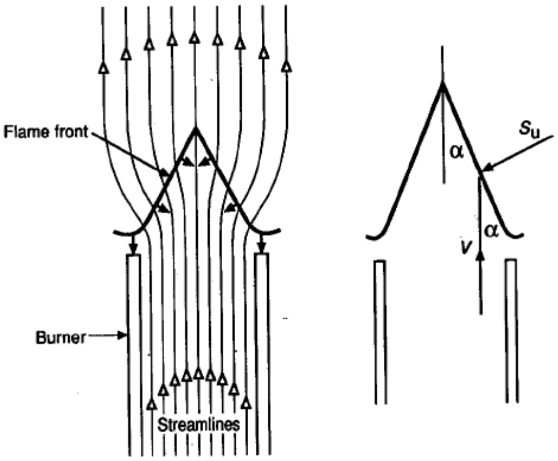
- Flammability limits are frequently quoted as percent of fuel by volume in the mixture, or as a percentage of the stoichiometric fuel requirement.
- A premixed laminar flame will propagate only within a range of mixture strengths:
  - Lower limit (lean limit) of flammability, $\Phi < 1$
  - Upper limit (rich limit) of flammability $\Phi > 1$
- There are enormous variations between fuels, the flammability range in air

For acetylene is 2.5-80% by vol.

For propane the range is 2.2-9.5%.

Flame Stabilization

- Important design criteria: avoid flashback and lift off.
    - In flashback, flame enters and propagates through the burner upstream without quenching (safety hazard).
    - In liftoff, flame is not attached to the burner, but stabilized at a distance from it.
    - Liftoff: issues related to incomplete burning, ignition problems, control of the flame position.



Flame Stabilization

- Both flashback and liftoff are related to matching the local laminar flame speed to the local flow velocity.
    - A flame can be stabilized on the burner only between certain flow velocity limits.
    - If the gas velocity is progressively reduced, a point will be reached eventually at which the burning velocity exceeds the gas velocity somewhere across the burner.
    - At this point, flame will propagate back down the burner.