Premixed Flames

**Structure of 1D Premixed Flame**

- **Pre-heat zone**: Temperature of the unburnt gases rises to some arbitrary value $T_i$.
- **Reaction zone**: Where most of the combustion occurs and the location where the visible portion of the flame resides.

**Propagating Flame Front**

- $\rho_u V_u = S_L$
- $\rho_b V_b$

**Flame thickness** $\delta$

**Visible portion of the flame**

**Diffusion of heat and radicals**
Premixed Flames

Structure of 1D Premixed Flame

- Rate of Fuel depletion = molar concentration of reactants [mole/vol] \( * \) \( k \) (rate const.)

\[
\frac{d[F]}{dt} = -[F]^n[O_2]^m \cdot k
\]

\[
\frac{d[F]}{dt} = -[F]^n[O_2]^m \cdot B \cdot \exp \left( \frac{-E_a}{\mathcal{R}T} \right)
\]

where:

- \( E_a \) – Activation energy
- \( \mathcal{R} \) – Universal Gas Constant
- \( k \) – Rate constant for a specific fuel (~ Arrhenius Eq)
- \( n \) & \( m \) – provided in the following table

### Table 4.1 Overall reaction rates for fuels burning in air (from Westbrook and Dryer [2])

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Formula</th>
<th>( B )</th>
<th>( E_{(\text{cal/mole})} )</th>
<th>( n )</th>
<th>( m )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>( \text{CH}_4 )</td>
<td>( 8.3 \times 10^5 )</td>
<td>30.0</td>
<td>(-0.3)</td>
<td>1.3</td>
</tr>
<tr>
<td>Ethane</td>
<td>( \text{C}_2\text{H}_6 )</td>
<td>( 1.1 \times 10^{3} )</td>
<td>30.0</td>
<td>( 0.1)</td>
<td>1.65</td>
</tr>
<tr>
<td>Propane</td>
<td>( \text{C}_3\text{H}_8 )</td>
<td>( 8.6 \times 10^{1} )</td>
<td>30.0</td>
<td>( 0.1)</td>
<td>1.65</td>
</tr>
<tr>
<td>( n ) Hexane</td>
<td>( \text{C}_2\text{H}_6 )</td>
<td>( 5.7 \times 10^{1} )</td>
<td>30.0</td>
<td>( 0.25)</td>
<td>1.5</td>
</tr>
<tr>
<td>( n ) Heptane</td>
<td>( \text{C}<em>7\text{H}</em>{16} )</td>
<td>( 5.1 \times 10^{1} )</td>
<td>30.0</td>
<td>( 0.25)</td>
<td>1.5</td>
</tr>
<tr>
<td>Octane</td>
<td>( \text{C}<em>8\text{H}</em>{18} )</td>
<td>( 4.6 \times 10^{1} )</td>
<td>30.0</td>
<td>( 0.25)</td>
<td>1.5</td>
</tr>
<tr>
<td>Methanol</td>
<td>( \text{CH}_2\text{OH} )</td>
<td>( 3.2 \times 10^{2} )</td>
<td>30.0</td>
<td>( 0.25)</td>
<td>1.5</td>
</tr>
<tr>
<td>Ethanol</td>
<td>( \text{C}_2\text{H}_5\text{OH} )</td>
<td>( 1.5 \times 10^{2} )</td>
<td>30.0</td>
<td>( 0.15)</td>
<td>1.6</td>
</tr>
</tbody>
</table>

- Or

\[
\dot{m}^{m} F_r = A \cdot \exp \left( \frac{-E_a}{\mathcal{R}T} \right)
\]

- Commonly referred to as the Arrhenius eq where “A” is a constant.
Premixed Flames

Characteristics of Laminar Premixed Flames

- A 1D laminar premixed flame propagates relative to the fresh unburned gases at a speed referred to as the laminar flame speed $S_L$.

- When the fresh unburned gases are in a turbulent state, the flame speed is referred to as the turbulent flame speed ($S_T$).

- The turbulent flame speed is always larger than the laminar flame speed ($S_T > S_L$).

- Laminar vs. Turbulent Flames: both have same type of physical process and many turbulent flame theories are based on an underlying laminar flame structure.

Characteristics of Laminar Premixed Flames

- Since the burned product density is less than the reactant density, so by the conservation of mass the velocity of the burned gases is greater than the velocity of the unburned gases.

- Typical $S_L$ for fuels is between 0.1 to 1 m/s.

- For a typical hydrocarbon/air flame at atmospheric pressure, the density ratio is about 7.

- A flame is divided into two zones;
  i) **Preheat zone**: reactant $T$ increases, but little heat release.
  ii) **Reaction zone**: most of the chemical energy is released.
    - This zone is further divided into regions of slow and fast chemistry.
Premixed Flames

Characteristics of Laminar Premixed Flames

- Characteristics of the thin region of fast reaction chemistry
  - Destruction of fuel molecules and creation of intermediate species
  - Dominated by molecular reactions to produce CO
  - Thickness of the fast zone is usually < 1 mm @ atm pressure
  - Temperature & species concentration gradients are very large
  - These large gradients provide the driving forces for the flame to be self-sustaining, i.e. diffusion of heat & radical species from the reaction zone to the preheat zone.

- Characteristics of the region of slow reaction chemistry
  - Chemistry is dominated by three-body radical recombination reactions, such as the final burn-out of CO via
    \[ CO + OH \rightarrow CO_2 + H \]
  - At atmospheric pressure, this zone may extend several mm.

Premixed Flames

Laminar Premixed Flame

- A flame represents an interface separating the unburned gas (u) from the combustion products (burned gas, b).
- Pressure is roughly constant across the flame so \( \rho \sim 1/T \)
- This interface (i.e., the flame) can propagate (as found in an IC engine) or be stationary (i.e., fuel burner application).
Premixed Flames

Burning Velocity vs. Flame Speed

- **Burning velocity** ($S_u$) is a measure of the speed at which reactants ($\rho_u$) move into the flame (i.e., stationary flame) from a reference point located on the moving flame.

- **Flame speed** ($S_L$) is a measure of how quickly a flame moves away from a fixed reference point.

\[
\rho_b = \rho_u \quad \text{Products} \\
\text{Unburned Reactants}
\]

\[
\text{Stationary flame}
\]

\[
\rho_b = \rho_u \quad \text{Products} \\
\text{Unburned Reactants}
\]

\[
\text{Moving flame}
\]

Premixed Flames

Laminar Burning Velocity

- Maillard-LeChatelier theory gives:

\[
S_i^L \approx \alpha \cdot T_u \cdot P^{n-1} \exp\left(-\frac{E}{\mathcal{R} T_{ad}}\right)
\]

- High flame velocity corresponds to:
  1) higher unburned gas temperature
  2) lower pressure
  3) higher adiabatic flame temperature (higher chemical reaction rate)
  4) higher thermal diffusivity $\alpha (= \frac{k_{\text{cond}}}{\rho c_p})$
Premixed Flames

Laminar Premixed Flame

• Remember a flame represents an interface separating the unburned gas from the combustion products.

• Pressure is approximately constant across the flame front, so $\rho \sim 1/T$

• A flame under laminar conditions at a given $P$, $T$, and $\phi$ has two basic properties:
  a) the adiabatic flame temperature, $T_{ad}$
  b) laminar burning velocity, $S_u$ defined in terms of the approaching unburned gas velocity.

Premixed Flames

Premixed Flame Structure

• Fundamental Burning Velocity ($S_u$) – velocity of the flame as it propagates into an unburnt mixture with no turbulence.

$$S_u = \frac{2k}{\rho_c c'_p(T_r - T_i)} \dot{Q}_{avg}^{\frac{1}{2}}$$

$\dot{Q}_{avg}$ - average rate of heat released in reaction zone ($W/m^3$)

$T_i$ - temperature at initial conditions ($K$)

$T_r$ - flame temperature ($K$)

$\rho_c$ - density at initial conditions ($kg/m^3$)

$k$ - thermal conductivity ($W/[m*K]$)

$c'_p$ - thermal capacity of the products ($J/K$)

Note: As a premixed flame comes close to a surface, heat is transferred to the surface, & the flame cools, slowing flame propagation.
Premixed Flames

Premixed Flame Structure

• For any given premixed fuel/air mixture there is one and only one burning velocity ($S_u$).

• However, the burning velocity depends on:
  - Equivalence ratio
  - Mixture T & P
  - Test apparatus (environmental conditions)

• The burning velocity is maximum for a slightly fuel rich mixture, which is compatible with experimental observation.

• This is due to highly mobile hydrogen atoms which diffuse ahead of the reaction zone and contribute significantly to the mechanism of flame propagation. Their concentration is higher in the fuel-rich flame.

Laminar Flame Speed

Burning velocity ($S_{u,max}$) for hydrocarbons is ~ 35 cm/s at $\phi = 1.1$. 

$S_u + S_g = S_{s}$
Premixed Flames

Laminar Burning Velocity

Laminar Burning Velocity vs. Equivalence Ratio

Methane Dominated Flame

Su is larger at lower pressures
Su is larger at higher T
Premixed Burning Velocity

- Many studies have examined the variation of burning velocity with experimental parameters such as flammable gas concentration and temperature.
- Mixtures close to the flammability limits have finite burning velocities and there is no evidence that $S_u \to 0$ in the limit.
- The burning velocity is increased if the oxygen concentration in the atmosphere is increased.
- Also the addition of turbulence and low pressure can accelerate a flame to detonation.
- Gaseous fuel/air mixtures whose $T$'s are above 800 K will undergo slow oxidation and pyrolysis (pre-flame reactions), changing their chemical composition and $S_u$.

**Premixed Flames**

**Premixed Burning Velocity**

**EFFECT OF TEMPERATURE ON BURNING VELOCITIES OF FOUR PARAFFINS IN AIR AT ATMOSPHERIC PRESSURE**

- $S_u = 10 + 0.000342T^2$
- Temperature of the unburned F/A mixture

REF: BUREAU OF MINES BULLETIN 680
INTEGRATES DATA FOR METHANE, PROPAINE, ETHANE, ISO OCTANE.
Addition of Suppressants

- A flammable mixture may be rendered non-flammable by the addition of a suitable suppressant.
- Additives such as nitrogen and carbon dioxide act as inert diluents, increasing the thermal capacity of the mixture and reducing the flame temperature.
  - Ultimately below a critical value where flame propagation is not possible.
Premixed Flames

Premixed Burning Velocity

- If chemical inhibitors are present in the unburnt vapor/air mixture, significant reductions in the burning velocity without a corresponding reduction in $T_{\text{flame}}$ will occur.

- Example - adding 2% methyl bromide to a stoichiometric mixture of ethylene and air, reduces the burning velocity from 0.66 m/s to 0.25 m/s.

- These species inhibit the oxidation chain reactions, by reacting with the chain carriers and replacing them by relatively inert atoms or radicals.

- Halon is very efficient at suppressing ignition by a small spark. However, higher concentrations are required to suppress flame propagation when a larger source of ignition such as a flame is used.