8. Laminar Diffusion Flames (Laminar Non-Premixed Flames)

- In a *diffusion flame* combustion occurs at the interface between the fuel gas and the oxidant gas, and the burning depends more on rate of diffusion of reactants than on the rates of chemical processes involved.
- It is more difficult to give a general treatment of diffusion flames, largely because no simple, measurable parameter, analogous to the burning velocity in premixed flames, can be defined.
• Used in certain applications (e.g., residential gas appliances).
  - mostly partially-premixed flames
• Used in fundamental flame research.
• Primary concern in design is the flame geometry.
• Parameters that control the flame shape,
  - Fuel flow rate
  - Fuel type
  - Other factors
Candle Flame.
8. Laminar Diffusion (Non-Premixed) Flames

Diffusion Flame Structure.
Diffusion Flame Regimes.

8. Laminar Diffusion (Non-Premixed) Flames
A Simple Approach

• For simple laminar diffusion flames on circular nozzles (similar to a candle flame), flame height is mostly used to characterize the flame.

• For simple treatments, reaction zone is defined as the region where the fuel and air mixture is stoichiometric. This assumption is, of course, clearly incorrect as reaction will be occurring over an extremely wide range of fuel/air ratios.

• Diffusion process is rate-determining so that rate of reaction is directly related to the amounts of fuel and oxidant diffusing into the reaction zone.
• For a simple conical laminar diffusion flame, molecular diffusion is considered only in radial direction.

• Average square displacement (Einstein diffusion equation) is given by

\[ \bar{y}^2 = 2Dt \]

• Height of the flame is taken as the point where the average depth of penetration is equal to the tube radius.

• Approximating \( \bar{y}^2 \) by \( R^2 \) yields

\[ t = \frac{R^2}{2D} \]
- Since

\[ t = \frac{L_f}{\nu} \]

then,

\[ L_f \approx \frac{\nu R^2}{2D} \]

- Volume flow rate

\[ Q_F = \nu \pi R^2 \]

so that

\[ L_f \approx \frac{Q_F}{\pi D} \]
• Although very crude, this approximation permits certain predictions:

  - At a given flow rate, flame height is independent of the burner diameter.

  - Since the diffusion coefficient $D$ is inversely proportional to pressure, the height of the flame is independent of pressure at given mass flow rate.

  - Flame height is proportional to volume flow rate of fuel.
Methane diffusion flames at high pressures.
Nonreacting Constant-Density Laminar Jet

Physical Description:

- Analysis presented in the previous section is very crude and provides only very qualitative features of laminar diffusion flames.

- To develop an understanding of the reacting laminar jet, we start with a nonreacting laminar jet of a fluid flowing into an infinite reservoir.

- Important points: basic flow and diffusional processes.
8. Laminar Diffusion (Non-Premixed) Flames
• **Potential core**: the effects of viscous shear and molecular diffusion are not in effect yet; so the velocity and nozzle-fluid (fuel) mass fraction remain unchanged from their nozzle-exit values and are uniform in this region.

• In the region between the potential core and the jet edge, both the velocity and fuel concentration decrease monotonically to zero at the jet edge.

• Beyond the potential core the viscous shear and diffusion effects are active across whole field of the jet.
• Initial jet momentum is conserved throughout the entire flowfield.

• As the jet moves into surroundings, some of the momentum is transferred to air, decreasing the velocity of the jet.

• Along the jet increasing quantities of air are entrained into the jet as it proceeds downstream.

- We can express this mathematically using an integral form of momentum conservation:
\[ 2\pi \int_{0}^{\infty} \rho(r, x)v_x^2(r, x)r \, dr = \rho_e v_e^2 \pi R^2 \]

where subscript \( e \) specifies the nozzle exit conditions.

- The process that control the diffusion and convection of momentum are similar to the processes that control the fuel concentration field (convection and diffusion of fuel mass).
• Distribution of fuel mass fraction, $Y_F(r, x)$, should be similar to dimensionless velocity distribution, $v_x(r, x)/v_e$.

• Fuel molecules diffuse radially outward according to Fick’s law.

• The effect of moving downstream is to increase time available for diffusion.

• The width of the region containing fuel grows with $x$ and centerline fuel concentration decays.

• The mass of fluid issuing from nozzle is conserved:
\[
2\pi \int_{0}^{\infty} \rho(r, x) v_x(r, x) Y_F(r, x) r \, dr = \rho_e v_e \pi R^2 Y_{F,e}
\]

(8.2)

where \( Y_{F,e} = 1 \).

- To determine the velocity and mass fraction fields we need to make some assumptions.

**Assumptions:**

1. \( MW_e = MW_\infty \). \( P = \text{const.} \). \( T = \text{const.: Uniform density field.} \)

2. Species transport is by Fick’s diffusion law.
3. Momentum and species diffusivities are constant and equal, i.e. the Schmidt Number is unity,

\[ Sc \equiv \frac{\nu}{D} = 1 \]

4. Diffusion is considered only in radial direction; axial diffusion is neglected.

(This may not be a good assumption very near to the nozzle exit; since near the exit it is expected that the axial diffusion will be significant in comparison with the downstream locations.)
Conservation Laws (Boundary-layer equations):

- **Mass Conservation:**
  \[
  \frac{\partial v_x}{\partial x} + \frac{1}{r} \frac{\partial (v_r r)}{\partial r} = 0 \quad (8.3)
  \]

- **Axial Momentum Conservation:**
  \[
  v_x \frac{\partial v_x}{\partial x} + v_r \frac{\partial v_x}{\partial r} = \nu \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_x}{\partial r} \right) \quad (8.4)
  \]

- **Species Conservation:** For the jet fluid (fuel)
  \[
  v_x \frac{\partial Y_F}{\partial x} + v_r \frac{\partial Y_F}{\partial r} = D \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_x}{\partial r} \right) \quad (8.5)
  \]
In addition, we have,

\[ Y_{Ox} = 1 - Y_F \]  \hspace{1cm} (8.6)

**Boundary Conditions:**

- To solve Eqns.8.3-8.5 for the unknown functions:
  - \( v_x(r, x) \), \( v_r(r, x) \), and \( Y_F(r, x) \)

requires,

  - three boundary conditions each for \( v_x \) and \( Y_F \), and
  - one boundary condition for \( v_r \).
Along the jet centreline, \( r = 0 \),

\[ v_r(0, x) = 0 \]  \hspace{1cm} (8.7a)

\[ \frac{\partial v_x}{\partial r}(0, x) = 0 \]  \hspace{1cm} (8.7b)

\[ \frac{\partial Y_F}{\partial r}(0, x) = 0 \]  \hspace{1cm} (8.7c)

where the last two result from symmetry.

At large radii \((r \to \infty)\),

\[ v_x(\infty, x) = 0 \]  \hspace{1cm} (8.7d)

\[ Y_F(\infty, x) = 0 \]  \hspace{1cm} (8.7e)
• At the jet exit, \( x = 0 \), we assume uniform axial velocity and fuel mass fraction, and zero elsewhere:

\[
    v_x(r \leq R, 0) = v_e
\]

\[
    v_x(r > R, 0) = 0
\]

\[
    Y_F(r \leq R, 0) = Y_{F,e} = 1
\]

\[
    Y_F(r > R, 0) = 0
\]

\textbf{Solution:}

• Velocity field can be obtained by assuming the profiles to be similar.
• Intrinsic shape of the velocity profiles is the same everywhere in the flowfield.

• Radial distribution of \( v_x(r, x) \), when normalized by the local centreline velocity \( v_x(0, x) \), is a universal function that depends only on the similarity variable \( r/x \).

- Solutions for axial and radial velocities:

\[
v_x = \frac{3}{8\pi} \frac{J_e}{\mu x} \left[ 1 + \frac{\xi^2}{4} \right]^{-2}
\]

(8.8)
\[ v_r = \left( \frac{3J_e}{16\pi \rho_e} \right)^{1/2} \frac{1}{x} \frac{\xi - \frac{\xi^3}{4}}{(1 + \frac{\xi^2}{4})^2} \]  

(8.9)

where \( J_e \) is the jet initial momentum flow,

\[ J_e = \rho_e v_e^2 \pi R^2 \]  

(8.10)

and,

\[ \xi = \left( \frac{3\rho_e J_e}{16\pi} \right)^{1/2} \frac{1}{\mu} \frac{r}{x} \]  

(8.11)
• Axial velocity distribution in dimensionless form (substitute Eqn.8.10 into 8.8),
\[
\frac{v_x}{v_e} = 0.375 \left( \frac{\rho_e v_e R}{\mu} \right) \left( \frac{x}{R} \right)^{-1} \left[ 1 + \frac{\xi^2}{4} \right]^{-2}
\] (8.12)

• Dimensionless centreline velocity decay obtained by setting \( r = 0 \) (\( \xi = 0 \)),
\[
\frac{v_{x,0}}{v_e} = 0.375 \left( \frac{\rho_e v_e R}{\mu} \right) \left( \frac{x}{R} \right)^{-1}
\] (8.13)
• Velocity decays inversely with axial distance, and proportional to the jet Reynolds number,

\[ \text{Re}_j \equiv \frac{\rho_e v_e R}{\mu} \]

• From Eqn. 8.13, we see that the solution is not valid near the nozzle;
  - at small values of \( x \), the dimensionless centerline velocity becomes larger than unity, which is not physically correct.
• Other parameters used to characterize jets are the spreading rate and spreading angle, $\alpha$.  
• We introduce jet half-width, $r_{1/2}$.  
  - *Half-width*: radial location where jet velocity has decayed to one-half of its centreline value.  
• An expression for $r_{1/2}$ can be derived by setting $v_x/v_{x,0}$ to be one half and solving for $r$.  
• *Jet spreading rate* = $r_{1/2}/x$.  
• *Jet spreading angle* is the angle whose tangent is the spreading rate.
8. Laminar Diffusion (Non-Premixed) Flames
\[ r_{1/2}/x = 2.97 \left( \frac{\mu}{\rho_e v_e R} \right) = 2.97 \text{Re}_j^{-1} \tag{8.14} \]

\[ \alpha \equiv \tan^{-1}(r_{1/2}/x) \tag{8.15} \]

- High-Re\(_j\) jets are narrow, while low-Re\(_j\) jets are wide.
- Comparing Eqns. 8.4 and 8.5, we see that \( Y_F \) plays the same mathematical role as \( v_x/v_e \), if the Schmidt number is unity, i.e., \( \nu = D \).
• Then the functional form of the solution for $Y_F$ is identical to that for $v_x/v_e$,

$$Y_F = \frac{3}{8\pi} \frac{Q_F}{Dx} \left[ 1 + \frac{\xi^2}{4} \right]^{-2}$$

(8.16)

where $Q_F = v_e \pi R^2$, volumetric flow rate of fuel.

• By applying $Sc = 1$ to Eqn.8.16,

$$Y_F = 0.375\text{Re}_j \left( \frac{x}{R} \right)^{-1} \left[ 1 + \frac{\xi^2}{4} \right]^{-2}$$

(8.17)
• Centreline values of mass fraction,

\[ Y_{F,0} = 0.375 \text{Re}_j \left( \frac{x}{R} \right)^{-1} \]  

(8.18)

• Again, it should be noted that the solutions are valid far from the nozzle. The dimensionless distance downstream where the solution is valid must exceed the jet Reynolds number, that is,

\[ \left( \frac{x}{R} \right) \geq 0.375 \text{Re}_j \]  

(8.19)
Jet Flame Physical Description

- The burning laminar fuel jet has much in common with our previous discussion of the non-reacting jet.

- As the fuel flows along the flame axis, it diffuses radially outward, while the oxidizer diffuses radially inward.

- The “flame surface” can be defined as,

\[
\text{Flame Surface} \equiv \text{Locus of points where } \Phi \text{ equals unity}
\]  

(8.20)
8. Laminar Diffusion (Non-Premixed) Flames
• The products formed at the flame surface diffuse radially both inward and outward.

• An overventilated flame is where there is more than enough oxidizer in the immediate surroundings to continuously burn the fuel.

• Underventilated flame is the opposite of above.

• Flame length for an overventilated flame is determined at the axial location where,

\[ \Phi(r = 0, x = L_f) = 1 \] (8.21)
• Chemical reaction zone is quite narrow (but significantly larger than laminar flame thickness).
• Flame temperature distribution exhibits an annular shape until the flame tip is reached.
• In the upper regions, the bouyant forces are important.
• As a result, the jet accelerates narrowing the flame.
• The narrowing of the flow increases the fuel concentration gradients, \( \frac{dY_F}{dr} \), thus enhancing diffusion.
By ignoring the effects of heat released by reaction, Eqn. 8.16 provides a crude description of flame boundaries when $Y_F = Y_{F,\text{stoic}}$.

$$Y_F = \frac{3}{8\pi} \frac{Q_F}{\mathcal{D} x} \left[ 1 + \frac{\xi^2}{4} \right]^{-2}$$  \hspace{1cm} (8.16)

- When $r$ equals zero, we get a flame length,

$$L_f \approx \frac{3}{8\pi} \frac{Q_F}{\mathcal{D} Y_{F,\text{stoic}}}$$  \hspace{1cm} (8.22)
- Flame length is proportional to volumetric flow rate of fuel.
- Flame length is inversely proportional to the stoichiometric fuel mass fraction.
- Since \( Q_F = v_e \pi R^2 \), various combinations of \( v_e \) and \( R \) can yield the same flame length.
- Since the diffusion coefficient \( D \) is inversely proportional to pressure, the height of the flame is independent of pressure at given mass flow rate.
Historical Theoretical Formulations:

- Burke and Schumann (1928)
  - constant velocity field parallel to flame axis.
  - reasonable predictions of $L_f$ for round burners.

- Roper and Roper et al (1977)
  - relaxed single constant velocity assumption.
  - provides extremely good predictions.
  - matched by experimental results/correlations.
  - round and slot-burners.
Roper’s Solutions and Correlations:
Circular Port:

\[
L_{f,thy} = \frac{Q_{F}(T_{\infty}/T_{F})}{4\pi D_{\infty} \ln(1 + 1/S)} \left(\frac{T_{\infty}}{T_{f}}\right)^{0.67}
\] (8.59)

\[
L_{f,expt} = 1330 \frac{Q_{F}(T_{\infty}/T_{F})}{\ln(1 + 1/S)}
\] (8.60)

where \(S\) is stoichiometric molar oxidizer-fuel ratio, \(D_{\infty}\) mean diffusion coefficient of oxidizer at \(T_{\infty}\), \(T_{F}\) and \(T_{f}\) are fuel stream and mean flame temperatures, respectively.
Square Port:

\[
L_{f,thy} = \frac{Q_F(T_\infty/T_F)}{16D_\infty \{\text{inverf}[(1 + S)^{-0.5}]\}^2} \left(\frac{T_\infty}{T_f}\right)^{0.67}
\] (8.61)

\[
L_{f,expt} = 1045 \frac{Q_F(T_\infty/T_F)}{\{\text{inverf}[(1 + S)^{-0.5}]\}^2}
\] (8.62)

where *inverf* is the inverse of error function *Erf*,

\[
\text{Erf}w = \frac{2}{\sqrt{\pi}} \int_0^w e^{-t^2} dt
\]
Slot Burner–Momentum Controlled:

\[
L_{f,\text{thy}} = \frac{b\beta^2 Q_F}{h ID_\infty Y_{F,\text{stoic}}} \left( \frac{T_\infty}{T_F} \right)^2 \left( \frac{T_f}{T_\infty} \right)^{0.33} \tag{8.63}
\]

\[
L_{f,\text{expt}} = 8.6 \cdot 10^4 \frac{b\beta^2 Q_F}{h I Y_{F,\text{stoic}}} \left( \frac{T_\infty}{T_F} \right)^2 \tag{8.64}
\]

where \(b\) is the slot width and \(h\) is the length, and,

\[
\beta = \frac{1}{4 \times \text{inverf}[1/(1 + S)]}
\]
$I$ is the ratio of actual initial momentum flow from the slot to that of uniform flow,

$$I = \frac{J_{e,act}}{\dot{m}_F v_e}$$

For uniform flow $I = 1$. For a fully developed flow, assuming parabolic exit velocity, $I = 1.5$.

- Equations 8.63 and 8.64 are only applicable to conditions where the oxidizer is stagnant.
Slot Burner–Buoyancy Controlled:

\[
L_{f, \text{thy}} = \left[ \frac{9\beta^4 Q_F^4 T_\infty^4}{8D_\infty^2 a \eta^4 T_F^4} \right]^{1/3} \left( \frac{T_f}{T_\infty} \right)^{2/9} \quad (8.65)
\]

\[
L_{f, \text{expt}} = 2 \cdot 10^3 \left[ \frac{\beta^4 Q_F^4 T_\infty^4}{a \eta^4 T_F^4} \right]^{1/3} \quad (8.66)
\]

where \( a \) is the mean buoyant acceleration,

\[
a \approx 0.6g \left( \frac{T_f}{T_\infty} - 1 \right) \quad (8.67)
\]

and \( g \) is the gravitational acceleration.
Slot Burner–Transition Regime:

- *Froude Number*,

\[
\text{Fr}_f \equiv \frac{(v_e Y_{F, \text{stoic}})^2}{aL_f}
\]  \hspace{1cm} (8.68)

- Froude number physically represent the ratio of the initial jet momentum flow to the buoyant force experienced by the flame.

\[
\begin{align*}
\text{Fr}_f &> > 1 & \text{Momentum-controlled} & \quad (8.69a) \\
\text{Fr}_f &\approx 1 & \text{Transition (mixed)} & \quad (8.69b) \\
\text{Fr}_f &<< 1 & \text{Buoyancy-controlled} & \quad (8.69c)
\end{align*}
\]
Note that $L_f$ must be known \textit{a priori} to establish the appropriate regime. So it requires a trial and error approach.

When $Fr_f \approx 1$,

$$L_{f,T} = \frac{4}{9} L_{f,M} \left( \frac{L_{f,B}}{L_{f,M}} \right)^3$$

$$\times \left\{ \left[ 1 + 3.38 \left( \frac{L_{f,M}}{L_{f,B}} \right)^3 \right]^{2/3} - 1 \right\}$$

(8.70)
Soot Formation in Diffusion Flames:

- Fuel type
  - Fuel chemical structure and composition
- Dilution
  - Inert or reactive diluents
- Turbulence
  - Turbulence time versus chemical time
- Temperature
- Pressure
• Soot does not form in premixed flames except when $\Phi \geq \Phi_{\text{crit}}$

• The details of soot formation process in diffusion flames is elusive

• Conversion of a hydrocarbon fuel with molecules containing a few carbon atoms into a carbonaceous agglomerate containing some millions of carbon atoms in a few milliseconds.

• Transition from a gaseous to solid phase

• Smallest detectable solid particles are about 1.5 nm in diameter (about 2000 amu)
Soot formation involves a series of chemical and physical processes:

- Formation and growth of large aromatic hydrocarbon molecules leading to soot inception, i.e., transition to first solid particles (primary particles)
- Surface growth and coagulation of primary particles to agglomerates
- Growth of agglomerates by picking up growth components from the gas phase
- Oxidation of agglomerates
• **Smoke Point:**

- An ASTM standard method to determine sooting tendency of a liquid fuel
- Fuel flow rate is increased until the smoke starts being emitted from the flame tip of a laminar flame on a standard burner
- Greater the fuel flow rate (height of the flame), the lower is the sooting propensity
- Generally used for aviation fuel specifications
- Dependent on the fuel chemical composition
Vinyl radical C$_2$H$_3$.

Vinyl acetylene.

Vinyl acetylene radical.

Linear C$_6$H$_5$.

Cyclic C$_6$H$_5$ (phenyl radical).

Pyrolysis / oxidative pyrolysis of FUEL.

ACETYLENE

HYDROGEN ATOM

MOLECULAR ZONE

PARTICLE ZONE

Soot Inception

Soot Surface Growth

Coagulation

Reaction Time Coordinate

Soot Particle Dia. = 1 nm to 40+ nm.
- fuel tube = 11 mm; fuel flow rate = 3.27 cm³/s
- air nozzle = 100 mm; air flow rate = 170 L/min
- visible flame height = 67 mm (Fuel: C₂H₄)
8. Laminar Diffusion (Non-Premixed) Flames
8. Laminar Diffusion (Non-Premixed) Flames

C$_2$H$_4$ Flame

Height Above Burner, mm

Primary Particle Diameter, nm

4.90 ml/min

3.85 ml/min

AER 1304–ÖLG
\[ z = 10 \text{ mm}; \ r = 5 \text{ mm} \]
\[ z = 33 \text{ mm}; \ r = 0 \text{ mm} \]
Predicted and Measured Results
C$_2$H$_4$-Air Flame

Temperature, K

Soot volume fraction, ppm